Electronic supplementary information

for

Multi-conformer molecules in solutions: an NMR-based DFT/MP2 conformational study of two glucopyranosides of vitamin E model compound

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Experimental section

General information

^{1}H and ^{13}C NMR spectra were recorded for solutions in $CDCl_3$ on a Bruker Advance III and II spectrometer operating at 600/400 and 150/100 MHz for ^{1}H and ^{13}C, respectively. In order to facilitate the detection of small *J* data, the 64 K time-domain ^{1}H NMR spectra were zero-filled to 512 K data point sets and additionally resolution enhanced with the Lorentzian-to-Gaussian function[1] prior to the Fourier transformation to change the line shape of the spectral peaks. Chemical shifts are reported in terms of δ data, in ppm, downfield from tetramethylsilane (TMS) used as an internal reference; δ = 0.000 ppm. Splitting patterns are designated as follows: by br, broad signal; s, singlet; d, doublet; t, triplet; dd, doublet of doublets, *etc*. *J*-couplings are given in Hz; J_{HH}s were obtained in the first-order analysis, whereas J_{CH}s extracted from $^{1}H/^{13}C$-HMBC plots as differences between off-diagonal cross-peaks arising from the ^{13}C satellites of H1' signals. The spectra were assigned with the aid of 2D shift correlation NMR experiments (COSY, HMQC, HMBC and NOESY) and all these assignments were positively verified by the DFT/GIAO-based predictions of δ data. The medium pressure liquid chromatography (MPLC) was done on a Büchi Sepacore Easy Purification System, by using cartridges packed with silica gel 230-400 mesh (Sigma-Aldrich) and appropriate solvent system as an eluent. Melting points (mps) were measured on a Boëtius apparatus and are uncorrected.

Synthesis and spectroscopic data

2,2,5,7,8-Pentamethylchroman-6-ol[2] (1 mmol), β-D-glucose pentaacetate (1.5 mmol; Sigma-Aldrich) and 0.25 equiv of anhydrous $ZnCl_2$ was heated on an oil bath at 130°C under diminished pressure (40 Torr) for 4 hrs. The reaction mixture was diluted with ethyl acetate (50 ml) and washed with water (3 x 30 ml). The organic layer was dried over $MgSO_4$ and evaporated to dryness. The crude reaction mixture was purified by MPLC (hexane-ethyl acetate, 15:1 v/v) giving inseparable mixture of **1α** and **1β** (48%; α/β 36:64). The glucosidic fraction was subjected to deacetylation according to Herzig *et al.* (MeOH, KCN, rt).[3] The α/β-anomers were separated in their deacetylated forms by MPLC chromatography (ethyl acetate) and resulted pure samples of both compounds were subjected to the acetylation procedure (Py/Ac_2O, 12 hrs, rt, yield 97%). After evaporation to dryness, the obtained glucopyranosides **1α** and **1β** were purified by MPLC (hexane-ethyl acetate, 5:1 v/v).

2,2,5,7,8-Pentamethylchroman-6-yl-2,3,4,6-tetra-*O*-acetyl-α-D-glucopyranoside[4] **(1α)**. White solid; δ_H (600 MHz, $CDCl_3$) 1.268 (3H, q, $J_{H,Hb}$ ~0.45, H2b), 1.298 (3H, q, $^{4}J_{H2a,H2b}$ ~0.45, H2a), 1.783 (2H, t, $^{3}J_{H3,H4}$ = 6.84, H3), 1.922 (3H, s, 2'-C$\underline{H}_3$CO), 2.042 (3H, s, 3'-C$\underline{H}_3$CO), 2.065 (3H, br s, H8b), 2.070 (3H, s, 4'-C$\underline{H}_3$CO), 2.076 (3H, s, 6'-C$\underline{H}_3$CO), 2.180 (3H, br s, H5a), 2.218 (3H, br s, H7a), 2.568 (2H, br t, $^{3}J_{H3,H4}$ = 6.84, H4), 4.147 (1H, dd, $^{3}J_{H6'R,H6'S}$ = 12.37, $^{3}J_{H5',H6'S}$ = 2.34, H6'*S*), 4.308 (1H, dd, $^{3}J_{H6'R,H6'S}$ = 12.37, $^{3}J_{H5',H6'R}$ = 4.68, H6'*R*), 4.528 (1H, dddd, $^{3}J_{H4',H5'}$ = 10.32, $^{3}J_{H5',H6'R}$ = 4.68, $^{3}J_{H5',H6'S}$ = 2.34, $^{4}J_{H1',H5'}$ = 0.52, H5'), 5.079 (1H, dd, $^{3}J_{H2',H3'}$ = 10.50, $^{3}J_{H1',H2'}$ = 3.54, H2'), 5.164 (1H, dd, $^{3}J_{H4',H5'}$ = 10.32, $^{3}J_{H3',H4'}$ = 9.30, H4'), 5.253 (1H, d, $^{3}J_{H1',H2'}$ = 3.54, H1'), 5.802 (1H, ddd, $^{3}J_{H2',H3'}$ = 10.51, $^{3}J_{H3',H4'}$ = 9.32, $^{4}J_{H1,H3}$ = 0.40, H3'); δ_C (150 MHz, $CDCl_3$) 11.90 (C8b), 13.07 (C5a), 13.99 (C7a), 20.45 (C2', $\underline{C}H_3CO$), 20.65 (C4', $\underline{C}H_3CO$), 20.68 (C3', $\underline{C}H_3CO$), 20.68 (C6', $\underline{C}H_3CO$), 21.17 (C4), 26.48 (C2b), 27.04 (C2a), 32.92 (C3), 62.14 (C6'), 68.63 (C4'), 69.10 (C5'), 70.06 (C3'), 71.14 (C2'), 72.85 (C2), 98.78 (C1'), 117.59 (C4a), 123.31 (C8), 124.86 (C5), 126.91 (C7), 147.79 (C6), 148.23 (C8a), 169.60 (C4', $CH_3\underline{C}O$), 169.84 (C2', $CH_3\underline{C}O$), 170.12 (C3', $CH_3\underline{C}O$), 170.63 (C6', $CH_3\underline{C}O$).

2,2,5,7,8-Pentamethylchroman-6-yl-2,3,4,6-tetra-*O*-acetyl-β-D-glucopyranoside[4] **(1β)**. Colorless needles, mp 141-143°C; δ_H (600 MHz, $CDCl_3$) 1.281 (3H, q, $^{4}J_{H2a,H2b}$ ~0.45, H2b), 1.293 (3H, q, $^{4}J_{H2a,H2b}$ ~0.45, H2a), 1.783 (2H, t, $^{3}J_{H3,H4}$ = 6.85, H3), 2.007 (3H, s, 4'-C$\underline{H}_3$CO), 2.011 (3H, s, 3'-C$\underline{H}_3$CO), 2.029 (3H, s, 6'-C$\underline{H}_3$CO), 2.070 (3H, br s, H8b), 2.100 (3H, br s, H5a), 2.105 (3H, s, 2'-C$\underline{H}_3$CO), 2.142 (3H, br s, H7a), 2.576 (2H, br t, $^{3}J_{H3',H4'}$ = 6.85, H4), 3.527 (1H, ddd, $^{3}J_{H4',H5'}$ = 9.95, $^{3}J_{H5',H6'R}$ = 4.72, $^{3}J_{H5',H6'S}$ = 2.74, H5'), 4.055 (1H, dd, $^{3}J_{H6'R,H6'S}$ = 12.18, $^{3}J_{H5',H6'S}$ = 2.74, H6'*S*), 4.190 (1H, dd, $^{3}J_{H6'R,H6'S}$ = 12.18, $^{3}J_{H5',H6'R}$ = 4.72, H6'*R*), 4.714 (1H, d, $^{3}J_{H1',H2'}$ = 8.00,

H1'), 5.162 (1H, dd, $^3J_{H4',H5'}$ = 9.95, $^3J_{H3',H4'}$ = 9.26, H4'), 5.243 (1H, dd, $^3J_{H2',H3'}$ = 9.71, $^3J_{H3',H4'}$ = 9.26, H3'), 5.323 (1H, dd, $^3J_{H2',H3'}$ = 9.71, $^3J_{H1',H2'}$ = 8.00, H2'); δ_C (150 MHz, $CDCl_3$) 11.82 (C8b), 12.65 (C5a), 13.38 (C7a), 20.56 (C4', $\underline{C}H_3CO$), 20.58 (C3', $\underline{C}H_3CO$), 20.63 (C6', $\underline{C}H_3CO$), 20.72 (C2', $\underline{C}H_3CO$), 21.04 (C4), 26.70 (C2b), 26.92 (C2a), 32.90 (C3), 61.85 (C6'), 68.73 (C4'), 71.53 (C5'), 72.00 (C2'), 72.89 (C2), 73.19 (C3'), 102.08 (C1'), 117.30 (C4a), 122.89 (C8), 126.89 (C5), 128.31 (C7), 145.37 (C6), 148.76 (C8a), 169.24 (C2', $CH_3\underline{C}O$), 169.40 (C4', $CH_3\underline{C}O$), 170.38 (C3', $CH_3\underline{C}O$), 170.52 (C6', $CH_3\underline{C}O$).

1-*O*-Methyl-2,3,4,6-tetra-*O*-acetyl-α-D-glucopyranoside[5] **(2α)**. Obtained by acetylation (Py/Ac_2O) of methyl α-D-glucopyranoside (Sigma-Aldrich). Colorless crystals; δ_H (600 MHz, $CDCl_3$) 2.004 (3H, s, 3-$C\underline{H}_3CO$), 2.025 (3H, s, 4-$C\underline{H}_3CO$), 2.071 (3H, s, 2-$C\underline{H}_3CO$), 2.093 (3H, s, 6-$C\underline{H}_3CO$), 3.414 (3H s, $OC\underline{H}_3$), 3.986 (1H, dddd, $^3J_{H4,H5}$ = 10.26, $^3J_{H5,H6R}$ = 4.69, $^3J_{H5,H6S}$ = 2.40, $^4J_{H1,H5}$ = 0.54, H5), 4.114 (1H, dd, $^3J_{H6R,H6S}$ = 12.31, $^3J_{H5,H6S}$ = 2.40, H6*S*), 4.258 (1H, dd, $^3J_{H6R,H6S}$ = 12.31, $^3J_{H5,H6R}$ = 4.74, H6*R*), 4.894 (1H, dd, $^3J_{H2,H3}$ = 10.20, $^3J_{H1,H2}$ = 3.66, H2), 4.951 (1H, br d, $^3J_{H1,H2}$ = 3.66, H1), 5.061 (1H, dd, $^3J_{H4,H5}$ = 10.26, $^3J_{H3,H4}$ = 9.36, H4), 5.474 (1H, ddd, $^3J_{H2,H3}$ = 10.20, $^3J_{H3,H4}$ = 9.32, $^4J_{H1,H5}$ = 0.36, H3); δ_C (150 MHz; $CDCl_3$) 20.59 (C4, $\underline{C}H_3CO$), 20.65 (C3, $\underline{C}H_3CO$), 20.68 (C6, $\underline{C}H_3CO$), 20.69 (C2, $\underline{C}H_3CO$), 55.48 ($O\underline{C}H_3$), 62.02 (C6), 67.23 (C5), 68.69 (C4), 70.21 (C3), 70.89 (C2), 96.87 (C1), 169.57 (C4, $CH_3\underline{C}O$), 170.02 (C3, $CH_3\underline{C}O$), 170.11 (C2, $CH_3\underline{C}O$), 170.60 (C6, $CH_3\underline{C}O$).

References

1 See *e.g.*, (a) J. C. Lindon and A. G. Ferrige, *Prog. Nucl. Magn. Reson. Spectrosc.*, 1980, **14**, 27–66; (b) T. Kupka and J. O. Dzięgielewski, *Magn. Reson. Chem.,* 1988, **26**, 353–357; (c) F. A. Anet and D. J. O'Leary, *Tetrahedron Lett.,* 1989, **30**, 2755–2758; (d) L. Griffiths, *Magn. Reson. Chem.,* 2001, **39**, 194–202.

2 (a) L. I. Smith, H. E. Ungnade, H. H. Hoehn and S. Wawzonek, *J. Org. Chem.,* 1939, **4**, 311–317; (b). Y. Yamamoto and K. Itonaga, *Org. Lett.*, 2009, **11**, 717–720.

3 J. Herzig, A. Nudelman, H. E. Gottlieb and B. Fischer, *J. Org. Chem.*, 1986, **51**, 727–730.

4 S. Witkowski and P. Wałejko, *Z. Naturforsch. B*, 2002, **57**, 571–578.

5 L. Shi, G. Zhang and F. Pan, *Tetrahedron*, 2008, **64**, 2572–2575.

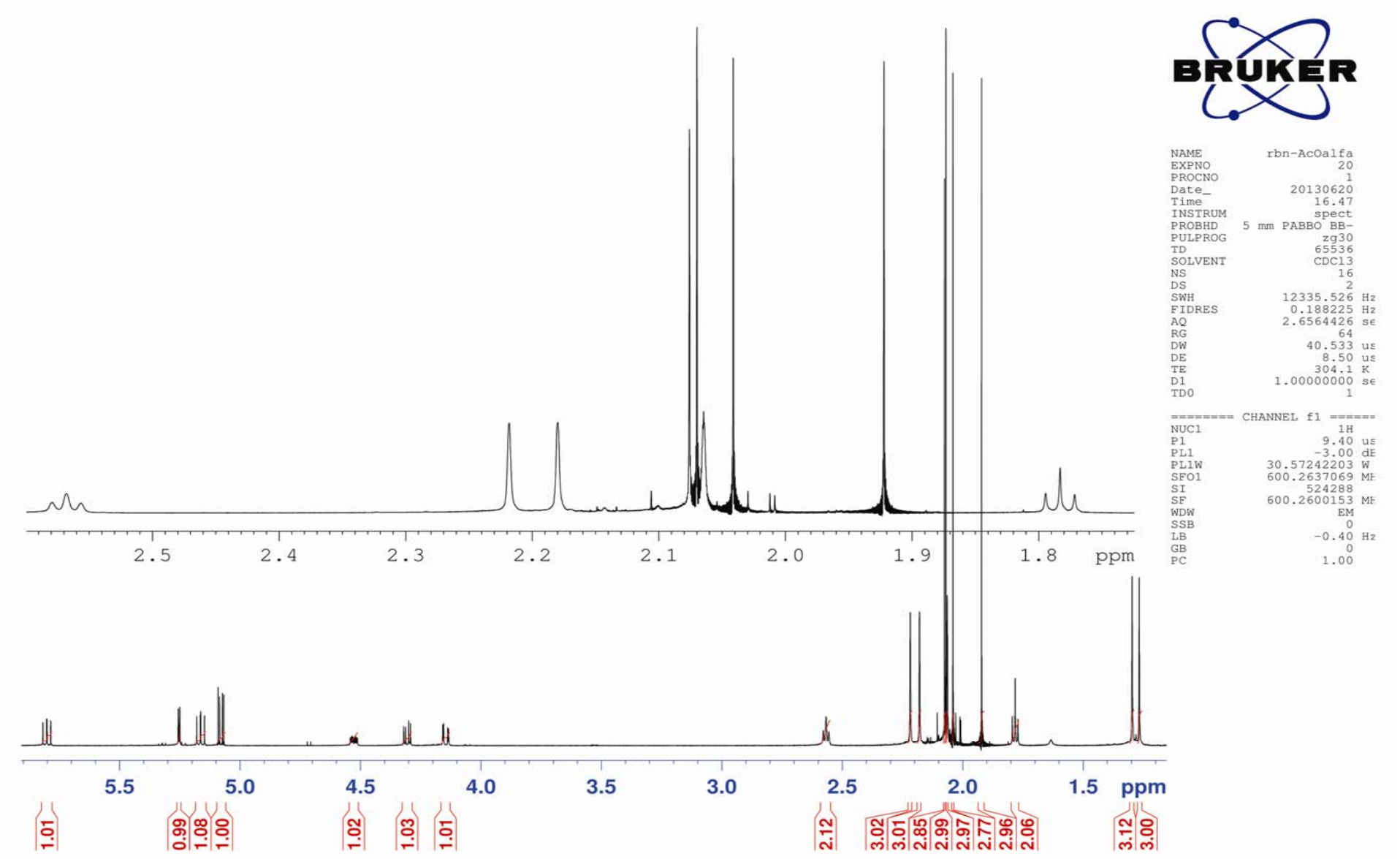


Figure S1. The 600 MHz ^{1}H NMR spectrum of glucoside **1α** in $CDCl_3$/TMS.

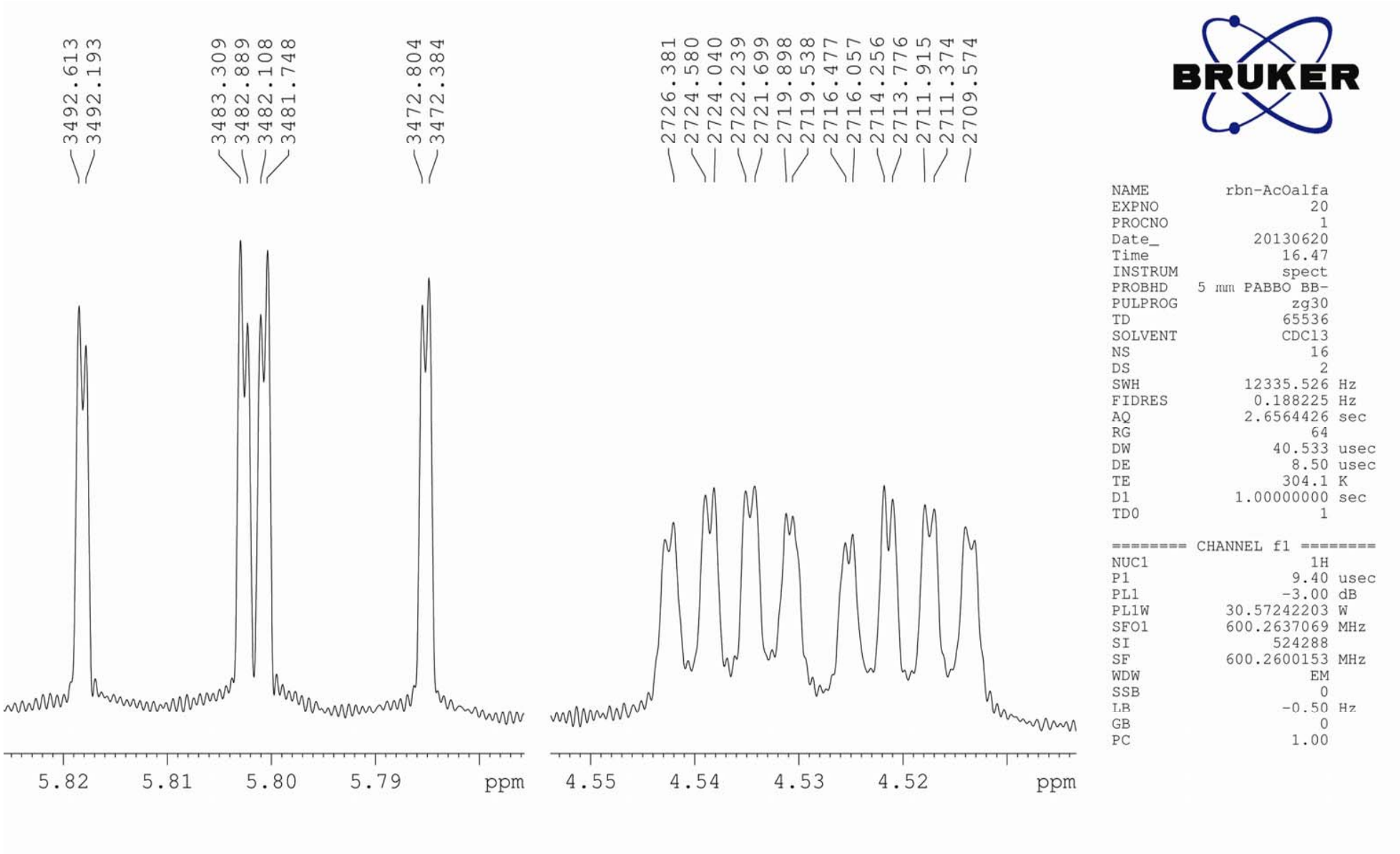


Figure S2. Two regions of the 600 MHz ^{1}H NMR spectrum of glucoside **1α** in $CDCl_3$/TMS.

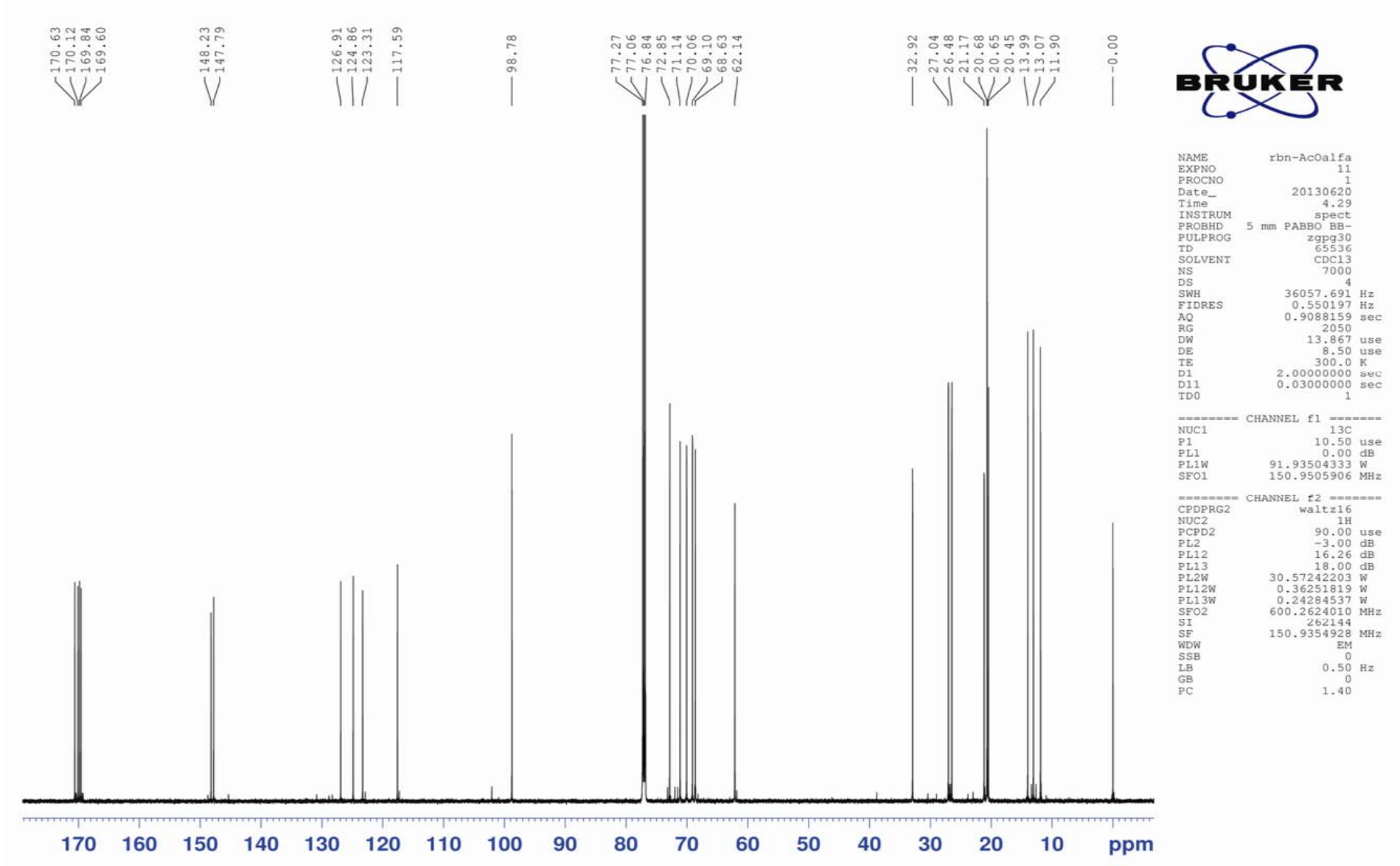


Figure S3. The 150 MHz ^{13}C NMR spectrum of glucoside **1α** in $CDCl_3$/TMS.

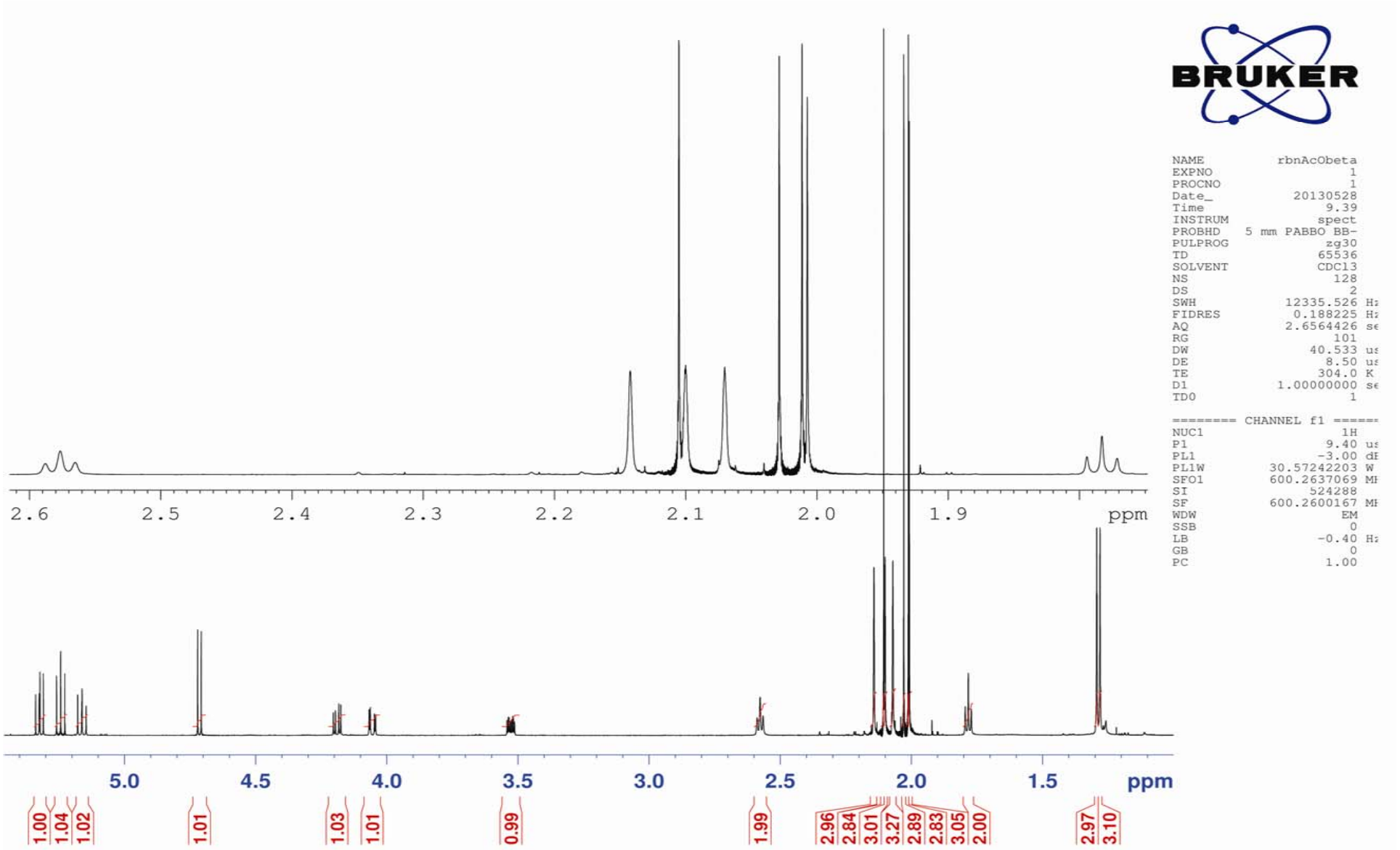


Figure S4. The 600 MHz ^{1}H NMR spectrum of glucoside **1β** in $CDCl_3$/TMS.

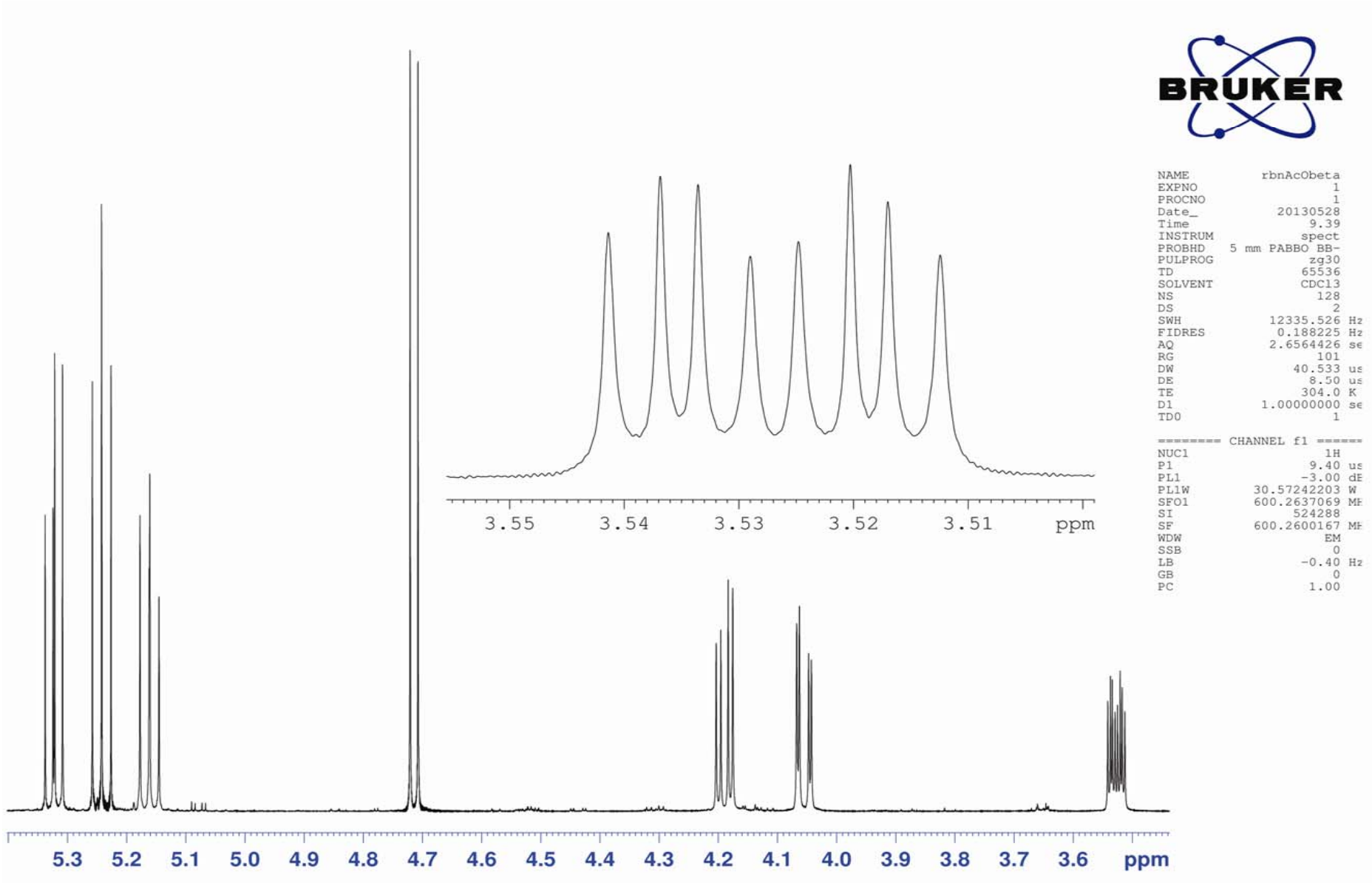


Figure S5. Two regions of the 600 MHz ^{1}H NMR spectrum of glucoside **1β** in $CDCl_3$/TMS.

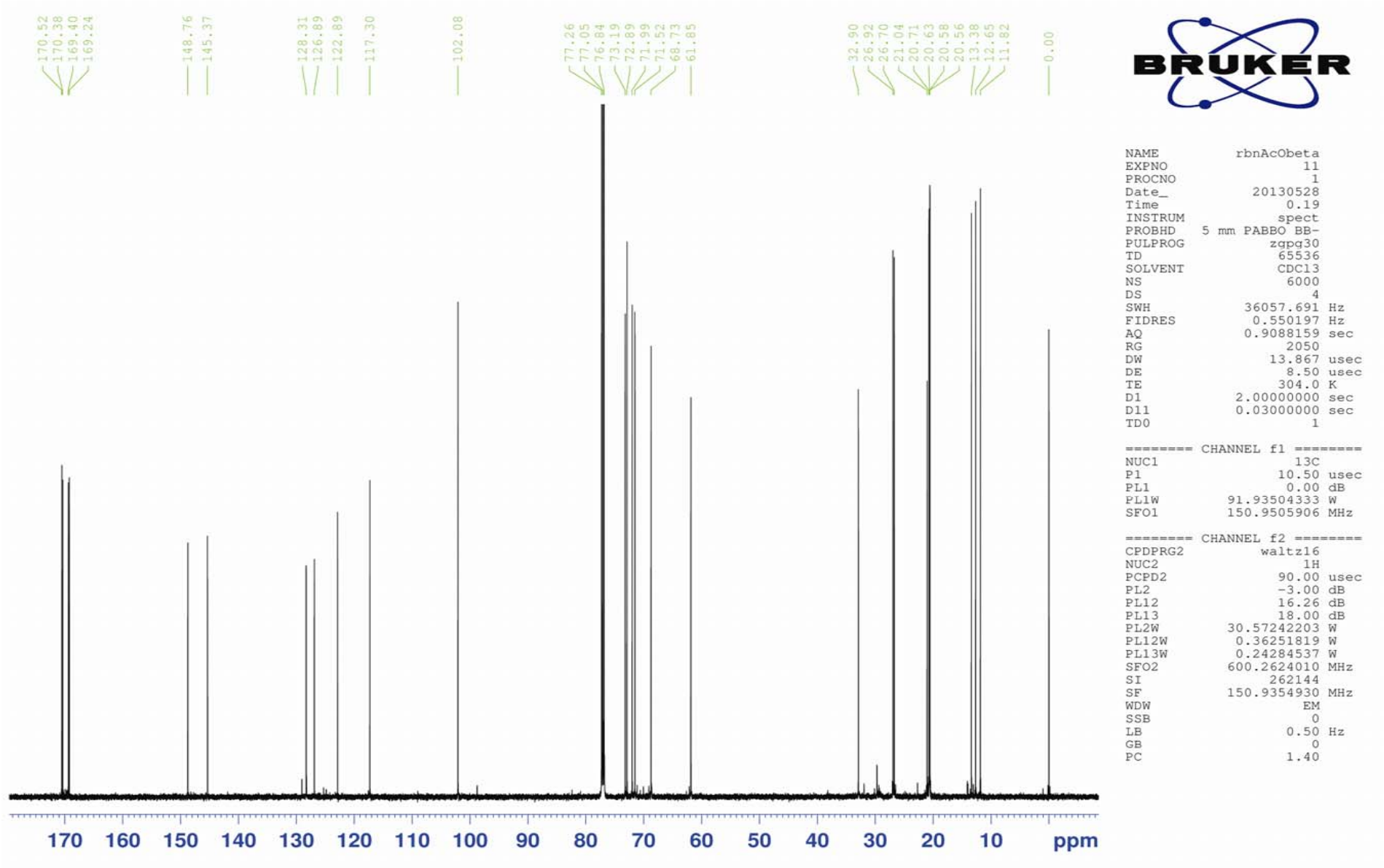


Figure S6. The 150 MHz ^{13}C NMR spectrum of glucoside **1β** in $CDCl_3$/TMS.

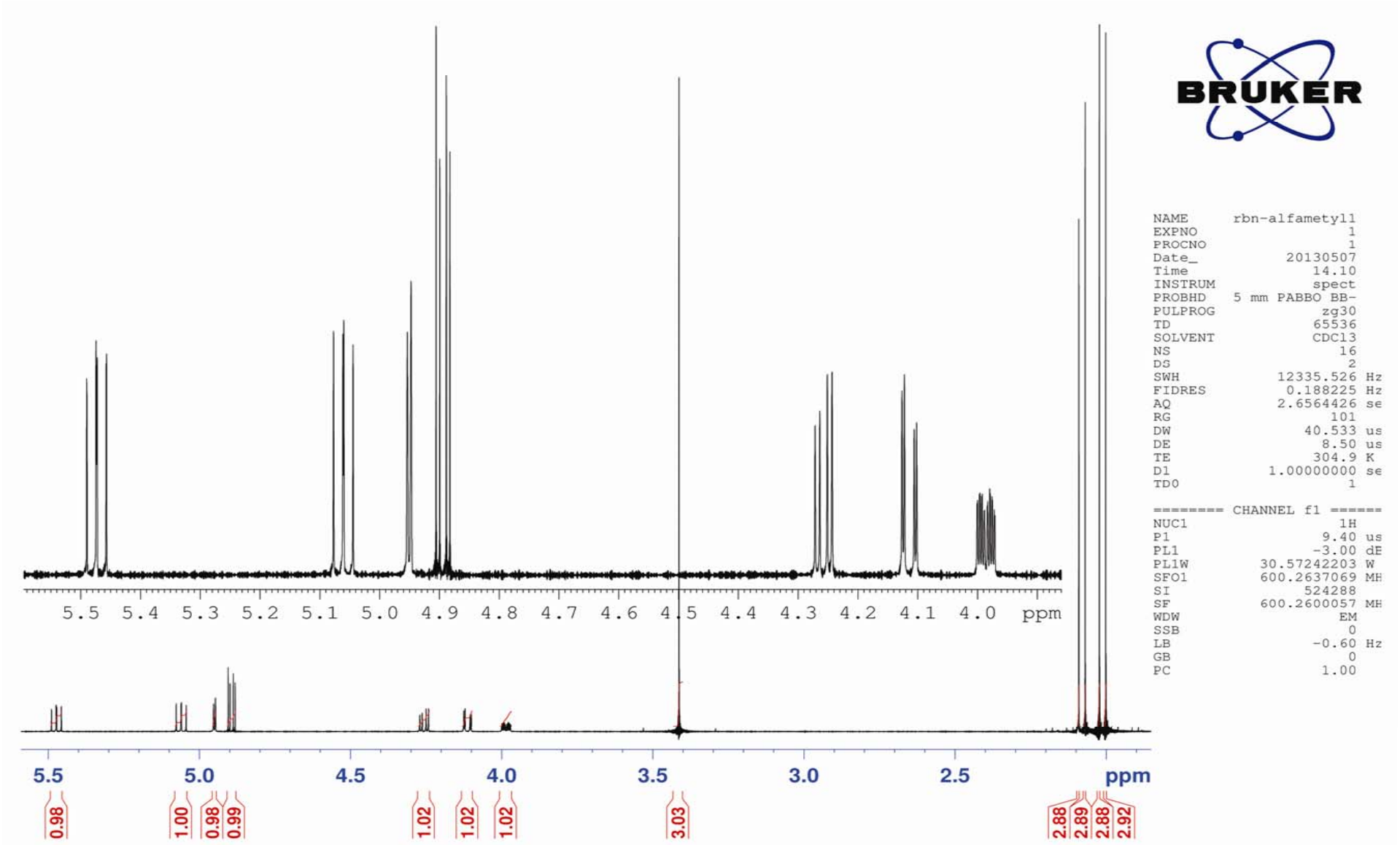


Figure S7. The 600 MHz ^{1}H NMR spectrum of glucoside **2α** in $CDCl_3$/TMS.

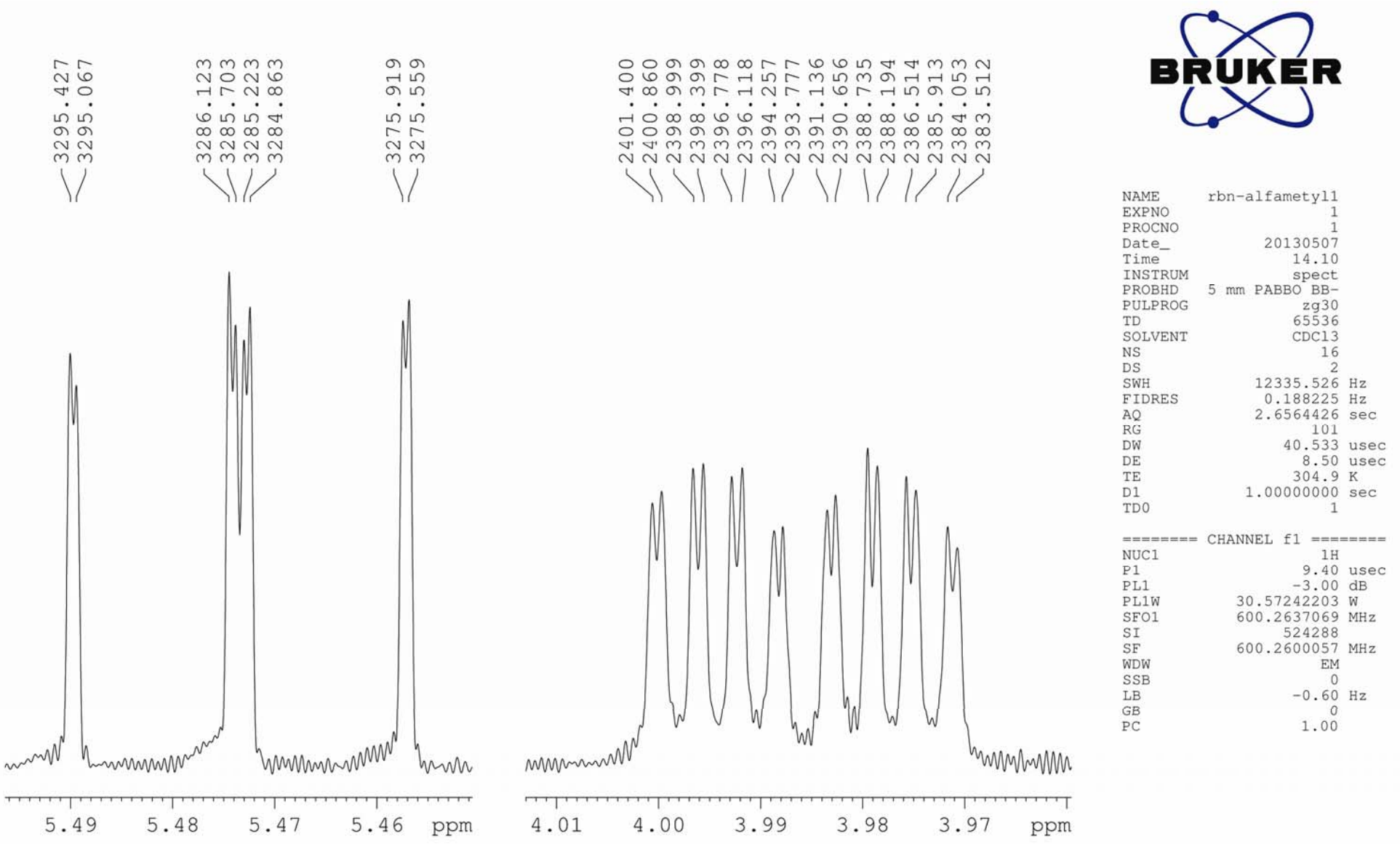


Figure S8. Two regions of the 600 MHz ^{1}H NMR spectrum of glucoside **2α** in $CDCl_3$/TMS.

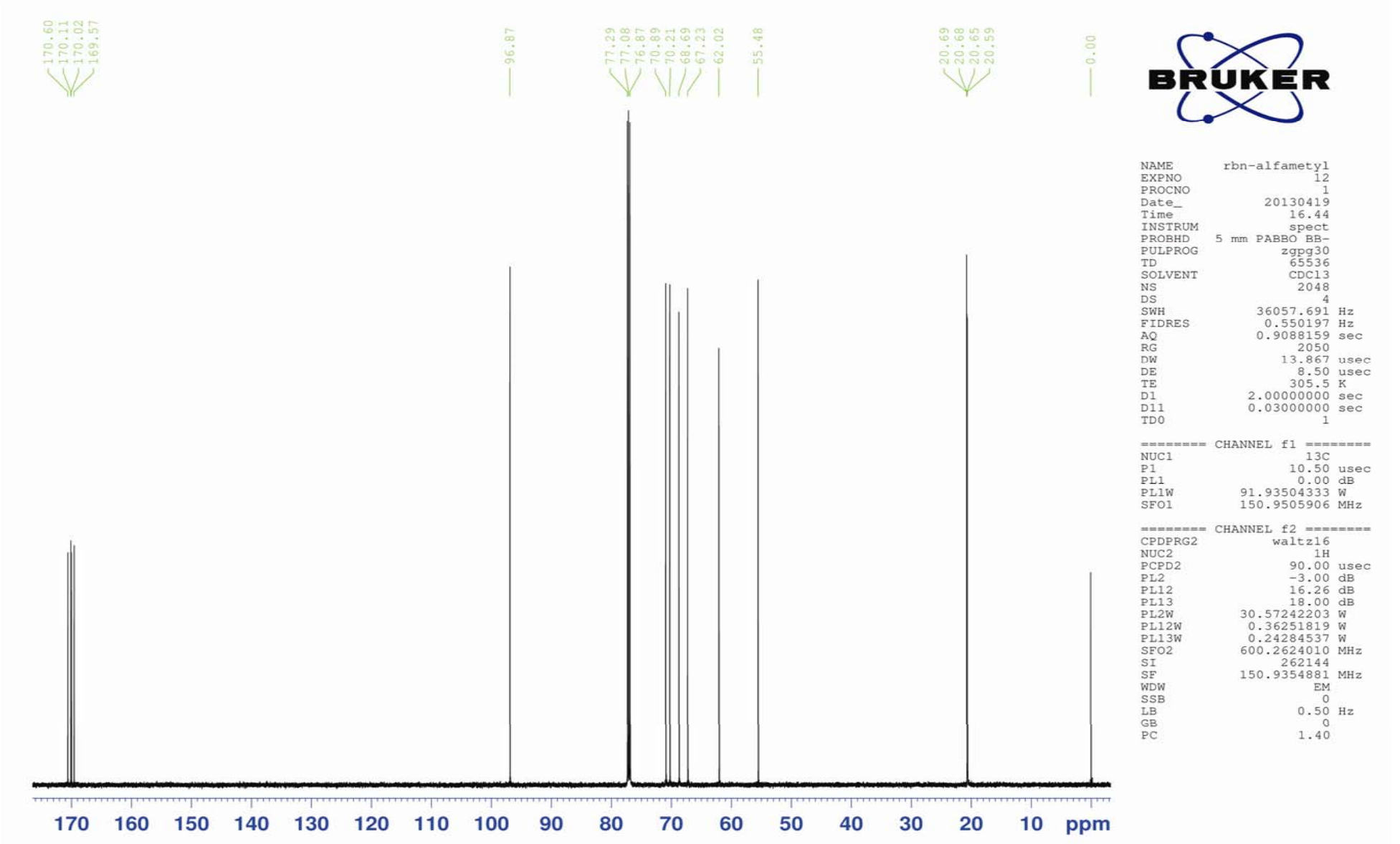
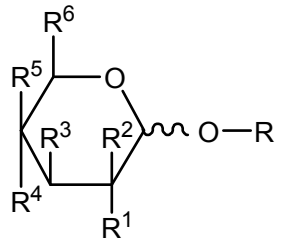
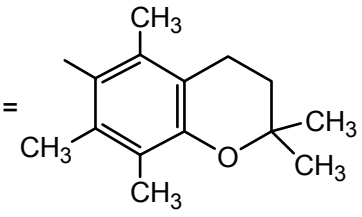


Figure S9. The 150 MHz ^{13}C NMR spectrum of glucoside **2α** in $CDCl_3$/TMS.

Table S1. Structures of glycopyranosides **1-8**



PMC' =



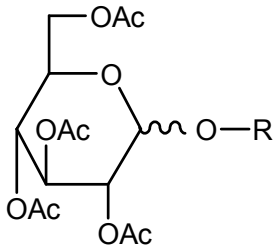
Compound	R	R^1	R^2	R^3	R^4	R^5	R^6
1	PMC′	OAc	H	OAc	OAc	H	OAc
2	Me	OAc	H	OAc	OAc	H	OAc
3	PMC′	OH	H	OH	OH	H	OH
4	PMC′	H	OAc	OAc	OAc	H	OAc
5	PMC′	H	OH	OH	OH	H	OH
6	PMC′	OAc	H	OAc	H	OAc	OAc
7	PMC′	OH	H	OH	H	OH	OH
8	PMC′	H	H	OAc	OAc	H	OAc

Table S2. Selected 400/100 MHz $^1H/^{13}C$ NMR data for **1-8**.

Compound	α/β	δ_{H1} [ppm]	Δ_{H1}[a] [ppm]	δ_{H5} [ppm]	Δ_{H5}[b] [ppm]	δ_{C1} [ppm]	Δ_{C1}[c] [ppm]	δ_{H6}[d] [ppm]
1[e]	α	5.25	**0.53**	4.54	**1.00**	98.6	**-3.3**	4.10–4.40
	β	4.72		3.54		101.9		4.06, 4.12
2[e]	α	4.94	**0.52**	3.97	**0.32**	96.7	**-4.9**	4.09, 4.25
	β	4.42		3.65		101.6		4.13, 4.27
3[f]	α	5.18	**0.63**	4.06	**1.05**	103.2	**-2.4**	3.40–3.92
	β	4.55		3.01		105.6		3.58, 3.78
4[e]	α	4.91	**0.17**	4.51	**1.01**	101.5	**1.2**	4.12–4.38
	β	4.74		3.50		100.3		4.14–4.37
5[f]	α	4.83	**0.16**	4.21	**1.13**	105.0	**3.0**	3.40–3.72
	β	4.67		3.08		102.0		3.50–4.07
6[e]	α	5.18	**0.50**	4.75	**1.00**	99.2	**-3.3**	4.00–4.40
	β	4.68		3.75		102.5		4.07, 4.09
7[f]	α	5.23	**0.77**	4.25	**0.94**	103.0	**-3.2**	3.60–4.10
	β	4.46		3.31		106.2		3.51–3.87
8[e]	α	f	**f**	4.38	**0.70**	100.7	**-0.2**	3.88–4.25
	β	f		3.68		100.9		3.84–4.30

[a] $\Delta_{H1} = \delta_{H1\alpha} - \delta_{H1\beta}$. [b] $\Delta_{H5} = \delta_{H5\alpha} - \delta_{H5\beta}$. [c] $\Delta_{C1} = \delta_{C1\alpha} - \delta_{C1\beta}$. [d] The range of δ_H values or centers of two multiplets. [e] For $CDCl_3$ solution. [f] For CD_3OD solution. [f] Not determined due to strong signal overlapping for the analyzed α/β mixture.

Table S3. Differences in chemical shifts of the $H_{5\alpha}$ and $H_{5\beta}$ protons in a series of glucosides (400 MHz ^1H NMR/$CDCl_3$ solution).



	$\delta_{H5\alpha}$ [ppm]	$\delta_{H5\beta}$ [ppm]	$\Delta_{H5} = \delta_{H5\alpha} - \delta_{H5\beta}$ [ppm]
R = Ac	4.06	3.77	0.29
R = Me (compd. **2**)	3.97	3.65	0.32
R = Ph	4.30	3.86	0.44
Compd. **8**[a]	4.38	3.68	0.70
R = 2,6-dimethylphenyl	4.52	3.57	0.95
R = PMC' (compd. **1**)	4.54	3.54	1.00
R = α-tocopheryl	4.56	3.51	1.05

[a/] For the structure see Table S1.

Table S4. Key torsion angles[a] [°] and G^{o} data [hartrees] for all 12 initial conformers of **1α** obtained by four DFT/PCM(UFF,$CHCl_3$) methods with the 6-31+G(*d*,*p*) basis set.

Form[b]	Functional	phi (φ)	psi (ψ)	omega (ω)	chi (χ)	theta (θ)	G^{o}
13762 1αB	B3LYP	127.5	122.4	71.3	176.6	58.4	-1916.982281
	M06-2X	141.2	118.1	69.5	179.1	61.2	-1916.179273
	ωB97X-D	146.2	117.2	70.4	178.3	59.9	**-1916.407534**
	B3LYP-GD3BJ	146.9	117.8	70.9	178.4	59.8	-1917.143472
13787	B3LYP	127.8	122.5	68.3	93.3	58.4	-1916.981720
	M06-2X	141.2	118.0	65.4	82.0	61.1	-1916.178834
	ωB97X-D	145.4	117.0	65.8	83.1	60.0	-1916.406536
	B3LYP-GD3BJ	147.5	117.7	66.4	83.1	59.9	-7.27[c]
13874 1αH	B3LYP	127.2	122.0	-64.9	-175.5	58.4	-1916.981351
	M06-2X	141.6	118.1	-64.6	-148.9	61.2	-1916.179948
	ωB97X-D	150.9	117.3	-70.3	-123.4	60.1	-1916.405846
	B3LYP-GD3BJ	151.1	117.8	-70.8	-123.5	60.0	-7.58[c]
13942[d] **1αF**	B3LYP	124.6	123.2	70.8	177.1	-58.7	-1916.981751
	M06-2X	138.3	118.6	69.0	179.8	-60.8	-1916.178409
	ωB97X-D	139.4	118.0	69.9	179.0	-59.7	-1916.407117
	B3LYP-GD3BJ	140.9	118.9	70.6	178.0	-59.6	-1917.142761
14072 1αC	B3LYP	126.2	-61.4	70.8	175.9	-58.5	-1916.982214
	M06-2X	140.7	-64.6	69.6	179.8	-61.0	-1916.180113
	ωB97X-D	143.6	-65.2	70.0	179.7	-59.8	-1916.406547
	B3LYP-GD3BJ	146.2	-64.5	70.7	179.0	-59.8	-6.96[c]
14082	**B3LYP**	125.6	123.6	68.1	93.1	-58.6	**-1916.982729**
	M06-2X	139.3	118.4	65.4	81.9	-60.8	-1916.178556
	ωB97X-D	140.4	117.9	65.2	82.9	-59.7	-1916.405742
	B3LYP-GD3BJ	140.6	118.6	65.7	82.9	-59.6	-1917.141332
14216 1αA	B3LYP	126.1	-61.2	-65.3	-175.3	-58.6	-1916.982435
	M06-2X	141.7	-64.6	-64.4	-149.8	-61.0	-1916.180019
	ωB97X-D	151.9	-65.0	-70.3	-124.1	-59.9	-1916.405535
	B3LYP-GD3BJ	152.7	-64.5	-70.7	-123.8	-59.8	-5.48[c]
14229[e]	*X-ray structure*	*137.0 (2)*	*-68.2 (3)*	*57.8 (3)*	*79.0 (3)*	*59.6 (5)*	–
	B3LYP	128.0	-62.7	68.4	93.4	58.6	-1916.981231
	M06-2X	141.5	-65.1	65.8	82.2	61.0	-1916.179731
	ωB97X-D	155.7	-65.4	66.8	83.4	60.1	-1916.406235
	B3LYP-GD3BJ	153.4	-65.1	67.1	83.7	60.1	-1917.141986
14322 1αD	B3LYP	125.5	123.5	-64.9	-175.0	-58.7	-1916.982145
	M06-2X	139.6	118.3	-64.8	-148.8	-60.7	-1916.179491
	ωB97X-D	142.0	118.0	-70.6	-123.0	-59.6	-1916.405298
	B3LYP-GD3BJ	142.7	119.1	-70.8	-123.1	-59.5	-1917.140439
14447[f] **1αG**	B3LYP	126.6	-62.8	71.1	176.3	58.6	-1916.981613
	M06-2X	141.6	-65.1	69.5	178.8	61.0	-1916.179671
	ωB97X-D	154.5	-65.3	70.5	178.2	60.0	-1916.407261
	B3LYP-GD3BJ	152.8	-65.1	70.8	177.3	60.0	-2.83[c]
14599 1αE	B3LYP	127.6	-62.8	-65.3	-175.1	58.5	-1916.982140
	M06-2X	142.5	-64.9	-64.3	-149.7	61.0	**-1916.180283**
	ωB97X-D	155.3	-65.4	-70.3	-123.2	60.0	-1916.405307
	B3LYP-GD3BJ	154.1	-65.1	-70.7	-123.2	60.0	-1917.140862
14913[e]	*X-ray structure*	*136.3 (2)*	*-69.3 (3)*	*50.8 (3)*	*78.2 (3)*	*-53.6 (13)*	–
	B3LYP	127.1	-61.2	67.9	93.6	-58.6	-1916.982710
	M06-2X	140.2	-64.7	65.9	82.2	-61.1	-1916.179539
	ωB97X-D	143.4	-65.2	66.1	83.7	-59.9	-1916.406842
	B3LYP-GD3BJ	146.2	-64.5	67.1	84.0	-59.8	-10.05[c]

[a/] For their detailed description, see the main text. [b/] Initial code names xxxxxx of all of the structures originate from the MMX energies (xx.xxx in kcal mol^{-1}) of their simple MMX models, after omission of the decimal point and final name below (if applicable). [c/] An imaginary vibrational frequency. [d/] Obtained from **13762** by DHP ring flipping (Hyperchem). [e/] Constructed from an incomplete geometry of such a conformer recognized in the crystal of **1α** (italicized numbers, see also main text). [f/] From **14072** by DHP ring flipping (Hyperchem).

Table S5. Key torsion angles[a] [°] and G^{o} data [hartrees] for all 12 initial conformers of **1β** obtained by four DFT/PCM(UFF,$CHCl_3$) methods with the 6-31+G(*d*,*p*) basis set.

Form[b]	Functional	phi (φ)	psi (ψ)	omega (ω)	chi (χ)	theta (θ)	G^{o}
12272 1βF	B3LYP	-73.0	106.2	72.4	-179.8	-58.5	-1916.984778
	M06-2X	-74.7	99.7	67.6	-174.0	-61.0	-1916.177993
	ωB97X-D	-74.0	105.8	63.2	-108.3	-59.3	-1916.406944
	B3LYP-GD3BJ	-73.1	105.4	65.0	-108.2	-59.0	-1917.140876
12302 1βG	B3LYP	-72.8	104.1	72.3	-180.0	58.5	-1916.984645
	M06-2X	-72.4	97.7	67.8	-165.3	61.1	-1916.178542
	ωB97X-D	-64.6	101.0	67.3	-110.2	59.8	-1916.407195
	B3LYP-GD3BJ	-63.7	101.4	68.2	-108.7	59.6	-8.08[c]
12506[d] 1βA	*X-ray structure*	*68.4 (10)*	*78.7 (11)*	*-78.4 (11)*	*166.3 (9)*	*58.3 (14)*	–
	B3LYP	-73.4	-79.7	72.2	-179.6	-58.5	**-1916.985973**
	M06-2X	-73.8	-84.7	66.0	-167.4	-61.0	-1916.177614
	ωB97X-D	-58.7	-79.6	66.3	-107.1	-59.9	-1916.406544
	B3LYP-GD3BJ	-61.7	-78.9	67.6	-107.9	-59.7	-1917.142420
13023 1βE	B3LYP	-73.1	-81.3	71.4	-179.4	58.6	-1916.985023
	M06-2X	-74.2	-86.1	66.1	-168.1	61.0	-1916.179069
	ωB97X-D	-62.3	-80.9	67.6	-110.0	59.9	-1916.406742
	B3LYP-GD3BJ	-63.0	-80.2	68.1	-109.3	59.9	-1917.142163
13597[e]	B3LYP	-74.0	-81.6	66.0	88.8	58.5	-1916.985200
	M06-2X	-70.1	-84.3	49.7	70.2	61.0	-1916.177621
	ωB97X-D	-69.5	-82.0	49.6	70.1	60.0	-1916.407702
	B3LYP-GD3BJ	-69.6	-81.8	49.4	69.2	60.0	-1917.141984
13599[f]	B3LYP	-72.8	105.6	67.3	89.8	-58.5	-1916.983669
	M06-2X	-76.0	99.7	46.5	67.1	-60.2	-1916.176962
	ωB97X-D	-76.9	101.2	46.0	67.5	-59.1	-1916.405339
	B3LYP-GD3BJ	-75.5	101.6	47.4	67.3	-58.8	-1917.143245
13620	B3LYP	-72.4	103.8	66.3	89.3	58.5	-1916.984464
	M06-2X	-72.6	96.3	48.9	70.0	61.2	-1916.177639
	ωB97X-D	-71.3	97.4	48.8	70.3	59.9	-1916.407435
	B3LYP-GD3BJ	-70.3	97.9	49.1	69.5	59.7	-1917.142129
13675 1βH	B3LYP	-72.6	105.1	-65.1	-175.6	-58.6	-1916.984495
	M06-2X	-74.1	100.8	-63.6	-149.4	-61.0	-1916.178995
	ωB97X-D	-75.4	102.0	-69.8	-122.8	-59.8	-1916.405495
	B3LYP-GD3BJ	-75.0	102.3	-70.1	-122.8	-59.8	-2.15[c]
13731[g]	B3LYP	-73.9	-79.9	66.0	88.5	-58.5	-1916.985279
	M06-2X	-73.2	-84.1	48.0	69.3	-61.1	-1916.177227
	ωB97X-D	-72.6	-82.4	48.2	69.4	-59.8	**-1916.408001**
	B3LYP-GD3BJ	-69.7	-81.4	48.8	69.0	-59.7	-1917.142328
13878 1βD	B3LYP	-72.7	103.3	-65.3	-175.7	58.5	-1916.985094
	M06-2X	-73.1	98.9	-63.9	-147.3	61.0	-1916.179344
	ωB97X-D	-75.2	100.2	-69.8	-123.2	59.8	-1916.405967
	B3LYP-GD3BJ	-74.8	100.7	-70.1	-123.1	59.8	-1917.142655
14572[h] 1βB	B3LYP	-72.8	-80.0	-65.0	-174.8	-58.6	-1916.985754
	M06-2X	-73.8	-83.0	-71.0	-118.9	-61.1	-1916.177884
	ωB97X-D	-75.1	-82.2	-69.8	-123.2	-59.9	-1916.405960
	B3LYP-GD3BJ	-75.0	-81.5	-70.1	-123.2	-59.9	-1917.140828
14866[i] 1βC	B3LYP	-72.7	-81.3	-65.2	-175.3	58.6	-1916.985289
	M06-2X	-74.8	-85.2	-63.6	-149.7	61.0	**-1916.180120**
	ωB97X-D	-76.0	-84.2	-69.7	-123.1	59.9	-1916.405601
	B3LYP-GD3BJ	-75.3	-83.3	-70.0	-123.2	59.8	-1917.142008

[a/] For their detailed description, see the main text. [b/] Initial code names xxxxxx of all of the structures originate from the MMX energies (xx.xxx in kcal mol^{-1}) of their simple MMX models, after omission of the decimal point and final name below (if applicable). [c/] The imaginary vibrational frequency. [d/] Found later as an enantiomeric specimen in the crystal structure of **1β** (italicized numbers); see main text. [e/] Obtained from **13023** by the C6'–O6' bond rotation (Hyperchem). [f/] From **13620** by DHP ring flipping (Hyperchem). [g/] From **13597** by DHP ring flipping (Hyperchem). [h/] From **14866** by DHP ring flipping (Hyperchem). [i/] From **13023** by the C5'–C6' bond rotation (Hyperchem).

Table S6. Key torsion angles[a] [°] and two values of the first harmonic vibrational frequency ω_e [cm^{-1}] obtained with the PCM($CHCl_3$)/B3LYP-GD3BJ/6-31+G(*d*,*p*) method for all initial forms of **1α** and **1β** having one small imaginary frequency (see Tables S4 and S5 and the main text), by using four different van der Waals radii

Alpha anomer

Form[b]	SCRF method	phi (φ)	psi (ψ)	omega (ω)	chi (χ)	theta (θ)	ω_e	ω_e[c]
13787	PCM/UFF	147.5	117.7	66.4	83.1	59.9	-7.27	2.03
	PCM/UA0	152.6	117.7	66.3	83.7	59.9	**7.55**	10.39
	PCM/Bondi	146.0	117.2	66.1	84.3	59.9	**-12.49**	0.00
	PCM/IDSCRF	153.1	117.7	66.5	83.3	59.9	**2.44**	5.85
13874 1αH	PCM/UFF	151.1	117.8	-70.8	-123.5	60.0	-7.58	0.00
	PCM/UA0	152.0	117.8	-71.2	-123.5	60.0	-2.56	4.37
	PCM/Bondi	152.1	117.7	-68.8	-124.8	60.0	-6.86	6.31
	PCM/IDSCRF	154.6	118.0	-71.1	-123.6	59.9	**-2.38**	3.96
14072 1αC	PCM/UFF	146.2	-64.5	70.7	179.0	-59.8	-6.96	2.03
	PCM/UA0	151.8	-64.7	70.6	178.2	-59.8	-6.82	3.22
	PCM/Bondi	144.2	-64.9	69.8	178.3	-59.8	-4.71	3.50
	PCM/IDSCRF	151.1	-64.7	70.6	177.3	-59.8	**1.43**	5.86
14216 1αA	PCM/UFF	152.7	-64.5	-70.7	-123.8	-59.8	-5.48	0.00
	PCM/UA0	153.6	-64.5	-71.2	-123.4	-59.8	-5.49	3.76
	PCM/Bondi	149.1	-64.7	-68.4	-126.5	-59.9	-6.36	0.00
	PCM/IDSCRF	153.9	-64.5	-71.1	-123.5	-59.8	**-6.38**	0.00
14447 1αG	PCM/UFF	152.8	-65.1	70.8	177.3	60.0	-2.83	6.41
	PCM/UA0	153.4	-65.0	70.7	178.6	60.0	-6.58	3.29
	PCM/Bondi	154.3	-65.3	69.9	179.7	60.1	**1.89**	9.10
	PCM/IDSCRF	153.7	-64.9	70.9	179.6	60.0	**-6.79**	0.00
14913	PCM/UFF	146.2	-64.5	67.1	84.0	-59.8	-10.05	0.00
	PCM/UA0	154.3	-64.7	66.8	84.3	-59.8	-10.01	0.00
	PCM/Bondi	147.3	-64.8	66.1	84.6	-59.8	-6.21	0.00
	PCM/IDSCRF	154.3	-64.6	66.6	84.0	-59.8	**-3.51**	6.82

Beta anomer

12302 1βG	PCM/UFF	-63.7	101.4	68.2	-108.7	59.6	-8.08	0.00
	PCM/UA0	-63.2	101.2	67.8	-108.6	59.7	-6.43	0.00
	PCM/Bondi	-65.1	102.4	67.7	-109.8	59.7	6.21	9.81
	PCM/IDSCRF	-61.0	100.9	67.9	-108.0	59.5	**9.70**	10.51
13675 1βH	PCM/UFF	-75.0	102.3	-70.1	-122.8	-59.8	-2.15	3.99
	PCM/UA0	-74.9	101.4	-70.6	-122.8	-59.8	-2.96	3.16
	PCM/Bondi	-75.0	102.7	-67.5	-126.5	-59.8	-0.70	5.02
	PCM/IDSCRF	-74.8	101.4	-70.6	-122.7	-59.8	**7.83**	8.41

[a/] For their detailed description, see the main text. [b/] Initial code names xxxxxx of all of the structures originate from the MMX energies (xx.xxx in kcal mol^{-1}) of their simple MMX models, after omission of the decimal point, see also Tables S4 and S5 for their origin. [c/] From the full mass-weighted force constant matrix calculations.

Table S7. DFT-computed[a] energetics and abundances of the forms **A-H** of **1α**.

Form	Initial code name	$G_{B3LYP\ 298}{}^{o}$ [b] [hartrees]	$\Delta G_{B3LYP}{}^{o}$ [c] [kJ/mol]	Abundance [d] [%]	E_{D3} (DFT-D V3) [e] [hartrees]	$G_{DFT-D3}{}^{o}$ [f] [hartrees]	$\Delta G_{DFT-D3}{}^{o}$ [g] [kJ/mol]	Abundance [h] [%]
1αA	14216	-1916.982435[i]	**0.00**	**18.8**	-0.096995	-1917.079430	**0.00**	**24.6_5**
1αB	13762	-1916.982281	0.40	15.9	-0.096414	-1917.078695	1.93	11.3
1αC	14072	-1916.982214	0.58	14.8_5	-0.096466	-1917.078680	1.97	11.1
1αD	14322	-1916.982145	0.76	13.8	-0.096944	-1917.079089	0.89	17.2
1αE	14599	-1916.982140	0.77	13.7	-0.096980	-1917.079120	0.81	17.7_5
1αF	13942	-1916.981751	1.80	9.1	-0.096524	-1917.077875	4.08	4.7_5
1αG	14447	-1916.981613	2.16	7.9	-0.096401	-1917.078152	3.35	6.4
1αH	13874	-1916.981351	2.85	5.9_5	-0.096989	-1917.078220	3.18	6.8

[a/] At the PCM($CHCl_3$)/B3LYP/6-31+G(*d*,*p*) level. [b/] Without the correction for van der Waals (vdW) dispersion forces. [c/] Relative values of the uncorrected standard Gibbs free energy. [d/] Standard populations (Boltzmann 1). [e/] The B3LYP specific vdW correction (DFT-D V3 term). [f/] With the vdW correction. [g/] Relative values of the corrected standard Gibbs free energy. [h/] The vdW corrected populations (Boltzmann 2). [i/] -1917.025093 Ha at 390 K.

Table S8. MP2-computed[a] energy data and abundances of the forms **A-H** of **1α**.

Form	Initial code name	E_0 [hartrees]	ΔE_0 [kJ/mol]	Abundance [b] [%]	ZPVE [c] [hartrees]	E (estim.) [d] [hartrees]	ΔE (estim.) [kJ/mol]	Abundance [e] [%]
1aA	14216	-1913.1230923	0.04	21.9	0.632940	-1912.4901523	**0.00**	**21.4**
1aB	13762	-1913.1215579	4.07	4.3	0.632805	-1912.4887529	3.67	4.9
1aC	14072	-1913.1216256	3.89	4.6	0.632945	-1912.4886806	3.86	4.5
1aD	14322	-1913.1231071	**0.00**	**22.2**	0.632960	-1912.4901471	0.01	21.3
1aE	14599	-1913.1228668	0.63	17.2	0.632785	-1912.4900818	0.19	19.8_5
1aF	13942	-1913.1216691	3.78	4.8_5	0.632894	-1912.4887751	3.62	5.0
1aG	14447	-1913.1212265	4.94	3.0	0.632843	-1912.4883835	4.64	3.3
1aH	13874	-1913.1230909	0.04	21.8_5	0.633008	-1912.4900829	0.18	19.9

[a/] At the PCM($CHCl_3$)/MP2/6-311+G(*2d*,*p*)//PCM($CHCl_3$)/B3LYP/6-31+G(*d*,*p*) level. [b/] The MP2 data (not corrected for $ZPVE_{DFT}$)-based populations (Boltzmann 3). [c/] The non-scaled ZPVE contribution computed at the PCM($CHCl_3$)/B3LYP/6-31+G(*d*,*p*) level. [d/] Estimated values, $E \cong E_0 + ZPVE_{DFT}$. [e/] The MP2 data (corrected for $ZPVE_{DFT}$)-based populations (Boltzmann 4).

Table S9. DFT-computed[a] energetics and abundances of the forms **A-H** of **1β**.

Form	Initial code name	$G_{B3LYP\ 298}{}^{o\ a}$ [hartrees]	$\Delta G_{B3LYP}{}^{o\ b}$ [kJ/mol]	Abundance [c] [%]	E_{D3} (DFT-D V3) [d] [hartrees]	$G_{DFT-D3}{}^{o\ e}$ [hartrees]	$\Delta G_{DFT-D3}{}^{o\ f}$ [kJ/mol]	Abundance [g] [%]
1βA	12506	-1916.985973	**0.00**	**26.5**	-0.093900	-1917.079873	0.85	19.2
1βB	14572	-1916.985754[h]	0.57	21.0	-0.094443	-1917.080197	**0.00**	**27.0**
1βC	14866	-1916.985289	1.80	12.8	-0.094389	-1917.079678	1.36	15.6
1βD	13878	-1916.985094	2.31	10.4_5	-0.094458	-1917.079552	1.70	13.6_5
1βE	13023	-1916.985023	2.49	9.7	-0.093975	-1917.078998	3.15	7.6
1βF	12272	-1916.984778	3.14	7.5	-0.093935	-1917.078713	3.90	5.6
1βG	12302	-1916.984645	3.49	6.5	-0.093887	-1917.078532	4.37	4.6
1βH	13675	-1916.984495	3.88	5.5	-0.094383	-1917.078878	3.46	6.7

[a/] At the PCM($CHCl_3$)/B3LYP/6-31+G(*d*,*p*) level. [a/] Without the correction for van der Waals (vdW) dispersion forces. [b/] Relative values of the uncorrected standard Gibbs free energy. [c/] Standard populations (Boltzmann 1). [d/] The B3LYP specific vdW correction (DFT-D V3 term). [e/] With the vdW correction. [f/] Relative values of the corrected standard Gibbs free energy. [g/] The vdW corrected populations (Boltzmann 2). [h/] -1917.028562 Ha at 390 K.

Table S10. MP2-computed[a] energy data and abundances of the forms **A-H** of **1β**.

Form	Initial code name	E_0 [hartrees]	ΔE_0 [kJ/mol]	Abundance [b] [%]	ZPVE [c] [hartrees]	E (estim.) [d] [hartrees]	ΔE (estim.) [kJ/mol]	Abundance [e] [%]
1βA	12506	-1913.1215858	4.26	4.3	0.632461	-1912.4891248	3.74	4.8
1βB	14572	-1913.1229473	0.69	18.3	0.632465	-1912.4904823	0.18	20.1_5
1βC	14866	-1913.1227982	1.08	15.6	0.632494	-1912.4903042	0.65	16.7
1βD	13878	-1913.1231359	0.19	22.3	0.632585	-1912.4905509	**0.00**	**21.7**
1βE	13023	-1913.1216488	4.10	4.6	0.632405	-1912.4892438	3.43	5.4
1βF	12272	-1913.1217597	3.80	5.2	0.632494	-1912.4892657	3.37	5.6
1βG	12302	-1913.1218238	3.64	5.6	0.632544	-1912.4892798	3.34	5.6
1βH	13675	-1913.1232086	**0.00**	**24.1**	0.632730	-1912.4904786	0.19	20.1

[a/] At the PCM($CHCl_3$)/MP2/6-311+G(*2d*,*p*)//PCM($CHCl_3$)/B3LYP/6-31+G(*d*,*p*) level. [b/] The MP2 data (not corrected for $ZPVE_{DFT}$)-based populations (Boltzmann 3). [c/] The non-scaled ZPVE contribution computed at the PCM($CHCl_3$)/B3LYP/6-31+G(*d*,*p*) level. [d/] Estimated values, $E \cong E_0 + ZPVE_{DFT}$. [e/] The MP2 data (corrected for $ZPVE_{DFT}$)-based populations (Boltzmann 4).

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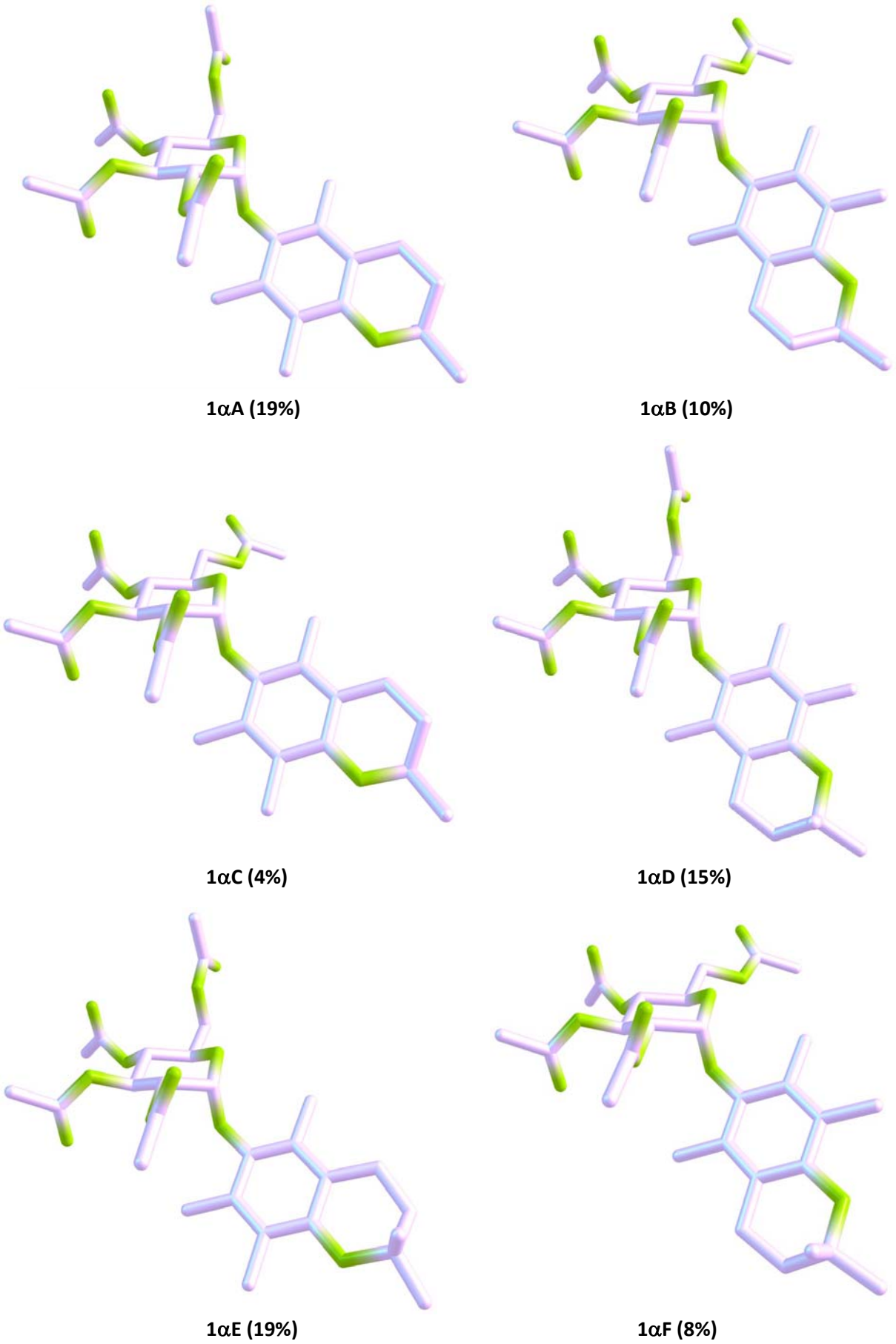
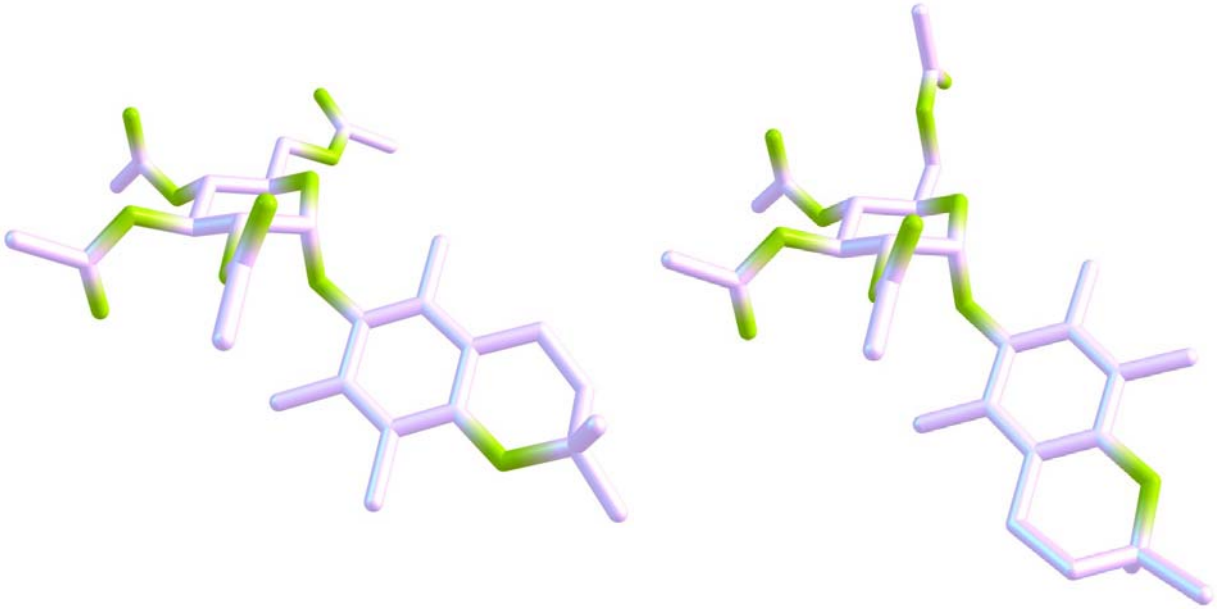


Figure S10. Chemcraft plots of the analyzed forms of glucoside **1α** with their abundances estimated according to DFT/NMR data (given in parentheses),



1αG (10%) **1αH (15%)**

Figure S10 (cont). Chemcraft plots of the analyzed forms of glucoside **1α** with their abundances estimated according to DFT/NMR data (given in parentheses),

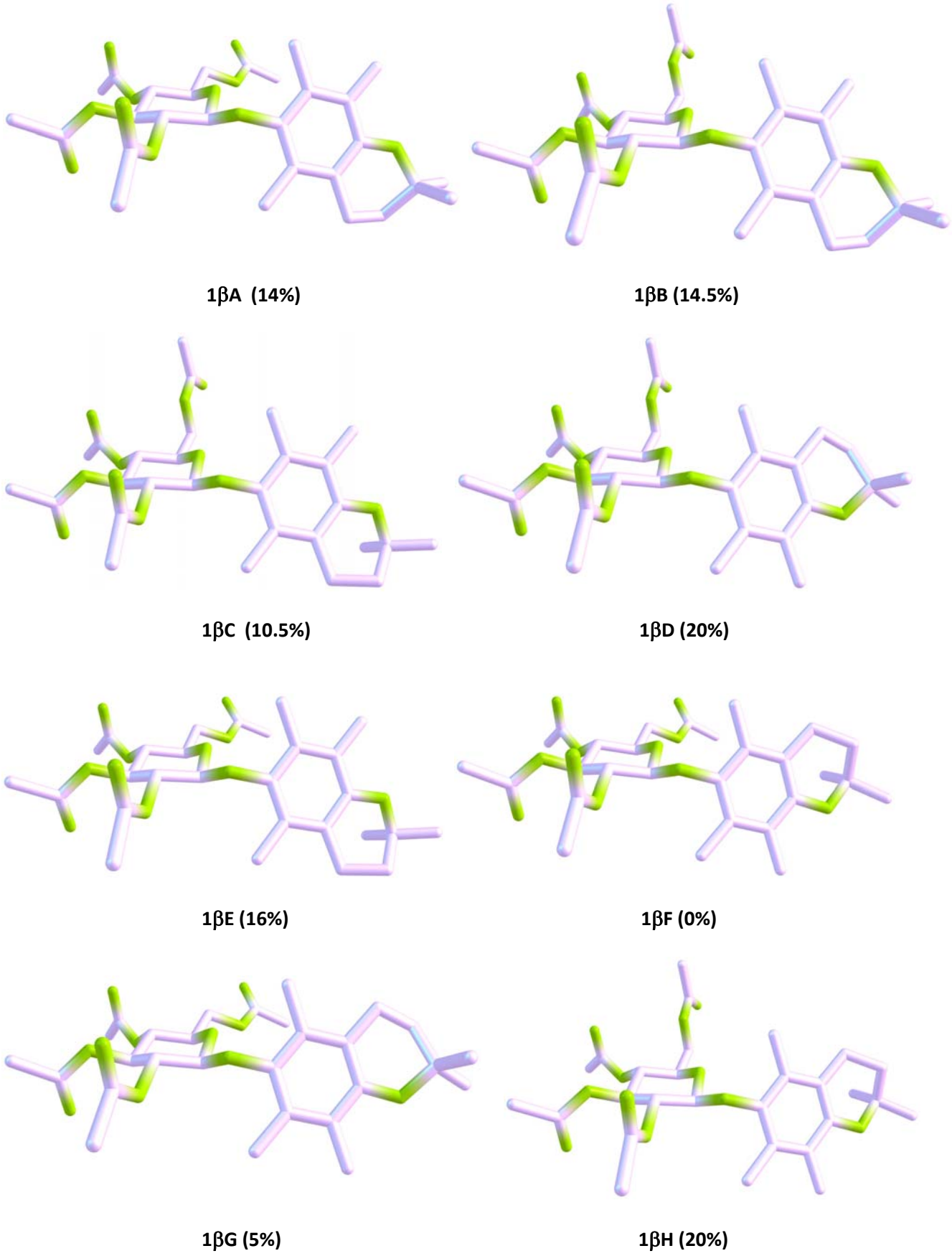


Figure S11. Chemcraft plots of the analyzed forms of glucoside **1β** with their abundances estimated according to DFT/NMR data (given in parentheses),

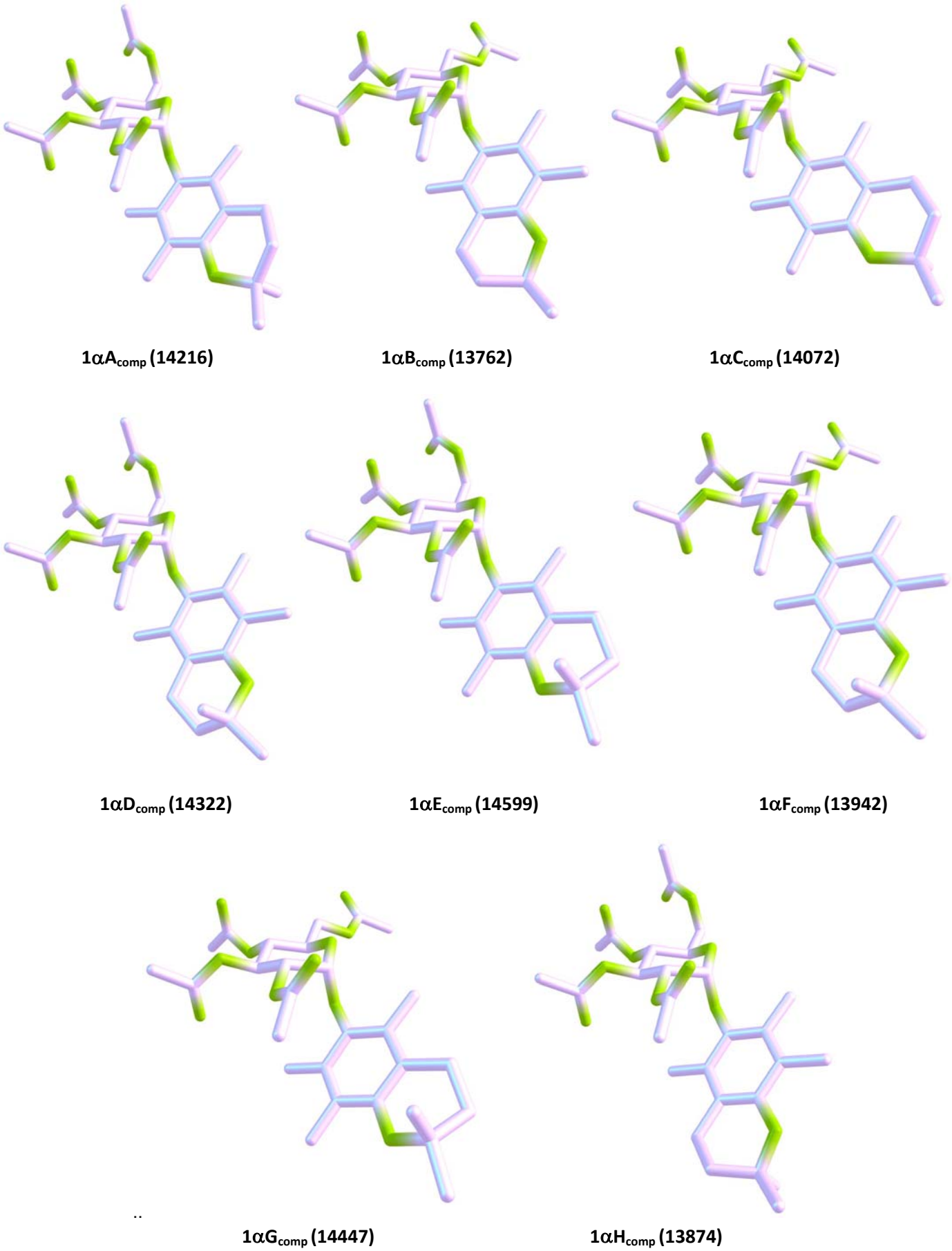
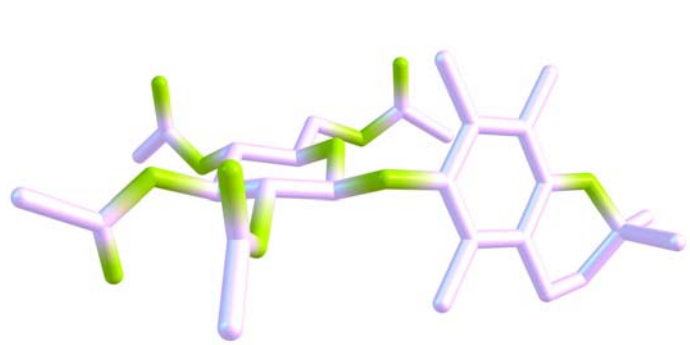
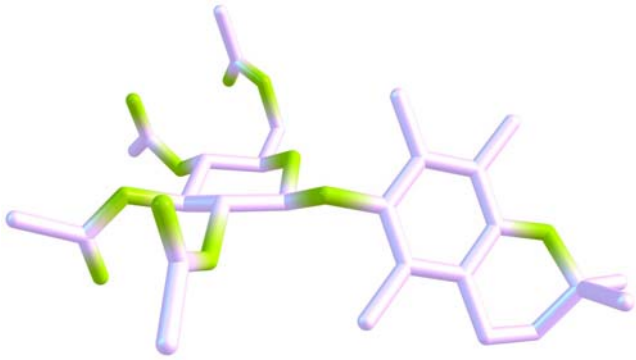


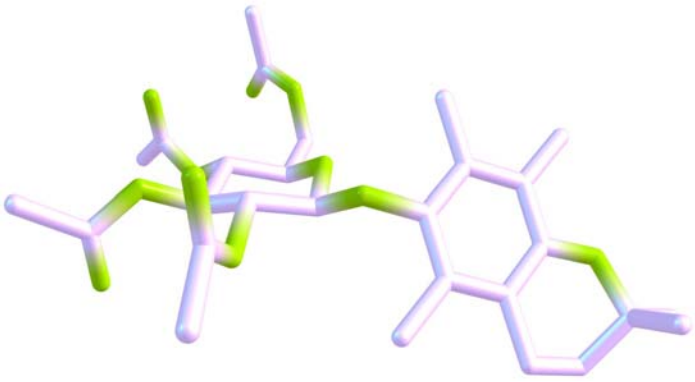
Figure S12. Chemcraft plots of the compact structures of the **A-H** forms of glucoside **1**α obtained at the PCM($CHCl_3$)/B3LYP-GD3BJ/6-31+G(*d*,*p*) level.



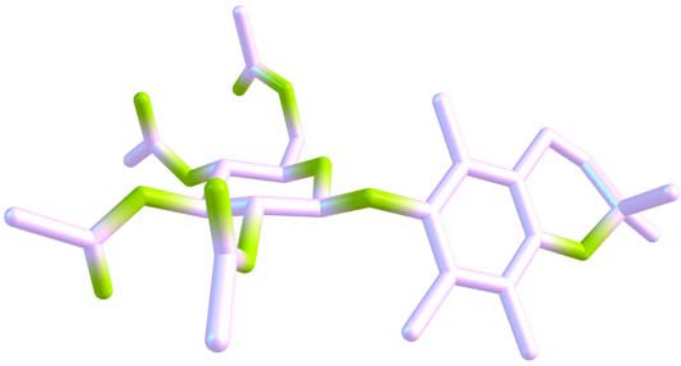
1βA$_{comp}$ (12506)



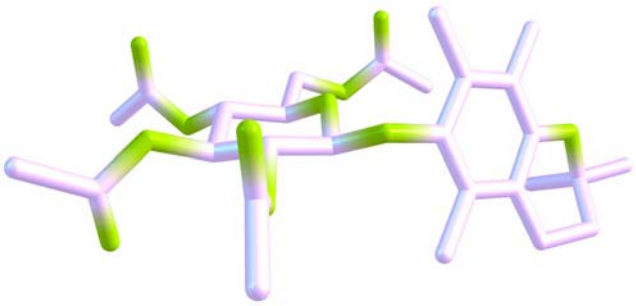
1βB$_{comp}$ (14572)



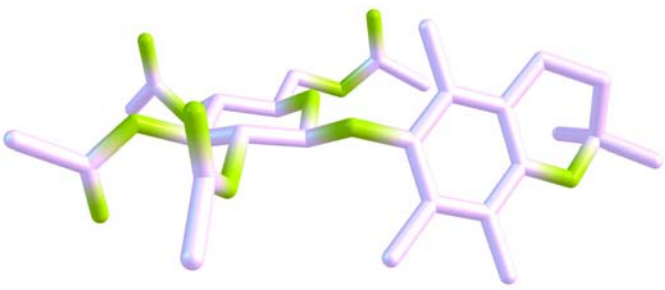
1βC$_{comp}$ (14866)



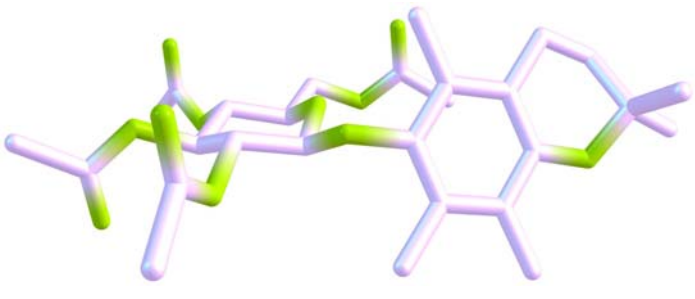
1βD$_{comp}$ (13878)



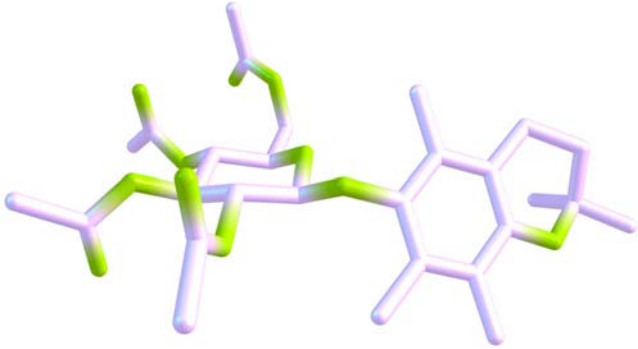
1βE$_{comp}$ (13023)



1βF$_{comp}$ (12272)



1βG$_{comp}$ (12302)



1βH$_{comp}$ (13675)

Figure S13. Chemcraft plots of the compact structures of the **A-H** forms of glucoside **1β** obtained at the PCM($CHCl_3$)/B3LYP-GD3BJ/6-31+G(*d*,*p*) level.

Table S11. Selected $^{1}H/^{13}C$ chemical shifts [ppm] and J_{HH} couplings [Hz] relating to the 2a/2b *gem*-dimethyl and C*H*CH_2OAc units of the forms A-H, respectively, found for the 'Boltzmann 1' based data (DFT-level *p*1 values).

	α-anomer (**1α**)				β-anomer (**1β**)			
Nucleus *j*	**Exp.**	**Calcd** [a]	**Scaled** [b]	$-\Delta_{scaled-exp}$	**Exp.**	**Calcd** [a]	**Scaled** [b]	$-\Delta_{scaled-exp}$
H2a	1.298	1.204	1.197	0.101	1.293	1.211	1.239	0.054
H2b	1.268	1.232	1.224	–0.044	1.281	1.266	1.294	–0.013
C2a	27.04	26.08	24.71	2.33	26.92	25.88	24.52	2.40
C2b	26.48	27.05	25.62	0.86	26.70	27.44	26.00	0.70
Coupling *k,l*	**Exp.**	**Calcd** [d]	–	$-\Delta_{calcd-exp}$	**Exp.**	**Calcd** [d]	–	$-\Delta_{calcd-exp}$
$^{3}J_{H5',H6'S}$	2.34	1.91	–	0.43	2.74	1.83	–	0.91
$^{3}J_{H5',H6'R}$	4.68	5.57	–	–0.89	4.72	5.59	–	–0.87
$^{2}J_{H6'R,H6'S}$	**(–)**12.37	-12.46_5	–	0.09_5	**(–)**12.18	–12.37	–	0.19
	$r_{C/H}^2$ **= 0.99982** [c] ***gg/gt* = 1.09** CRMSE = 0.78 CMAE = 0.52 $\delta^{calcd} = 1.0580\ \delta^{obsd} - 0.0630$				$r_{C/H}^2$ **= 0.99975** [c] ***gg/gt* = 0.99** CRMSE = 0.92 CMAE = 0.63 $\delta^{calcd} = 1.0566\ \delta^{obsd} - 0.0278$			

[a/] $\delta_{K,j}^{calcd} = \sigma_{K,TMS} - (p3_A \cdot \sigma_{K,A,j} + p3_B \cdot \sigma_{K,B,j} + \ldots + p3_H \cdot \sigma_{K,H,j})$, K = H or C. [b/] $\delta_{K,j}^{scaled} = (\delta_{K,j}^{calcd} - b)/a$. [c/] A binuclear (H/C, 1:1) regression analysis was applied, see Computational details (main text). [d/] $J_{HH} = p3_A \cdot J_{A,HH} + p3_B \cdot J_{B,HH} + \ldots + p3_H \cdot J_{H,HH}$ see also Computational details.

Table S12. Selected $^{1}H/^{13}C$ chemical shifts [ppm] and J_{HH} couplings [Hz] relating to the 2a/2b *gem*-dimethyl and C*H*CH_2OAc units of the forms A-H, respectively, found for the 'Boltzmann 2' based data (DFT-level *p*2 values).[#]

	α-anomer (**1α**)				β-anomer (**1β**)			
Nucleus *j*	**Exp.**	**Calcd** [a]	**Scaled** [b]	$-\Delta_{scaled-exp}$	**Exp.**	**Calcd** [a]	**Scaled** [b]	$-\Delta_{scaled-exp}$
H2a	1.298	1.216	1.175	0.123	1.293	1.216	1.249	0.044
H2b	1.268	1.249	1.206	0.062	1.281	1.259	1.292	–0.011
C2a	27.04	26.07	24.67	2.37	26.92	26.03	24.66	2.22_5
C2b	26.48	27.21	25.74_5	0.73_5	26.70	27.29	25.86	0.84
Coupling *k,l*	**Exp.**	**Calcd** [d]	–	$-\Delta_{calcd-exp}$	**Exp.**	**Calcd** [d]	–	$-\Delta_{calcd-exp}$
$^{3}J_{H5',H6'S}$	2.34	2.04	–	0.30	2.74	1.955	–	0.785
$^{3}J_{H5',H6'R}$	4.68	4.57	–	0.11	4.72	4.71	–	0.01
$^{2}J_{H6'R,H6'S}$	**(–)**12.37	–12.61	–	0.24	**(–)**12.18	–12.49	–	0.31
	$r_{C/H}^2$ **= 0.99982** [c] ***gg/gt* = 1.98** CRMSE = 0.78 CMAE = 0.53 $\delta^{calcd} = 1.0578\ \delta^{obsd} - 0.0271$				$r_{C/H}^2$ **= 0.99975** [c] ***gg/gt* = 1.70** CRMSE = 0.91 CMAE = 0.63 $\delta^{calcd} = 1.0566\ \delta^{obsd} - 0.0333$			

[#/] See footnotes to Table S11.

Table S13. Selected $^{1}H/^{13}C$ chemical shifts [ppm] and J_{HH} couplings [Hz] relating to the 2a/2b *gem*-dimethyl and C*H*CH_2OAc units of the forms A-H, respectively, found for the 'Boltzmann 3' based data (MP2-level *p*3 values).

	α-anomer (**1α**)				β-anomer (**1β**)			
Nucleus *j*	**Exp.**	**Calcd** [a]	**Scaled** [b]	$-\Delta_{scaled-exp}$	**Exp.**	**Calcd** [a]	**Scaled** [b]	$-\Delta_{scaled-exp}$
H2a	1.298	1.350	0.980	0.318	1.293	1.331	0.997	0.296
H2b	1.268	1.366	0.995	0.273	1.281	1.341	1.007	0.274
C2a	27.04	28.96	26.58	0.46	26.92	28.93	26.70	0.22
C2b	26.48	29.51	27.09	–0.61	26.70	29.21	26.96	–0.26
Coupling *k,l*	**Exp.**	**Calcd** [d]	–	$-\Delta_{calcd-exp}$	**Exp.**	**Calcd** [d]	–	$-\Delta_{calcd-exp}$
$^{3}J_{H5',H6'S}$	2.34	2.21	–	0.13	2.74	2.12	–	0.62
$^{3}J_{H5',H6'R}$	4.68	3.38	–	1.30	4.72	3.56	–	1.16
$^{2}J_{H6'R,H6'S}$	**(–)**12.37	–12.78	–	0.41	**(–)**12.18	–12.65	–	0.47
	$r_{C/H}^2$ **= 0.99918** [c] ***gg/gt* = 4.96** CRMSE = 0.78 CMAE = 0.66 $\delta^{calcd} = 1.0784\ \delta^{obsd} + 0.2931$				$r_{C/H}^2$ **= 0.99924** [c] ***gg/gt* = 4.08** CRMSE = 0.78 CMAE = 0.67 $\delta^{calcd} = 1.0738\ \delta^{obsd} + 0.2601$			

[a/] $\delta_{K,j}^{calcd} = \sigma_{K,TMS} - (p3_A \cdot \sigma_{K,A,j} + p3_B \cdot \sigma_{K,B,j} + \ldots + p3_H \cdot \sigma_{K,H,j})$, K = H or C. [b/] $\delta_{K,j}^{scaled} = (\delta_{K,j}^{calcd} - b)/a$. [c/] A binuclear (H/C, 1:1) regression analysis was applied, see Computational (main text). [d/] $J_{HH} = p3_A \cdot J_{A,HH} + p3_B \cdot J_{B,HH} + \ldots + p3_H \cdot J_{H,HH}$ (found for the DFT-level *J*-data), see also Computational.

Table S14. Selected $^{1}H/^{13}C$ chemical shifts [ppm] and J_{HH} couplings [Hz] relating to the 2a/2b *gem*-dimethyl and C*H*CH_2OAc units of the forms A-H, respectively, found for the 'Boltzmann 4' based data (MP2-level *p*4 values).[#]

	α-anomer (**1α**)				β-anomer (**1β**)			
Nucleus *j*	**Exp.**	**Calcd** [a]	**Scaled** [b]	$-\Delta_{scaled-exp}$	**Exp.**	**Calcd** [a]	**Scaled** [b]	$-\Delta_{scaled-exp}$
H2a	1.298	1.278	1.093	0.205	1.293	1.320	1.024	0.269
H2b	1.268	1.285	1.099	0.169	1.281	1.322	1.026	0.255
C2a	27.04	28.65	26.53	0.51	26.92	28.95	26.76	0.16
C2b	26.48	28.96	26.82	–0.34	26.70	29.03	26.84	–0.14
Coupling *k,l*	**Exp.**	**Calcd** [d]	–	$-\Delta_{calcd-exp}$	**Exp.**	**Calcd** [d]	–	$-\Delta_{calcd-exp}$
$^{3}J_{H5',H6'S}$	2.34	2.20	–	0.14	2.74	2.11	–	0.63
$^{3}J_{H5',H6'R}$	4.68	3.45	–	1.23	4.72	3.67	–	1.05
$^{2}J_{H6'R,H6'S}$	**(–)**12.37	–12.80	–	0.43	**(–)**12.18	–12.65	–	0.46
	$r_{C/H}^2$ **= 0.99939** [c] ***gg/gt* = 4.66** CRMSE = 0.68 CMAE = 0.54 $\delta^{calcd} = 1.0761\ \delta^{obsd} + 0.1025$				$r_{C/H}^2$ **= 0.99928** [c] ***gg/gt* = 3.68** CRMSE = 0.75 CMAE = 0.64 $\delta^{calcd} = 1.0735\ \delta^{obsd} + 0.2207$			

[#] See footnotes to Table S13.

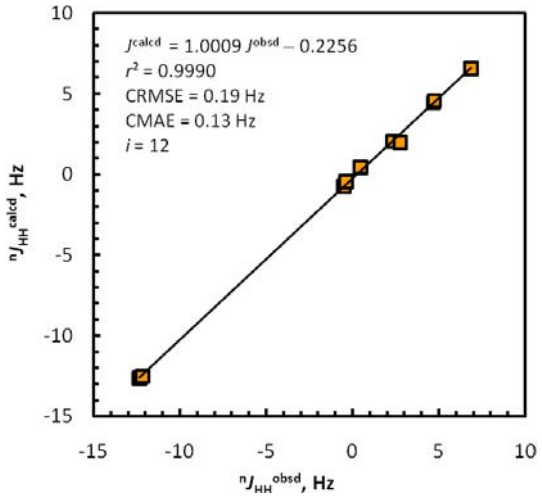


Figure S14. The scatter plot of the selected pairs of predicted *vs.* experimental $^{n}J_{HH}$ data found at the PCM($CHCl_3$)/B3LYP/IGLO-II//PCM($CHCl_3$)/B3LYP/6-31+G(*d*,*p*) level for the overall multi-component (*p*5 data) conformations of systems **1α** and **1β**; for all details see main text, Table 2, and Computational.

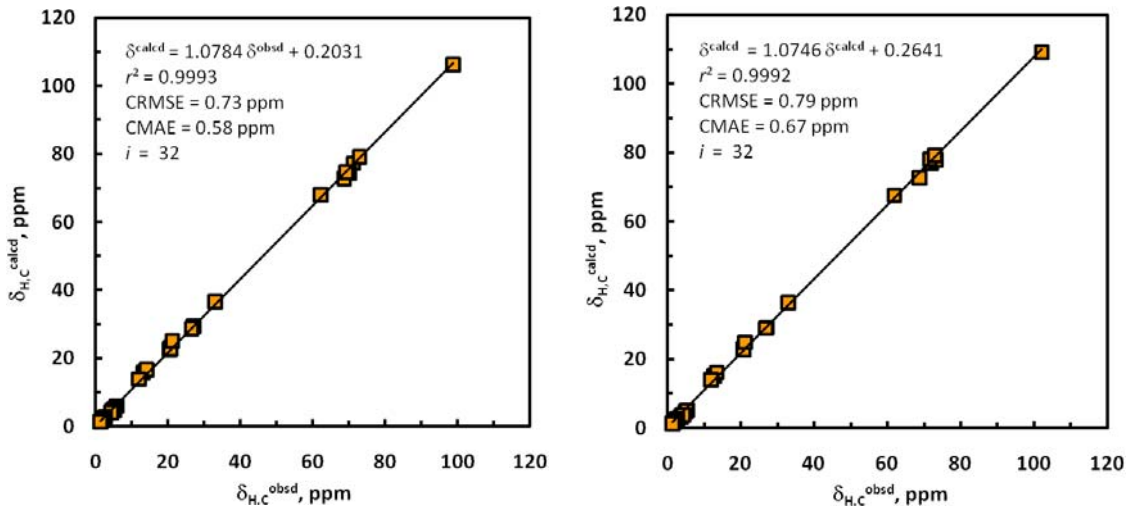


Figure S15. Scatter plots of the MP2 predicted *vs.* experimental (1:1) $\delta_{H,C}$ data sets for the overall multi-component (*p*6 results) solution conformation of **1α** (left side) and**1β** (right side); for the additional information see text and Computational details.

Table S15. B3LYP/6-31+G(*d*,*p*) optimized Cartesian coordinates for the forms **A-H** of **1**α.

The conformer **A** of **1**α (form **1**α**A**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.366988	0.357680	0.670844
2	6	0	-1.206565	-0.880939	1.039322
3	6	0	-2.260975	-1.166610	-0.026516
4	6	0	-3.104894	0.086852	-0.271996
5	6	0	-2.201800	1.304291	-0.547542
6	8	0	-1.249284	1.449845	0.517105
7	8	0	-0.380376	-2.049707	1.171014
8	8	0	-3.129302	-2.209322	0.462152
9	8	0	-3.913075	-0.134114	-1.446872
10	6	0	-2.953742	2.615626	-0.670876
11	8	0	-3.723134	2.827754	0.530678
12	6	0	-4.535656	3.907599	0.550386
13	8	0	-4.629837	4.681955	-0.385122
14	6	0	0.123630	-2.332656	2.401828
15	6	0	0.956396	-3.584753	2.371964
16	6	0	-3.207023	-3.379964	-0.226722
17	6	0	-4.132104	-4.343278	0.467411
18	6	0	-5.267384	-0.213372	-1.316924
19	6	0	-5.914183	-0.456370	-2.653888
20	8	0	-5.849761	-0.096597	-0.257875
21	8	0	-2.602285	-3.597673	-1.257840
22	8	0	-0.074897	-1.636409	3.378843
23	6	0	-5.284840	4.006980	1.852194
24	8	0	0.371219	0.149822	-0.521832
25	6	0	2.511241	1.215285	-0.015961
26	6	0	1.773852	0.107107	-0.462092
27	6	0	2.397112	-1.055991	-0.951157
28	6	0	3.801030	-1.136495	-0.935334
29	6	0	4.543507	-0.055839	-0.420078
30	6	0	3.917492	1.112823	0.040970
31	8	0	5.910358	-0.225050	-0.385006
32	6	0	4.753410	2.257201	0.579092
33	6	0	6.185383	1.816533	0.895162
34	6	0	6.768169	0.941226	-0.220911
35	6	0	1.847544	2.520215	0.367468
36	6	0	1.593540	-2.195654	-1.532416
37	6	0	4.501327	-2.368919	-1.460765
38	6	0	6.863684	1.676820	-1.565556
39	6	0	8.126616	0.366849	0.178499
40	1	0	0.297341	0.614942	1.497667
41	1	0	-1.687800	-0.678149	1.999289
42	1	0	-1.795964	-1.500194	-0.955878
43	1	0	-3.755603	0.278195	0.583162
44	1	0	-1.670940	1.149255	-1.495560
45	1	0	-2.243790	3.436741	-0.798402
46	1	0	-3.620263	2.592142	-1.536287
47	1	0	0.440604	-4.380337	1.828996
48	1	0	1.178461	-3.899236	3.391342
49	1	0	1.894147	-3.377622	1.845880
50	1	0	-5.103274	-3.873343	0.645209
51	1	0	-4.252214	-5.238630	-0.141639
52	1	0	-3.715226	-4.613883	1.442629
53	1	0	-6.994192	-0.527090	-2.529806
54	1	0	-5.525871	-1.379432	-3.094199
55	1	0	-5.671310	0.361301	-3.339141
56	1	0	-5.913427	3.121314	1.985717

57	1	0	-5.904302	4.903241	1.850271
58	1	0	-4.580690	4.040356	2.688642
59	1	0	4.292600	2.664453	1.485715
60	1	0	4.766417	3.085403	-0.143703
61	1	0	6.196793	1.232104	1.823202
62	1	0	6.828352	2.688991	1.053804
63	1	0	2.404391	3.368180	-0.042802
64	1	0	0.826327	2.578340	-0.007723
65	1	0	1.808749	2.664415	1.455379
66	1	0	1.862206	-2.362518	-2.582614
67	1	0	0.525486	-1.998943	-1.483094
68	1	0	1.789227	-3.135664	-1.004051
69	1	0	5.583668	-2.255221	-1.414162
70	1	0	4.228609	-3.261325	-0.883468
71	1	0	4.221943	-2.570861	-2.501783
72	1	0	5.881733	1.998153	-1.923233
73	1	0	7.499216	2.563612	-1.469118
74	1	0	7.301506	1.018922	-2.322393
75	1	0	8.052599	-0.177910	1.124719
76	1	0	8.493475	-0.320429	-0.590220
77	1	0	8.857344	1.173198	0.297275

The conformer **B** of **1α** (form **1αB**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.615421	0.238934	1.065812
2	6	0	-1.269969	-1.151738	1.175728
3	6	0	-2.284798	-1.369378	0.057201
4	6	0	-3.297680	-0.220675	0.038738
5	6	0	-2.576150	1.141541	0.018559
6	8	0	-1.646233	1.203862	1.111282
7	8	0	-0.287387	-2.197701	1.096457
8	8	0	-2.999333	-2.593373	0.322753
9	8	0	-4.081033	-0.339388	-1.166256
10	6	0	-3.546203	2.294758	0.191326
11	8	0	-2.829957	3.513112	-0.100920
12	6	0	-3.548188	4.657773	-0.071601
13	8	0	-4.741490	4.684900	0.170375
14	6	0	0.235878	-2.662483	2.262609
15	6	0	1.243717	-3.750114	2.009999
16	6	0	-2.918855	-3.612428	-0.575844
17	6	0	-3.700700	-4.805304	-0.095004
18	6	0	-5.424310	-0.550698	-1.064156
19	6	0	-6.048010	-0.669731	-2.427898
20	8	0	-6.013137	-0.620309	-0.004491
21	8	0	-2.294730	-3.546849	-1.616016
22	8	0	-0.074176	-2.224767	3.353765
23	6	0	-2.684620	5.856896	-0.360809
24	8	0	0.130673	0.373732	-0.131306
25	6	0	2.283090	-0.464846	-0.755350
26	6	0	1.528318	0.490037	-0.058359
27	6	0	2.127821	1.573418	0.612295
28	6	0	3.532584	1.646364	0.661547
29	6	0	4.295251	0.668837	-0.006520
30	6	0	3.689584	-0.380014	-0.716030
31	8	0	5.663382	0.802378	0.089587
32	6	0	4.545576	-1.405501	-1.431259
33	6	0	6.002163	-1.359199	-0.960809
34	6	0	6.515775	0.081341	-0.846574
35	6	0	1.620850	-1.553419	-1.568261

36	6	0	1.304944	2.680545	1.234658
37	6	0	4.219498	2.773427	1.400400
38	6	0	7.905883	0.124602	-0.213779
39	6	0	6.508470	0.823077	-2.191255
40	1	0	0.014233	0.422113	1.938296
41	1	0	-1.764987	-1.205921	2.148442
42	1	0	-1.787209	-1.452544	-0.910524
43	1	0	-3.959407	-0.293260	0.905761
44	1	0	-2.038771	1.255406	-0.930112
45	1	0	-4.387476	2.199373	-0.498540
46	1	0	-3.928388	2.331931	1.215401
47	1	0	1.468399	-4.262587	2.945102
48	1	0	2.162042	-3.299510	1.618865
49	1	0	0.875026	-4.457133	1.263304
50	1	0	-3.681608	-5.585900	-0.854780
51	1	0	-3.262272	-5.182415	0.834181
52	1	0	-4.732590	-4.516588	0.123637
53	1	0	-5.569407	-1.476930	-2.989786
54	1	0	-5.892473	0.257157	-2.988384
55	1	0	-7.114882	-0.864892	-2.325751
56	1	0	-3.311102	6.742545	-0.462890
57	1	0	-2.102302	5.697920	-1.272310
58	1	0	-1.977077	6.003077	0.461709
59	1	0	4.144240	-2.411518	-1.266744
60	1	0	4.493819	-1.242820	-2.517274
61	1	0	6.644212	-1.926376	-1.643433
62	1	0	6.087262	-1.826738	0.027768
63	1	0	2.034528	-1.586401	-2.582229
64	1	0	1.777074	-2.544437	-1.125912
65	1	0	0.547388	-1.393373	-1.644360
66	1	0	1.744296	3.656226	1.006424
67	1	0	1.265415	2.601853	2.329276
68	1	0	0.279830	2.680501	0.865585
69	1	0	5.281579	2.566085	1.527873
70	1	0	4.130013	3.723876	0.857353
71	1	0	3.777140	2.928446	2.389945
72	1	0	7.905149	-0.383195	0.755592
73	1	0	8.632625	-0.370470	-0.865631
74	1	0	8.226746	1.160083	-0.063258
75	1	0	5.500850	0.895912	-2.609397
76	1	0	6.895839	1.838119	-2.061149
77	1	0	7.142614	0.301464	-2.916079

The conformer **C** of **1**α (form **1**α**C**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.518002	0.069904	0.950923
2	6	0	-1.403941	-1.182586	1.097360
3	6	0	-2.527652	-1.182205	0.064762
4	6	0	-3.312312	0.130739	0.143187
5	6	0	-2.356475	1.337978	0.074974
6	8	0	-1.349617	1.203744	1.090276
7	8	0	-0.638881	-2.386350	0.920183
8	8	0	-3.429875	-2.263907	0.372547
9	8	0	-4.199142	0.184761	-0.992705
10	6	0	-3.079215	2.646265	0.332315
11	8	0	-2.168936	3.716406	0.001772
12	6	0	-2.658205	4.973619	0.083783
13	8	0	-3.808256	5.217800	0.401550
14	6	0	-0.098940	-2.961338	2.028026

15	6	0	0.665911	-4.207369	1.675117
16	6	0	-3.605846	-3.255848	-0.543083
17	6	0	-4.550689	-4.302052	-0.015877
18	6	0	-5.545327	0.225086	-0.779513
19	6	0	-6.289228	0.248422	-2.086773
20	8	0	-6.048700	0.246159	0.325313
21	8	0	-3.062644	-3.274969	-1.629405
22	8	0	-0.218628	-2.496445	3.145271
23	6	0	-1.605037	5.996896	-0.249600
24	8	0	0.145134	0.094780	-0.300841
25	6	0	2.361825	0.937223	0.285972
26	6	0	1.544341	-0.018320	-0.337777
27	6	0	2.077749	-1.075146	-1.098470
28	6	0	3.474052	-1.218537	-1.182817
29	6	0	4.299116	-0.303613	-0.499592
30	6	0	3.761625	0.766031	0.233409
31	8	0	5.654970	-0.533212	-0.585472
32	6	0	4.684846	1.735004	0.945226
33	6	0	6.105791	1.178719	1.072674
34	6	0	6.581705	0.534848	-0.235148
35	6	0	1.788679	2.155893	0.976483
36	6	0	1.184424	-2.027598	-1.858344
37	6	0	4.078591	-2.340725	-1.995731
38	6	0	6.647068	1.532973	-1.400285
39	6	0	7.925975	-0.167508	-0.049309
40	1	0	0.200286	0.114871	1.771499
41	1	0	-1.820581	-1.174494	2.107605
42	1	0	-2.131768	-1.326964	-0.941973
43	1	0	-3.903870	0.159057	1.061939
44	1	0	-1.881996	1.372073	-0.912740
45	1	0	-3.969442	2.726130	-0.295236
46	1	0	-3.374950	2.728970	1.382062
47	1	0	0.106118	-4.820030	0.964794
48	1	0	0.881236	-4.771670	2.582155
49	1	0	1.609565	-3.922110	1.198135
50	1	0	-4.742928	-5.044444	-0.789725
51	1	0	-4.109203	-4.787586	0.860088
52	1	0	-5.487778	-3.838279	0.304345
53	1	0	-6.023478	-0.628460	-2.684229
54	1	0	-6.003187	1.135153	-2.660537
55	1	0	-7.361700	0.261183	-1.896225
56	1	0	-0.856554	6.019601	0.549290
57	1	0	-2.066305	6.979905	-0.340569
58	1	0	-1.090758	5.731321	-1.176798
59	1	0	4.704382	2.695878	0.411431
60	1	0	4.294391	1.960404	1.943661
61	1	0	6.134596	0.412032	1.856459
62	1	0	6.802087	1.970848	1.368538
63	1	0	2.367680	3.048416	0.720010
64	1	0	0.753614	2.335080	0.687231
65	1	0	1.816611	2.065453	2.070615
66	1	0	1.300064	-3.058308	-1.503448
67	1	0	1.440003	-2.030009	-2.924413
68	1	0	0.135854	-1.756654	-1.760897
69	1	0	5.166062	-2.328493	-1.934683
70	1	0	3.727829	-3.320098	-1.648394
71	1	0	3.795600	-2.262597	-3.052869
72	1	0	5.667019	1.964860	-1.620262
73	1	0	7.335328	2.350757	-1.161466
74	1	0	7.006980	1.031372	-2.303697
75	1	0	7.871455	-0.896664	0.764885
76	1	0	8.215069	-0.691248	-0.965842
77	1	0	8.704286	0.564107	0.190025

The conformer **D** of **1**α (form **1**α**D**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.460766	-0.583798	0.681796
2	6	0	1.091470	0.768755	1.065670
3	6	0	2.064670	1.245193	-0.009464
4	6	0	3.100536	0.154818	-0.293786
5	6	0	2.408542	-1.192382	-0.578236
6	8	0	1.509209	-1.511584	0.494317
7	8	0	0.086114	1.781902	1.235251
8	8	0	2.757146	2.408729	0.487753
9	8	0	3.835964	0.529483	-1.477696
10	6	0	3.367949	-2.357274	-0.730259
11	8	0	4.169561	-2.459241	0.464516
12	6	0	5.154673	-3.384377	0.459425
13	8	0	5.374337	-4.111781	-0.492568
14	6	0	-0.411545	1.978106	2.485481
15	6	0	-1.433344	3.081925	2.493360
16	6	0	2.611642	3.592597	-0.166672
17	6	0	3.382948	4.681409	0.529864
18	6	0	5.167674	0.800398	-1.375934
19	6	0	5.734771	1.180289	-2.717155
20	8	0	5.790248	0.734404	-0.335545
21	8	0	1.945177	3.730100	-1.173252
22	8	0	-0.066104	1.324412	3.450655
23	6	0	5.916878	-3.381416	1.757523
24	8	0	-0.320480	-0.476329	-0.496529
25	6	0	-2.528672	0.361454	-0.883363
26	6	0	-1.708509	-0.679800	-0.422899
27	6	0	-2.237125	-1.913254	0.005351
28	6	0	-3.634604	-2.061484	0.082439
29	6	0	-4.461936	-1.003606	-0.341797
30	6	0	-3.927527	0.187861	-0.856114
31	8	0	-5.817988	-1.233774	-0.267879
32	6	0	-4.851049	1.273845	-1.369993
33	6	0	-6.282977	0.764917	-1.559672
34	6	0	-6.736033	-0.108176	-0.383043
35	6	0	-1.945842	1.637306	-1.445302
36	6	0	-1.347851	-3.089780	0.345342
37	6	0	-4.249063	-3.348658	0.584936
38	6	0	-6.755913	0.653231	0.950418
39	6	0	-8.095794	-0.747962	-0.659587
40	1	0	-0.139127	-0.963641	1.510803
41	1	0	1.616538	0.629709	2.013832
42	1	0	1.533887	1.514000	-0.924456
43	1	0	3.791616	0.060823	0.545803
44	1	0	1.846316	-1.114482	-1.517650
45	1	0	2.804737	-3.283302	-0.870866
46	1	0	4.015209	-2.206812	-1.597588
47	1	0	-2.313150	2.764468	1.924840
48	1	0	-1.033611	3.976951	2.009584
49	1	0	-1.723530	3.302871	3.520000
50	1	0	4.430202	4.387762	0.643703
51	1	0	3.311462	5.604900	-0.043755
52	1	0	2.975348	4.836774	1.533614
53	1	0	5.586508	0.363191	-3.429455
54	1	0	6.797817	1.396094	-2.616345
55	1	0	5.209942	2.056413	-3.109317
56	1	0	5.233855	-3.558769	2.593396
57	1	0	6.380300	-2.402398	1.912530
58	1	0	6.684246	-4.154444	1.733080
59	1	0	-4.842308	2.129805	-0.680061
60	1	0	-4.477326	1.662913	-2.323508

61	1	0	-6.342185	0.157828	-2.471138
62	1	0	-6.975169	1.604591	-1.684531
63	1	0	-2.156527	1.723310	-2.518891
64	1	0	-2.378825	2.522102	-0.965635
65	1	0	-0.867913	1.675745	-1.311442
66	1	0	-1.758585	-4.011789	-0.076585
67	1	0	-1.263964	-3.248428	1.428649
68	1	0	-0.339548	-2.961165	-0.046587
69	1	0	-5.298091	-3.202034	0.842450
70	1	0	-4.204707	-4.140385	-0.175227
71	1	0	-3.724296	-3.723529	1.469167
72	1	0	-5.764587	1.028543	1.218317
73	1	0	-7.439724	1.506665	0.890049
74	1	0	-7.097304	-0.006605	1.753779
75	1	0	-8.073612	-1.311511	-1.597331
76	1	0	-8.369743	-1.431653	0.149960
77	1	0	-8.868049	0.024095	-0.735344

The conformer **E** of **1**α (form **1**α**E**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.344187	0.428808	0.571672
2	6	0	-1.117748	-0.829036	1.011888
3	6	0	-2.210401	-1.181797	0.006679
4	6	0	-3.110401	0.033679	-0.231751
5	6	0	-2.268411	1.276831	-0.577473
6	8	0	-1.273271	1.483988	0.437024
7	8	0	-0.242572	-1.962921	1.134013
8	8	0	-3.015625	-2.239570	0.566570
9	8	0	-3.960330	-0.248133	-1.363574
10	6	0	-3.075415	2.555445	-0.694837
11	8	0	-3.794592	2.768863	0.537194
12	6	0	-4.648211	3.816174	0.569723
13	8	0	-4.816738	4.562002	-0.378415
14	6	0	0.327095	-2.193228	2.346802
15	6	0	1.205619	-3.413645	2.311617
16	6	0	-3.098966	-3.426002	-0.093920
17	6	0	-3.949954	-4.401569	0.674008
18	6	0	-5.305421	-0.358060	-1.174384
19	6	0	-5.999682	-0.663673	-2.474171
20	8	0	-5.846678	-0.221269	-0.096072
21	8	0	-2.552048	-3.647170	-1.156090
22	8	0	0.147725	-1.477925	3.313822
23	6	0	-5.340319	3.919134	1.902508
24	8	0	0.340581	0.222608	-0.652749
25	6	0	2.482246	1.339193	-0.283347
26	6	0	1.745240	0.203551	-0.655326
27	6	0	2.364282	-0.967691	-1.129629
28	6	0	3.767860	-1.043710	-1.131268
29	6	0	4.513401	0.063653	-0.680923
30	6	0	3.892400	1.259457	-0.286793
31	8	0	5.882681	-0.086476	-0.700513
32	6	0	4.737428	2.447603	0.128027
33	6	0	6.209919	2.271802	-0.254656
34	6	0	6.710198	0.853832	0.043414
35	6	0	1.810285	2.644399	0.083664
36	6	0	1.550858	-2.124871	-1.662160
37	6	0	4.469682	-2.291763	-1.616594
38	6	0	8.121714	0.637695	-0.500362
39	6	0	6.643671	0.500868	1.536479

40	1	0	0.350675	0.730912	1.357508
41	1	0	-1.559333	-0.617271	1.988804
42	1	0	-1.777981	-1.526441	-0.934252
43	1	0	-3.730025	0.223057	0.646624
44	1	0	-1.776626	1.118663	-1.545729
45	1	0	-2.404618	3.399103	-0.875850
46	1	0	-3.780650	2.484941	-1.526394
47	1	0	2.124332	-3.175372	1.765175
48	1	0	0.710494	-4.234683	1.787965
49	1	0	1.461575	-3.707537	3.329277
50	1	0	-4.925647	-3.959663	0.894238
51	1	0	-4.072647	-5.315714	0.094122
52	1	0	-3.471156	-4.632677	1.630701
53	1	0	-7.072377	-0.748935	-2.304234
54	1	0	-5.611389	-1.596468	-2.893652
55	1	0	-5.799435	0.130392	-3.199649
56	1	0	-5.930243	3.015401	2.083249
57	1	0	-5.991083	4.792911	1.910166
58	1	0	-4.600817	3.995797	2.704858
59	1	0	4.357383	3.363154	-0.337588
60	1	0	4.642914	2.609406	1.211232
61	1	0	6.831871	3.002565	0.273500
62	1	0	6.337070	2.453955	-1.328663
63	1	0	2.255433	3.476156	-0.472270
64	1	0	0.745116	2.633007	-0.141472
65	1	0	1.926661	2.881491	1.149155
66	1	0	1.916207	-2.430326	-2.648654
67	1	0	0.498971	-1.862399	-1.754258
68	1	0	1.617811	-3.003740	-1.010291
69	1	0	5.524670	-2.278486	-1.343789
70	1	0	4.014629	-3.195593	-1.198051
71	1	0	4.409672	-2.383079	-2.709384
72	1	0	8.161824	0.863003	-1.570462
73	1	0	8.830694	1.289765	0.019574
74	1	0	8.435299	-0.400386	-0.352045
75	1	0	5.621149	0.549548	1.920586
76	1	0	7.019874	-0.513756	1.698994
77	1	0	7.259961	1.194874	2.117962

The conformer **F** of **1α** (form **1αF**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.582239	-0.236053	1.002324
2	6	0	1.221834	1.158343	1.148345
3	6	0	2.274627	1.391859	0.068166
4	6	0	3.298197	0.252721	0.076824
5	6	0	2.590285	-1.115597	0.025044
6	8	0	1.621141	-1.191190	1.081588
7	8	0	0.238144	2.200552	1.040309
8	8	0	2.969083	2.619940	0.366023
9	8	0	4.118933	0.385365	-1.101615
10	6	0	3.563314	-2.260794	0.231065
11	8	0	2.865711	-3.484745	-0.081891
12	6	0	3.588017	-4.625304	-0.015688
13	8	0	4.770597	-4.644363	0.274879
14	6	0	-0.344654	2.642347	2.186899
15	6	0	-1.324004	3.748209	1.903352
16	6	0	2.900469	3.648534	-0.522725
17	6	0	3.661239	4.842227	-0.011116
18	6	0	5.455876	0.610350	-0.955838

19	6	0	6.121381	0.741551	-2.298567
20	8	0	6.009912	0.681692	0.122319
21	8	0	2.301155	3.589503	-1.577746
22	8	0	-0.093795	2.179581	3.282824
23	6	0	2.743014	-5.831173	-0.330564
24	8	0	-0.116284	-0.359451	-0.224025
25	6	0	-2.286051	0.385683	-0.905832
26	6	0	-1.508142	-0.549195	-0.206190
27	6	0	-2.075287	-1.681731	0.409898
28	6	0	-3.476363	-1.815210	0.423049
29	6	0	-4.264044	-0.856234	-0.242994
30	6	0	-3.685623	0.218475	-0.935935
31	8	0	-5.624654	-1.069404	-0.213383
32	6	0	-4.563134	1.188217	-1.701272
33	6	0	-5.986449	0.652512	-1.881811
34	6	0	-6.520858	0.014652	-0.593561
35	6	0	-1.655017	1.533852	-1.658782
36	6	0	-1.220457	-2.771454	1.019933
37	6	0	-4.134661	-2.986812	1.116570
38	6	0	-6.613393	1.012061	0.570343
39	6	0	-7.868638	-0.665386	-0.830045
40	1	0	-0.079692	-0.433681	1.847464
41	1	0	1.680839	1.207211	2.138824
42	1	0	1.810877	1.476698	-0.916205
43	1	0	3.930736	0.326410	0.965273
44	1	0	2.090140	-1.230391	-0.943759
45	1	0	4.425767	-2.159891	-0.431449
46	1	0	3.912232	-2.293503	1.267054
47	1	0	-1.712758	4.141094	2.842180
48	1	0	-2.148023	3.358707	1.297699
49	1	0	-0.842203	4.544719	1.329843
50	1	0	3.649863	5.632248	-0.761232
51	1	0	3.201464	5.203421	0.914023
52	1	0	4.691345	4.560032	0.223945
53	1	0	5.995187	-0.185307	-2.866448
54	1	0	7.181980	0.949186	-2.161692
55	1	0	5.651217	1.544709	-2.873210
56	1	0	3.379128	-6.712044	-0.412605
57	1	0	2.186881	-5.677441	-1.259072
58	1	0	2.012607	-5.982575	0.470819
59	1	0	-4.587148	2.158550	-1.184921
60	1	0	-4.126733	1.391371	-2.685398
61	1	0	-5.996668	-0.114180	-2.665991
62	1	0	-6.659918	1.454044	-2.203961
63	1	0	-1.803262	1.420106	-2.740184
64	1	0	-2.102743	2.493443	-1.377161
65	1	0	-0.586009	1.593575	-1.471465
66	1	0	-1.617747	-3.756753	0.758841
67	1	0	-1.201567	-2.719550	2.116719
68	1	0	-0.189791	-2.721270	0.670653
69	1	0	-5.197397	-2.798997	1.269747
70	1	0	-4.045613	-3.907718	0.524418
71	1	0	-3.674104	-3.185489	2.089343
72	1	0	-5.636167	1.431571	0.824103
73	1	0	-7.282957	1.838512	0.309299
74	1	0	-7.010216	0.514059	1.460170
75	1	0	-7.796076	-1.394168	-1.643105
76	1	0	-8.199747	-1.185724	0.074116
77	1	0	-8.625573	0.079253	-1.096272

The conformer **G** of **1α** (form **1αG**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.482397	0.120155	0.883790
2	6	0	-1.301816	-1.170284	1.078152
3	6	0	-2.464186	-1.235029	0.091480
4	6	0	-3.306341	0.040834	0.187000
5	6	0	-2.413180	1.292207	0.076108
6	8	0	-1.361606	1.213978	1.051188
7	8	0	-0.489313	-2.340011	0.884902
8	8	0	-3.302361	-2.352736	0.448279
9	8	0	-4.232963	0.042723	-0.918148
10	6	0	-3.187205	2.565865	0.357044
11	8	0	-2.345188	3.675667	-0.020218
12	6	0	-2.887835	4.909151	0.083462
13	8	0	-4.029821	5.101046	0.460626
14	6	0	0.122927	-2.870915	1.976857
15	6	0	0.929897	-4.086158	1.610432
16	6	0	-3.466421	-3.366088	-0.445641
17	6	0	-4.343509	-4.444512	0.131463
18	6	0	-5.571665	0.021874	-0.659784
19	6	0	-6.359275	0.000373	-1.941191
20	8	0	-6.038024	0.028712	0.461347
21	8	0	-2.963935	-3.378070	-1.551490
22	8	0	0.029332	-2.393213	3.091242
23	6	0	-1.903466	5.978125	-0.311105
24	8	0	0.124293	0.168018	-0.395424
25	6	0	2.325867	1.122113	0.068407
26	6	0	1.524712	0.114576	-0.492279
27	6	0	2.068816	-0.939808	-1.248735
28	6	0	3.465771	-1.047869	-1.360948
29	6	0	4.279019	-0.084733	-0.732111
30	6	0	3.729261	1.010107	-0.046447
31	8	0	5.637972	-0.260218	-0.875695
32	6	0	4.643105	2.056775	0.559827
33	6	0	6.082918	1.931849	0.052572
34	6	0	6.543416	0.470788	0.000495
35	6	0	1.728063	2.330542	0.755426
36	6	0	1.182251	-1.933098	-1.963809
37	6	0	4.087915	-2.176298	-2.151524
38	6	0	7.911532	0.343764	-0.668014
39	6	0	6.549281	-0.201394	1.381205
40	1	0	0.267823	0.206760	1.672204
41	1	0	-1.679115	-1.168213	2.103780
42	1	0	-2.102244	-1.374759	-0.928570
43	1	0	-3.866742	0.049057	1.125517
44	1	0	-1.980222	1.342787	-0.929713
45	1	0	-4.107269	2.597513	-0.230497
46	1	0	-3.439815	2.642462	1.418421
47	1	0	0.372991	-4.733329	0.929091
48	1	0	1.204160	-4.627563	2.515544
49	1	0	1.841561	-3.765076	1.095426
50	1	0	-4.515559	-5.216150	-0.618137
51	1	0	-3.859118	-4.882718	1.009578
52	1	0	-5.295834	-4.019531	0.460835
53	1	0	-6.067678	-0.863230	-2.545805
54	1	0	-6.140233	0.899101	-2.525762
55	1	0	-7.423892	-0.042588	-1.714513
56	1	0	-1.097890	6.022060	0.428973
57	1	0	-2.408927	6.942391	-0.354840
58	1	0	-1.450701	5.743510	-1.278075
59	1	0	4.272611	3.061409	0.329730
60	1	0	4.618354	1.979991	1.656176

61	1	0	6.763008	2.512318	0.685322
62	1	0	6.154369	2.342472	-0.961899
63	1	0	2.175070	3.252440	0.369009
64	1	0	0.652455	2.399148	0.601692
65	1	0	1.914633	2.321535	1.837269
66	1	0	1.462526	-2.007639	-3.020362
67	1	0	0.134918	-1.644248	-1.908113
68	1	0	1.273321	-2.939405	-1.538501
69	1	0	5.160366	-2.237225	-1.968294
70	1	0	3.637124	-3.140958	-1.895097
71	1	0	3.941162	-2.034776	-3.230598
72	1	0	7.899160	0.800200	-1.662514
73	1	0	8.674803	0.844917	-0.064312
74	1	0	8.191029	-0.709245	-0.772759
75	1	0	5.553152	-0.213110	1.831793
76	1	0	6.894405	-1.236045	1.292830
77	1	0	7.224427	0.331097	2.059520

The conformer **H** of **1**α (form **1**α**H**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.486805	-0.579092	0.751032
2	6	0	1.139742	0.772015	1.100838
3	6	0	2.070346	1.234723	-0.016842
4	6	0	3.089610	0.136118	-0.329026
5	6	0	2.380489	-1.209558	-0.576967
6	8	0	1.520399	-1.515859	0.531179
7	8	0	0.146321	1.790107	1.306642
8	8	0	2.786250	2.400717	0.439290
9	8	0	3.785237	0.495834	-1.541232
10	6	0	3.327095	-2.380869	-0.756607
11	8	0	4.173852	-2.478122	0.406927
12	6	0	5.147116	-3.415104	0.374582
13	8	0	5.320070	-4.156735	-0.576094
14	6	0	-0.289504	2.000994	2.577507
15	6	0	-1.321445	3.094522	2.622560
16	6	0	2.615703	3.578399	-0.220318
17	6	0	3.416419	4.672681	0.433114
18	6	0	5.120610	0.762849	-1.487007
19	6	0	5.644534	1.122934	-2.851070
20	8	0	5.777186	0.706867	-0.467140
21	8	0	1.908639	3.707280	-1.200018
22	8	0	0.106482	1.362171	3.533234
23	6	0	5.961858	-3.404000	1.640338
24	8	0	-0.335382	-0.478775	-0.399914
25	6	0	-2.530999	0.427160	-0.693903
26	6	0	-1.724429	-0.638040	-0.266910
27	6	0	-2.270173	-1.852877	0.190714
28	6	0	-3.668149	-1.966800	0.307584
29	6	0	-4.480812	-0.886653	-0.087884
30	6	0	-3.931293	0.303848	-0.588855
31	8	0	-5.838652	-1.069582	0.057790
32	6	0	-4.840542	1.439760	-1.011638
33	6	0	-6.264327	1.259035	-0.477486
34	6	0	-6.755549	-0.183786	-0.647661
35	6	0	-1.932460	1.680169	-1.290502
36	6	0	-1.399554	-3.048139	0.512237
37	6	0	-4.296355	-3.240861	0.827449
38	6	0	-8.102414	-0.394881	0.042558
39	6	0	-6.825849	-0.617700	-2.119085

40	1	0	-0.084810	-0.948191	1.604553
41	1	0	1.702819	0.635843	2.027363
42	1	0	1.504165	1.495942	-0.912410
43	1	0	3.809448	0.044983	0.486349
44	1	0	1.783521	-1.135671	-1.495000
45	1	0	2.753791	-3.304661	-0.868006
46	1	0	3.941058	-2.240633	-1.649578
47	1	0	-2.260111	2.715644	2.204613
48	1	0	-1.008955	3.949214	2.018094
49	1	0	-1.486979	3.396610	3.656384
50	1	0	3.045705	4.843265	1.448652
51	1	0	4.465880	4.375898	0.513207
52	1	0	3.327763	5.588864	-0.149759
53	1	0	5.486236	0.289324	-3.541920
54	1	0	6.707551	1.351957	-2.785159
55	1	0	5.098428	1.984498	-3.246124
56	1	0	5.309862	-3.537548	2.508336
57	1	0	6.461298	-2.436367	1.748993
58	1	0	6.704340	-4.200560	1.604800
59	1	0	-4.439509	2.395158	-0.655853
60	1	0	-4.855210	1.517974	-2.108070
61	1	0	-6.953266	1.944697	-0.982451
62	1	0	-6.292218	1.500651	0.592086
63	1	0	-2.407750	1.919038	-2.248355
64	1	0	-2.073004	2.549582	-0.637335
65	1	0	-0.863881	1.566636	-1.460119
66	1	0	-1.842617	-3.963204	0.108146
67	1	0	-1.290778	-3.202049	1.594006
68	1	0	-0.399650	-2.945640	0.091686
69	1	0	-5.350252	-3.089605	1.059295
70	1	0	-4.232116	-4.051609	0.089339
71	1	0	-3.791159	-3.592936	1.732857
72	1	0	-8.044977	-0.109011	1.097308
73	1	0	-8.873940	0.212462	-0.441326
74	1	0	-8.403103	-1.445585	-0.016394
75	1	0	-5.845709	-0.576518	-2.601774
76	1	0	-7.195678	-1.645088	-2.189460
77	1	0	-7.508239	0.034308	-2.674792

Table S16. B3LYP/6-31+G(*d*,*p*) optimized Cartesian coordinates for the forms **A-H** of **1**β.

The conformer **A** of **1**β (form **1**β**A**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.612961	-0.619728	0.206744
2	6	0	-1.915974	-1.380179	0.485353
3	6	0	-3.078100	-0.721059	-0.263424
4	6	0	-3.142795	0.784612	0.010469
5	6	0	-1.759502	1.422587	-0.227009
6	8	0	-0.803915	0.741128	0.585342
7	8	0	-1.787976	-2.730000	0.007321
8	8	0	-4.307955	-1.320134	0.186512
9	8	0	-4.088325	1.356946	-0.915406
10	6	0	-1.730520	2.890367	0.155401
11	8	0	-0.499914	3.443153	-0.356288
12	6	0	-0.276035	4.753506	-0.110465
13	8	0	-1.060826	5.455631	0.501163
14	6	0	-1.916737	-3.755066	0.896773
15	6	0	-1.680321	-5.078294	0.220561
16	6	0	-5.093560	-1.973427	-0.713913
17	6	0	-6.319642	-2.528476	-0.041248
18	6	0	-5.189181	1.996641	-0.425011
19	6	0	-6.055700	2.498667	-1.547443
20	8	0	-5.409764	2.135149	0.760650
21	8	0	-4.820335	-2.081393	-1.892848
22	8	0	-2.178220	-3.597589	2.071532
23	6	0	1.041126	5.202585	-0.685339
24	6	0	2.391564	-1.364588	-0.367006
25	6	0	1.713401	-0.781393	0.711989
26	6	0	2.328471	0.130561	1.585352
27	6	0	3.662680	0.504459	1.344416
28	6	0	4.338566	-0.045795	0.236850
29	6	0	3.719585	-0.967076	-0.623889
30	8	0	5.630855	0.389600	0.042820
31	6	0	4.481538	-1.533415	-1.805023
32	6	0	5.740388	-0.717976	-2.113455
33	6	0	6.513617	-0.365452	-0.836827
34	6	0	1.740242	-2.417517	-1.236106
35	6	0	1.595712	0.687579	2.782931
36	6	0	4.358699	1.483370	2.262359
37	6	0	7.015874	-1.606101	-0.084054
38	6	0	7.668340	0.589866	-1.134901
39	8	0	0.391815	-1.179994	0.992974
40	1	0	-0.348693	-0.657983	-0.861249
41	1	0	-2.097719	-1.389872	1.562276
42	1	0	-2.976770	-0.896480	-1.338159
43	1	0	-3.479287	0.971710	1.033126
44	1	0	-1.493411	1.322606	-1.290637
45	1	0	-2.574733	3.423765	-0.287295
46	1	0	-1.764487	3.008468	1.241708
47	1	0	-1.988969	-5.886728	0.882723
48	1	0	-0.612973	-5.181916	-0.001385
49	1	0	-2.222581	-5.131042	-0.726659
50	1	0	-6.949593	-3.023675	-0.779368
51	1	0	-6.025427	-3.240294	0.735894
52	1	0	-6.875324	-1.722977	0.447483
53	1	0	-6.335821	1.670853	-2.205035
54	1	0	-5.497989	3.222287	-2.149853
55	1	0	-6.947522	2.970710	-1.136877
56	1	0	1.057894	5.026482	-1.764986
57	1	0	1.856962	4.621754	-0.245073

58	1	0	1.187413	6.262528	-0.480005
59	1	0	3.838436	-1.553986	-2.691846
60	1	0	4.750150	-2.581608	-1.610623
61	1	0	6.393694	-1.266091	-2.800867
62	1	0	5.461752	0.219969	-2.609062
63	1	0	2.413987	-3.267237	-1.387969
64	1	0	1.489588	-2.030922	-2.232684
65	1	0	0.823531	-2.795368	-0.783854
66	1	0	2.162773	0.509357	3.703841
67	1	0	1.460893	1.772333	2.696248
68	1	0	0.611465	0.235574	2.890369
69	1	0	5.362245	1.712494	1.906017
70	1	0	4.442985	1.082923	3.280546
71	1	0	3.799056	2.423112	2.339300
72	1	0	6.191098	-2.249273	0.234416
73	1	0	7.573096	-1.303140	0.807527
74	1	0	7.681429	-2.195054	-0.724167
75	1	0	7.306106	1.484856	-1.650027
76	1	0	8.410673	0.097995	-1.771492
77	1	0	8.159911	0.898343	-0.206995

The conformer **B** of **1**β (form **1**β**B**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.337724	-0.596099	0.111087
2	6	0	-1.576654	-1.385913	0.551853
3	6	0	-2.764767	-1.042534	-0.351657
4	6	0	-2.973908	0.470924	-0.449805
5	6	0	-1.646259	1.167162	-0.808418
6	8	0	-0.656432	0.792429	0.148427
7	8	0	-1.310485	-2.792717	0.421233
8	8	0	-3.950434	-1.636108	0.211571
9	8	0	-3.913939	0.724773	-1.514470
10	6	0	-1.727715	2.682153	-0.840754
11	8	0	-2.207141	3.147882	0.436475
12	6	0	-2.444496	4.473710	0.550483
13	8	0	-2.267694	5.257941	-0.364592
14	6	0	-1.376108	-3.577488	1.533635
15	6	0	-0.995949	-4.996395	1.207193
16	6	0	-4.627014	-2.572869	-0.507980
17	6	0	-5.819768	-3.071865	0.261673
18	6	0	-5.126790	1.270869	-1.214719
19	6	0	-5.949412	1.450509	-2.462092
20	8	0	-5.471053	1.566383	-0.088819
21	8	0	-4.295052	-2.939692	-1.617984
22	8	0	-1.691075	-3.164634	2.630817
23	6	0	-2.944151	4.824902	1.926193
24	6	0	2.742059	-1.155848	-0.239710
25	6	0	1.975399	-0.404823	0.661681
26	6	0	2.471306	0.745297	1.297791
27	6	0	3.772192	1.182067	0.989882
28	6	0	4.536211	0.453115	0.056457
29	6	0	4.035938	-0.701569	-0.567481
30	8	0	5.790182	0.952814	-0.216794
31	6	0	4.888330	-1.453581	-1.569697
32	6	0	6.080730	-0.617652	-2.043158
33	6	0	6.769834	0.098315	-0.875148
34	6	0	2.222651	-2.442904	-0.841238
35	6	0	1.648195	1.494540	2.318893
36	6	0	4.339653	2.416583	1.652565
37	6	0	7.350091	-0.875495	0.160804

38	6	0	7.846746	1.060755	-1.373866
39	8	0	0.689017	-0.856268	1.016486
40	1	0	-0.038596	-0.865368	-0.914334
41	1	0	-1.795846	-1.150818	1.595639
42	1	0	-2.606781	-1.459892	-1.349932
43	1	0	-3.369987	0.866181	0.486950
44	1	0	-1.336764	0.845532	-1.816288
45	1	0	-0.736071	3.099626	-1.032955
46	1	0	-2.405864	3.010477	-1.632050
47	1	0	-1.478629	-5.325026	0.283714
48	1	0	-1.272213	-5.647877	2.035833
49	1	0	0.087181	-5.050034	1.054258
50	1	0	-6.478815	-2.235497	0.512157
51	1	0	-6.358710	-3.807075	-0.334953
52	1	0	-5.491825	-3.522507	1.203183
53	1	0	-6.921721	1.866914	-2.201303
54	1	0	-6.076183	0.489229	-2.968495
55	1	0	-5.432367	2.120992	-3.155222
56	1	0	-2.212002	4.518175	2.679002
57	1	0	-3.873599	4.285737	2.132298
58	1	0	-3.115935	5.898880	1.990411
59	1	0	4.282588	-1.741926	-2.436019
60	1	0	5.240947	-2.397049	-1.129092
61	1	0	6.806104	-1.247545	-2.569300
62	1	0	5.739396	0.146055	-2.752544
63	1	0	2.974562	-3.235897	-0.770867
64	1	0	1.980867	-2.330877	-1.906313
65	1	0	1.324943	-2.788122	-0.328874
66	1	0	2.194451	1.590264	3.264437
67	1	0	1.421542	2.511462	1.977039
68	1	0	0.704016	0.989658	2.513956
69	1	0	5.328788	2.653585	1.262693
70	1	0	4.425392	2.281698	2.738223
71	1	0	3.691184	3.286267	1.493379
72	1	0	6.573642	-1.499565	0.611352
73	1	0	7.844859	-0.318677	0.962286
74	1	0	8.088283	-1.534098	-0.309175
75	1	0	7.427912	1.769462	-2.094864
76	1	0	8.653838	0.504371	-1.861061
77	1	0	8.272528	1.625666	-0.538775

The conformer **C** of **1**β (form **1**β**C**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.326406	-0.649375	0.177554
2	6	0	-1.611477	-1.397631	0.554984
3	6	0	-2.748885	-0.989268	-0.386157
4	6	0	-2.893464	0.533202	-0.461298
5	6	0	-1.526310	1.181884	-0.754313
6	8	0	-0.591037	0.749912	0.232744
7	8	0	-1.396056	-2.811264	0.404751
8	8	0	-3.978164	-1.545307	0.118665
9	8	0	-3.780184	0.846520	-1.555398
10	6	0	-1.547154	2.699204	-0.759532
11	8	0	-2.062310	3.160064	0.505556
12	6	0	-2.243334	4.493007	0.638768
13	8	0	-1.986855	5.286660	-0.248933
14	6	0	-1.529236	-3.614143	1.498366
15	6	0	-1.196566	-5.040788	1.154454
16	6	0	-4.669162	-2.429729	-0.651601
17	6	0	-5.912564	-2.891578	0.058782

18	6	0	-4.987351	1.422109	-1.289603
19	6	0	-5.749187	1.666773	-2.564198
20	8	0	-5.370090	1.694792	-0.170399
21	8	0	-4.313376	-2.780489	-1.759448
22	8	0	-1.863247	-3.210077	2.593107
23	6	0	-2.794458	4.838857	1.996027
24	6	0	2.746305	-1.337327	-0.063111
25	6	0	1.970201	-0.562213	0.809771
26	6	0	2.477887	0.570167	1.468129
27	6	0	3.790217	0.986877	1.183242
28	6	0	4.559647	0.243917	0.265422
29	6	0	4.066212	-0.923505	-0.340272
30	8	0	5.835155	0.709397	0.035883
31	6	0	4.948920	-1.723162	-1.277236
32	6	0	6.419018	-1.304927	-1.179364
33	6	0	6.573418	0.219333	-1.120624
34	6	0	2.209393	-2.607577	-0.684147
35	6	0	1.648547	1.326960	2.479055
36	6	0	4.369043	2.210615	1.855943
37	6	0	8.022859	0.619320	-0.848897
38	6	0	6.043987	0.920630	-2.380028
39	8	0	0.656116	-0.970948	1.111859
40	1	0	-0.000606	-0.909156	-0.842438
41	1	0	-1.861772	-1.174614	1.594486
42	1	0	-2.569288	-1.393682	-1.386127
43	1	0	-3.309047	0.926359	0.467853
44	1	0	-1.189305	0.866998	-1.755487
45	1	0	-0.532794	3.080409	-0.901805
46	1	0	-2.177890	3.068563	-1.571745
47	1	0	-1.676208	-5.335392	0.217891
48	1	0	-1.511648	-5.694855	1.967010
49	1	0	-0.114055	-5.133232	1.017235
50	1	0	-6.559532	-2.034408	0.268225
51	1	0	-6.441599	-3.614026	-0.561810
52	1	0	-5.648240	-3.343425	1.019228
53	1	0	-6.723705	2.094084	-2.330706
54	1	0	-5.871534	0.729140	-3.113972
55	1	0	-5.187917	2.352954	-3.205815
56	1	0	-2.134286	4.453987	2.778607
57	1	0	-3.772399	4.366155	2.128828
58	1	0	-2.891080	5.920238	2.087424
59	1	0	4.591036	-1.612506	-2.310859
60	1	0	4.866254	-2.792134	-1.052368
61	1	0	6.862393	-1.722955	-0.267516
62	1	0	6.987685	-1.701858	-2.027240
63	1	0	2.871386	-3.454972	-0.472714
64	1	0	2.139439	-2.528248	-1.776303
65	1	0	1.222628	-2.858962	-0.297866
66	1	0	2.201628	1.454551	3.416260
67	1	0	1.394695	2.330362	2.116621
68	1	0	0.716581	0.806990	2.693995
69	1	0	5.313205	2.501485	1.396330
70	1	0	4.558430	2.027086	2.921826
71	1	0	3.679788	3.060067	1.798451
72	1	0	8.390903	0.140149	0.063464
73	1	0	8.105357	1.704031	-0.728908
74	1	0	8.661291	0.314924	-1.684328
75	1	0	4.978742	0.728716	-2.534585
76	1	0	6.586233	0.571021	-3.265075
77	1	0	6.185023	2.002282	-2.293845

The conformer **D** of **1**β (form **1**β**D**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.422517	-0.762750	-0.041192
2	6	0	-1.722888	-1.375575	0.494841
3	6	0	-2.918340	-0.847841	-0.304099
4	6	0	-2.912478	0.681657	-0.376543
5	6	0	-1.531327	1.187261	-0.837105
6	8	0	-0.533614	0.656397	0.033540
7	8	0	-1.675490	-2.803235	0.331984
8	8	0	-4.126923	-1.272799	0.355004
9	8	0	-3.888050	1.087250	-1.359005
10	6	0	-1.396290	2.698658	-0.851457
11	8	0	-1.706501	3.204349	0.462505
12	6	0	-1.722370	4.547896	0.608997
13	8	0	-1.480230	5.315473	-0.305302
14	6	0	-1.758230	-3.592461	1.440328
15	6	0	-1.627474	-5.044867	1.068976
16	6	0	-5.004487	-2.066083	-0.318461
17	6	0	-6.187966	-2.400626	0.548463
18	6	0	-4.987470	1.785776	-0.956397
19	6	0	-5.874120	2.100558	-2.131010
20	8	0	-5.198542	2.101172	0.196706
21	8	0	-4.834516	-2.440034	-1.462181
22	8	0	-1.909373	-3.160184	2.564463
23	6	0	-2.080483	4.942367	2.016709
24	6	0	2.629563	0.147461	0.907881
25	6	0	1.930495	-0.912371	0.317119
26	6	0	2.510799	-1.756179	-0.646146
27	6	0	3.825378	-1.495237	-1.072269
28	6	0	4.527590	-0.416260	-0.498644
29	6	0	3.946894	0.408308	0.478854
30	8	0	5.806471	-0.214885	-0.968061
31	6	0	4.733659	1.564496	1.061564
32	6	0	5.967164	1.896921	0.217293
33	6	0	6.719774	0.630903	-0.209788
34	6	0	2.008205	0.990674	1.996937
35	6	0	1.764923	-2.949012	-1.201202
36	6	0	4.482622	-2.369706	-2.116325
37	6	0	7.843735	0.959195	-1.191517
38	6	0	7.258163	-0.171897	0.983464
39	8	0	0.625892	-1.184740	0.773774
40	1	0	-0.249427	-1.051467	-1.090367
41	1	0	-1.820215	-1.131935	1.555027
42	1	0	-2.906789	-1.267128	-1.314072
43	1	0	-3.170634	1.112752	0.592025
44	1	0	-1.351226	0.844633	-1.868884
45	1	0	-0.372410	2.973739	-1.116884
46	1	0	-2.078120	3.134801	-1.585538
47	1	0	-0.592208	-5.250037	0.777023
48	1	0	-2.265780	-5.283570	0.214672
49	1	0	-1.889027	-5.665673	1.925393
50	1	0	-6.681653	-1.481261	0.876555
51	1	0	-6.887176	-3.021666	-0.010379
52	1	0	-5.852964	-2.929526	1.445728
53	1	0	-5.324315	2.699393	-2.863328
54	1	0	-6.751904	2.647925	-1.789433
55	1	0	-6.179226	1.174564	-2.627143
56	1	0	-1.417986	4.443731	2.729612
57	1	0	-3.103369	4.621893	2.238014
58	1	0	-2.002889	6.023757	2.124836
59	1	0	5.032899	1.331132	2.093256
60	1	0	4.095896	2.452247	1.134823

61	1	0	5.661338	2.430187	-0.691074
62	1	0	6.643101	2.558918	0.769224
63	1	0	2.676377	1.064486	2.862214
64	1	0	1.060186	0.569352	2.327041
65	1	0	1.814400	2.013026	1.650467
66	1	0	2.395174	-3.844141	-1.180050
67	1	0	0.863589	-3.160445	-0.626514
68	1	0	1.471572	-2.796080	-2.247947
69	1	0	5.429179	-1.942426	-2.445552
70	1	0	3.838179	-2.495203	-2.993494
71	1	0	4.687592	-3.375253	-1.725725
72	1	0	7.455016	1.509919	-2.053590
73	1	0	8.319049	0.041296	-1.551278
74	1	0	8.606027	1.572913	-0.701156
75	1	0	6.453236	-0.510410	1.641351
76	1	0	7.946863	0.441796	1.573957
77	1	0	7.799519	-1.053941	0.628150

The conformer **E** of **1β** (form **1β*E***)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.624023	-0.667198	0.242250
2	6	0	-1.974894	-1.354342	0.480446
3	6	0	-3.078062	-0.625306	-0.292276
4	6	0	-3.063707	0.879639	-0.007385
5	6	0	-1.640313	1.438986	-0.203195
6	8	0	-0.747536	0.699127	0.628943
7	8	0	-1.910594	-2.705997	-0.004781
8	8	0	-4.350991	-1.156637	0.121328
9	8	0	-3.950065	1.512636	-0.951950
10	6	0	-1.539775	2.900049	0.192346
11	8	0	-0.258570	3.381578	-0.263704
12	6	0	0.032875	4.673924	0.005786
13	8	0	-0.732326	5.415916	0.594739
14	6	0	-2.111305	-3.727780	0.875241
15	6	0	-1.929150	-5.057880	0.195838
16	6	0	-5.145631	-1.764284	-0.802802
17	6	0	-6.416611	-2.256391	-0.165431
18	6	0	-5.033604	2.197717	-0.484789
19	6	0	-5.837901	2.760519	-1.624597
20	8	0	-5.284824	2.328031	0.695655
21	8	0	-4.847467	-1.881633	-1.974783
22	8	0	-2.388639	-3.562934	2.045322
23	6	0	1.394986	5.049505	-0.514554
24	6	0	2.358366	-1.592848	-0.244269
25	6	0	1.675158	-0.962180	0.804641
26	6	0	2.304796	-0.069435	1.687645
27	6	0	3.652584	0.263464	1.465760
28	6	0	4.333225	-0.326714	0.381907
29	6	0	3.713830	-1.265975	-0.458968
30	8	0	5.651263	0.042415	0.228677
31	6	0	4.500543	-1.915913	-1.579282
32	6	0	6.007728	-1.688871	-1.429936
33	6	0	6.327592	-0.243814	-1.029631
34	6	0	1.683839	-2.623344	-1.122063
35	6	0	1.565400	0.517059	2.867508
36	6	0	4.364664	1.234903	2.379198
37	6	0	7.812994	-0.071579	-0.715651
38	6	0	5.873036	0.779473	-2.080655
39	8	0	0.326949	-1.292103	1.046357

40	1	0	-0.334909	-0.711237	-0.819528
41	1	0	-2.185279	-1.360956	1.552192
42	1	0	-2.960043	-0.798083	-1.365681
43	1	0	-3.415304	1.078355	1.008010
44	1	0	-1.350133	1.330446	-1.259774
45	1	0	-2.331864	3.485321	-0.280251
46	1	0	-1.611372	3.013635	1.277274
47	1	0	-2.299232	-5.852160	0.843491
48	1	0	-0.863102	-5.217985	0.002811
49	1	0	-2.446936	-5.075525	-0.766222
50	1	0	-7.049051	-2.721035	-0.921072
51	1	0	-6.180820	-2.979893	0.620727
52	1	0	-6.945352	-1.422947	0.306120
53	1	0	-6.130493	1.960022	-2.309939
54	1	0	-5.228357	3.471492	-2.190872
55	1	0	-6.721975	3.263158	-1.234078
56	1	0	1.431075	4.909679	-1.599201
57	1	0	2.156063	4.399161	-0.073756
58	1	0	1.606393	6.089676	-0.268798
59	1	0	4.153380	-1.531917	-2.549214
60	1	0	4.302508	-2.993054	-1.603629
61	1	0	6.405541	-2.349420	-0.650074
62	1	0	6.527192	-1.938178	-2.361502
63	1	0	2.253043	-3.559747	-1.132327
64	1	0	1.613802	-2.286376	-2.163965
65	1	0	0.678918	-2.855210	-0.771980
66	1	0	2.144452	0.393057	3.789055
67	1	0	1.393501	1.592217	2.736757
68	1	0	0.595314	0.040904	3.000736
69	1	0	5.314877	1.551473	1.949557
70	1	0	4.575847	0.781719	3.356964
71	1	0	3.754929	2.124857	2.567319
72	1	0	8.131450	-0.785912	0.049714
73	1	0	8.012714	0.940613	-0.350350
74	1	0	8.411123	-0.237251	-1.617330
75	1	0	4.791983	0.744630	-2.240389
76	1	0	6.366542	0.583878	-3.038654
77	1	0	6.136138	1.791120	-1.757043

The conformer **F** of **1**β (form **1**β**F**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.700160	-0.749365	0.041598
2	6	0	-2.076490	-1.310261	0.422469
3	6	0	-3.183455	-0.456251	-0.201277
4	6	0	-2.988355	1.031047	0.109704
5	6	0	-1.547428	1.460847	-0.232933
6	8	0	-0.641338	0.609627	0.468691
7	8	0	-2.202825	-2.646684	-0.091376
8	8	0	-4.446727	-0.875190	0.349222
9	8	0	-3.905017	1.776268	-0.716875
10	6	0	-1.261479	2.889541	0.189977
11	8	0	-0.011187	3.275887	-0.417527
12	6	0	0.425955	4.528263	-0.157622
13	8	0	-0.184884	5.309317	0.549341
14	6	0	-2.390801	-3.671404	0.788138
15	6	0	-2.427525	-4.990777	0.065755
16	6	0	-5.399415	-1.374419	-0.486433
17	6	0	-6.632299	-1.757661	0.286111
18	6	0	-4.866435	2.537433	-0.118666

19	6	0	-5.728468	3.211130	-1.151010
20	8	0	-4.982166	2.645163	1.084930
21	8	0	-5.251008	-1.485326	-1.687158
22	8	0	-2.503969	-3.516965	1.986716
23	6	0	1.729974	4.810907	-0.855474
24	6	0	2.430763	-0.557371	1.213563
25	6	0	1.608390	-1.288368	0.347255
26	6	0	2.096681	-1.902255	-0.819678
27	6	0	3.443155	-1.706487	-1.174985
28	6	0	4.270714	-0.948999	-0.322027
29	6	0	3.790712	-0.398102	0.877234
30	8	0	5.584265	-0.825056	-0.716682
31	6	0	4.728670	0.362537	1.791978
32	6	0	6.197564	0.128030	1.428180
33	6	0	6.423555	0.186652	-0.087512
34	6	0	1.896843	0.029550	2.499356
35	6	0	1.213280	-2.782373	-1.676287
36	6	0	4.005733	-2.318655	-2.437777
37	6	0	6.078820	1.557396	-0.687807
38	6	0	7.851264	-0.218761	-0.450860
39	8	0	0.265638	-1.487845	0.722106
40	1	0	-0.539082	-0.787769	-1.046941
41	1	0	-2.161301	-1.328291	1.511135
42	1	0	-3.207313	-0.608300	-1.283857
43	1	0	-3.206774	1.229898	1.161870
44	1	0	-1.389923	1.369342	-1.318707
45	1	0	-2.050264	3.562158	-0.154455
46	1	0	-1.180795	2.962561	1.277774
47	1	0	-2.757319	-5.772312	0.749583
48	1	0	-1.423271	-5.229511	-0.299600
49	1	0	-3.090860	-4.936775	-0.801156
50	1	0	-6.382421	-2.521269	1.028753
51	1	0	-7.018291	-0.889342	0.828008
52	1	0	-7.389515	-2.138166	-0.398514
53	1	0	-6.173931	2.463636	-1.813656
54	1	0	-5.115678	3.874421	-1.769108
55	1	0	-6.509448	3.786308	-0.655116
56	1	0	1.581596	4.782080	-1.939563
57	1	0	2.467417	4.043780	-0.604025
58	1	0	2.095868	5.794368	-0.562169
59	1	0	4.562625	0.062022	2.832268
60	1	0	4.495600	1.436258	1.756099
61	1	0	6.838525	0.864070	1.925461
62	1	0	6.511378	-0.863278	1.777040
63	1	0	2.075700	1.109901	2.547027
64	1	0	2.393871	-0.415303	3.370366
65	1	0	0.826534	-0.140642	2.595976
66	1	0	1.730782	-3.710798	-1.938049
67	1	0	0.291416	-3.047801	-1.158876
68	1	0	0.941307	-2.295444	-2.621990
69	1	0	4.961818	-1.864440	-2.698023
70	1	0	3.320930	-2.191856	-3.282417
71	1	0	4.174388	-3.397756	-2.320883
72	1	0	5.028148	1.815844	-0.530634
73	1	0	6.270258	1.553593	-1.765183
74	1	0	6.695365	2.338219	-0.229835
75	1	0	8.087457	-1.206675	-0.043788
76	1	0	8.564610	0.504991	-0.044036
77	1	0	7.975760	-0.252232	-1.537715

The conformer **G** of **1**β (form **1**β**G**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.691408	-0.717307	-0.022822
2	6	0	2.036815	-1.332629	-0.428732
3	6	0	3.186870	-0.526189	0.181000
4	6	0	3.048391	0.969011	-0.122285
5	6	0	1.631886	1.454572	0.246035
6	8	0	0.681775	0.644263	-0.445234
7	8	0	2.117335	-2.674983	0.079002
8	8	0	4.423881	-0.994752	-0.388657
9	8	0	4.008321	1.671975	0.692027
10	6	0	1.394591	2.896078	-0.163248
11	8	0	0.169166	3.324060	0.466731
12	6	0	-0.224637	4.594312	0.225218
13	8	0	0.402946	5.358086	-0.486052
14	6	0	2.258468	-3.702314	-0.805849
15	6	0	2.255545	-5.025077	-0.088691
16	6	0	5.366949	-1.535301	0.432014
17	6	0	6.570898	-1.968732	-0.359499
18	6	0	4.988304	2.398359	0.081176
19	6	0	5.892579	3.033499	1.101790
20	8	0	5.087445	2.508850	-1.123678
21	8	0	5.231798	-1.642616	1.634620
22	8	0	2.363589	-3.547570	-2.005193
23	6	0	-1.503560	4.920022	0.950189
24	6	0	-2.434839	-0.344970	-1.108369
25	6	0	-1.641564	-1.149098	-0.281127
26	6	0	-2.142049	-1.764442	0.879561
27	6	0	-3.474515	-1.518342	1.256025
28	6	0	-4.272667	-0.690984	0.440779
29	6	0	-3.770764	-0.100475	-0.730472
30	8	0	-5.564337	-0.488080	0.873931
31	6	0	-4.661309	0.789066	-1.573703
32	6	0	-5.917962	1.221157	-0.812900
33	6	0	-6.551710	0.049222	-0.053610
34	6	0	-1.891914	0.239757	-2.391452
35	6	0	-1.290284	-2.704836	1.702854
36	6	0	-4.049192	-2.146765	2.505655
37	6	0	-7.698920	0.522472	0.837949
38	6	0	-7.017947	-1.079504	-0.984658
39	8	0	-0.318154	-1.412772	-0.684833
40	1	0	0.549267	-0.752577	1.068580
41	1	0	2.104135	-1.349939	-1.518668
42	1	0	3.219789	-0.682159	1.262862
43	1	0	3.257516	1.163498	-1.177113
44	1	0	1.488564	1.362093	1.333622
45	1	0	2.213428	3.536182	0.173087
46	1	0	1.299607	2.979853	-1.249152
47	1	0	2.548666	-5.815238	-0.779281
48	1	0	1.247680	-5.228716	0.287796
49	1	0	2.930618	-4.998722	0.770402
50	1	0	7.323213	-2.378515	0.313544
51	1	0	6.278363	-2.722982	-1.096164
52	1	0	6.982629	-1.117649	-0.909674
53	1	0	6.301101	2.270421	1.770211
54	1	0	5.319702	3.735535	1.715618
55	1	0	6.699638	3.561799	0.595590
56	1	0	-1.328675	4.898742	2.030625
57	1	0	-2.268079	4.171302	0.726112
58	1	0	-1.848567	5.910754	0.655956
59	1	0	-4.941103	0.267952	-2.500299
60	1	0	-4.107648	1.678710	-1.893317

61	1	0	-5.659958	1.996775	-0.081483
62	1	0	-6.652446	1.655298	-1.499763
63	1	0	-2.568734	0.039626	-3.229377
64	1	0	-0.914885	-0.177638	-2.629827
65	1	0	-1.779624	1.328370	-2.319645
66	1	0	-1.842635	-3.619539	1.941248
67	1	0	-0.382232	-2.990789	1.172279
68	1	0	-0.995543	-2.256568	2.660726
69	1	0	-5.021314	-1.718477	2.747686
70	1	0	-3.385585	-2.002147	3.365169
71	1	0	-4.182719	-3.230036	2.384823
72	1	0	-7.360030	1.309922	1.518203
73	1	0	-8.088447	-0.308129	1.434823
74	1	0	-8.514589	0.919003	0.224998
75	1	0	-6.187312	-1.506087	-1.553375
76	1	0	-7.760927	-0.702418	-1.695559
77	1	0	-7.476211	-1.882561	-0.399521

The conformer **H** of **1**β (form **1**β**H**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.422797	-0.809252	0.006544
2	6	0	-1.763626	-1.372108	0.494723
3	6	0	-2.909074	-0.785862	-0.336168
4	6	0	-2.838400	0.742979	-0.387270
5	6	0	-1.422834	1.197488	-0.793878
6	8	0	-0.475805	0.612337	0.098136
7	8	0	-1.771304	-2.798611	0.317175
8	8	0	-4.155342	-1.169173	0.276474
9	8	0	-3.760873	1.200950	-1.397817
10	6	0	-1.225467	2.701971	-0.777303
11	8	0	-1.553738	3.198006	0.535885
12	6	0	-1.521814	4.538663	0.704774
13	8	0	-1.225247	5.310629	-0.189578
14	6	0	-1.911646	-3.594891	1.414742
15	6	0	-1.829952	-5.047530	1.030702
16	6	0	-5.038183	-1.923891	-0.433502
17	6	0	-6.260510	-2.223702	0.391184
18	6	0	-4.843370	1.941284	-1.024960
19	6	0	-5.672049	2.309099	-2.226139
20	8	0	-5.082542	2.250628	0.124271
21	8	0	-4.844512	-2.292579	-1.575134
22	8	0	-2.072352	-3.168072	2.539620
23	6	0	-1.901619	4.924205	2.109235
24	6	0	2.644469	-0.062697	1.084692
25	6	0	1.909327	-1.060154	0.432010
26	6	0	2.472000	-1.891820	-0.552335
27	6	0	3.797780	-1.658461	-0.958849
28	6	0	4.534359	-0.635241	-0.328825
29	6	0	3.986515	0.142844	0.704009
30	8	0	5.833140	-0.479972	-0.758892
31	6	0	4.831600	1.196067	1.390933
32	6	0	6.320741	1.032629	1.073170
33	6	0	6.554912	0.738429	-0.413529
34	6	0	2.038244	0.765931	2.193147
35	6	0	1.689786	-3.037335	-1.156241
36	6	0	4.435701	-2.504173	-2.037613
37	6	0	6.073643	1.874405	-1.327817
38	6	0	8.020914	0.407249	-0.688748
39	8	0	0.581918	-1.285107	0.846676

40	1	0	-0.230742	-1.091438	-1.040837
41	1	0	-1.884419	-1.135007	1.553995
42	1	0	-2.879602	-1.192291	-1.351034
43	1	0	-3.112986	1.172361	0.577552
44	1	0	-1.224295	0.864144	-1.825323
45	1	0	-0.183675	2.938781	-1.007680
46	1	0	-1.866614	3.178207	-1.522927
47	1	0	-0.797394	-5.290367	0.758787
48	1	0	-2.458322	-5.252273	0.160350
49	1	0	-2.134421	-5.665980	1.874546
50	1	0	-6.731454	-1.290360	0.713132
51	1	0	-6.962918	-2.813771	-0.196455
52	1	0	-5.974066	-2.772806	1.293094
53	1	0	-5.070384	2.893057	-2.929112
54	1	0	-6.537668	2.889418	-1.908783
55	1	0	-5.997838	1.403605	-2.746380
56	1	0	-1.268175	4.398805	2.829409
57	1	0	-2.937089	4.628118	2.304013
58	1	0	-1.797280	6.001540	2.234023
59	1	0	4.686577	1.143678	2.475576
60	1	0	4.488989	2.198448	1.097052
61	1	0	6.875876	1.931215	1.363302
62	1	0	6.732984	0.196299	1.650662
63	1	0	2.105743	1.837126	1.970752
64	1	0	2.568206	0.601983	3.139606
65	1	0	0.989600	0.517825	2.343034
66	1	0	2.295808	-3.948705	-1.179405
67	1	0	0.787176	-3.249594	-0.583467
68	1	0	1.391200	-2.830932	-2.192340
69	1	0	5.342746	-2.032727	-2.416035
70	1	0	3.751866	-2.662861	-2.877603
71	1	0	4.713647	-3.496902	-1.658349
72	1	0	5.000486	2.054465	-1.221311
73	1	0	6.274079	1.624202	-2.374068
74	1	0	6.601098	2.803713	-1.087695
75	1	0	8.355231	-0.420116	-0.055372
76	1	0	8.649871	1.279286	-0.483408
77	1	0	8.159511	0.120812	-1.735951