Supporting Information

2,3,5-*Tri-O*-Benzyl-D-Xylofuranose

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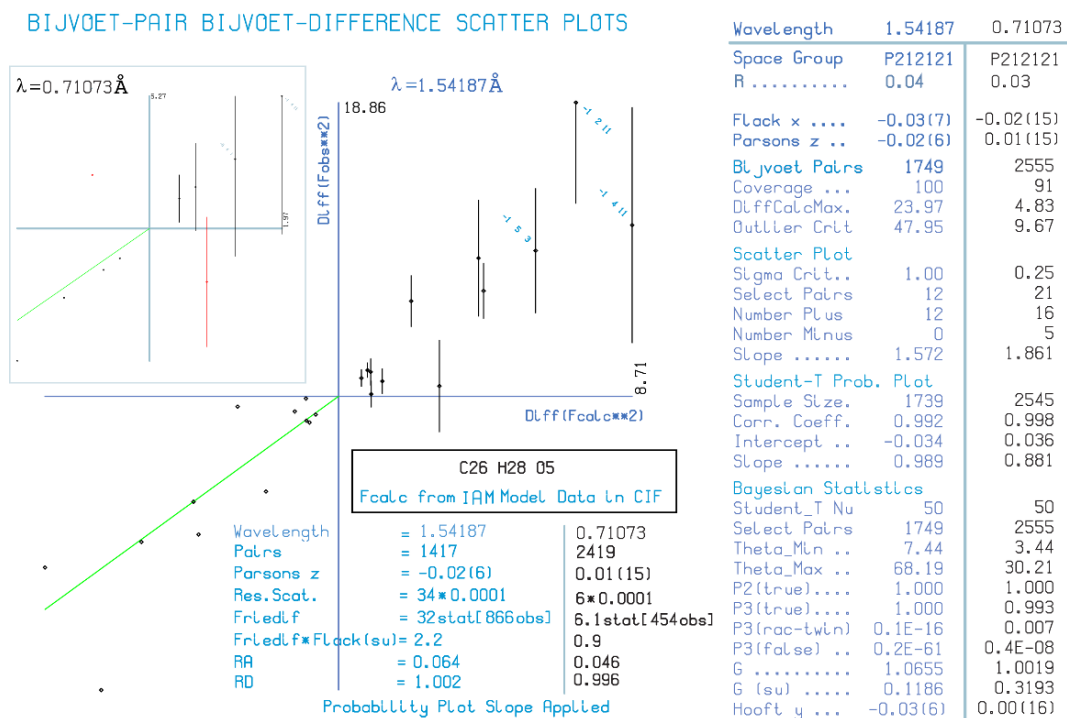
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1. Crystal Data, Data Collection and IAM Structure Refinement Details of Compound 1 (α/β, *ca* 89:11) Collected at Room Temperature.

Table S1. Crystal data, data collection and IAM structure refinement details of compound **1** collected at room temperature using copper radiation (statistics for Mo are recalled in comparison, right column)

Identification code	2,3,5-*Tri-O*-benzyl-α,β-D-xylofuranose (α,β)-**1** (α/β *ca.* 89:11)	
Empirical formula, (weight)	$C_{26}H_{28}O_5$, (420.48)	*Id.*
Temperature (K)	293(2)	*100(2)*
Diffractometer Rigaku®	mm007+Spider2	*XtaLabPro mm003+Pilatus200k*
Wavelength (Å)	1.54187	*0.71073*
Crystal system, space group	$P2_12_12_1$, Orthorhombic	*Id.*
Unit cell dimensions (Å, α=β=γ=90°)	a = 6.9071(1) b = 13.4121(3) c =24.3907(17)	*a = 6.9002(1) b = 13.1783(2) c = 23.9751(5)*
Volume (Å^3)	2259.52(17)	*2180.13(6)*
Z, Calculated density (Mg/m^3)	4, 1.236	*4, 1.281*
Absorption coefficient (mm^{-1})	0.686	*0.088*
F(000)	896	*Id.*
Theta range for data collection (°)	3.624 to 68.193	*2.98 to 30.25*
Limiting indices	−8 ≤ h ≤ 8, −16 ≤ k≤ 16, −29 ≤ l ≤ 26	*−9 ≤ h ≤ 9, −17 ≤ k ≤ 18, −33 ≤ l ≤ 33*
Reflections collected / unique R(int)	29687 / 4145 0.0448	*55919 / 6102 0.0370*
Completeness to $\theta_{max\ (iUCR)}$ (%)	100	*99.8*
Absorption correction method	Multi-scan 1.000 and 0.808	*Gauss. & M-scan 1.000 and 0.302*
Refinement method	IAM (*Shelxl software*)	*Id.*
Data / restraints / parameters	4145 / 426 / 421	*6102 / 416 / 419*
Goodness-of-fit on F^2	1.109	*1.028*
Final R indices [*I>2σ(I)*]	*R1, wR2*	0.0372, 0.0974	*0.0338, 0.0896*
Final R indices (all data)	*R1, wR2*	0.0410, 0.1032	*0.0352, 0.0903*
Absolute structure parameter [S1]	−0.03(7)	*−0.02(15)*
Largest diff. peak and hole (e.Å^{-3})	0.111 and −0.158	*0.273 and −0.192*

2. Bijvoet Analyses.

BIJVOET-PAIR BIJVOET-DIFFERENCE SCATTER PLOTS

λ=0.71073Å

λ=1.54187Å

C26 H28 O5

Fcalc from IAM Model Data in CIF

Wavelength	= 1.54187	0.71073
Pairs	= 1417	2419
Parsons z	= -0.02(6)	0.01(15)
Res.Scat.	= 34*0.0001	6*0.0001
Friedif	= 32stat[866obs]	6.1stat[454obs]
Friedif*Flack(su)	= 2.2	0.9
RA	= 0.064	0.046
RD	= 1.002	0.996

Probability Plot Slope Applied

|	1.54187	0.71073
Wavelength	1.54187	0.71073
Space Group	P212121	P212121
R	0.04	0.03
Flack x	-0.03(7)	-0.02(15)
Parsons z . .	-0.02(6)	0.01(15)
Bijvoet Pairs	1749	2555
Coverage . . .	100	91
DiffCalcMax.	23.97	4.83
Outlier Crit	47.95	9.67
Scatter Plot		
Sigma Crit..	1.00	0.25
Select Pairs	12	21
Number Plus	12	16
Number Minus	0	5
Slope	1.572	1.861
Student-T Prob. Plot		
Sample Size.	1739	2545
Corr. Coeff.	0.992	0.998
Intercept ..	-0.034	0.036
Slope	0.989	0.881
Bayesian Statistics		
Student_T Nu	50	50
Select Pairs	1749	2555
Theta_Min ..	7.44	3.44
Theta_Max ..	68.19	30.21
P2(true)....	1.000	1.000
P3(true)....	1.000	0.993
P3(rac-twin)	0.1E-16	0.007
P3(false) ..	0.2E-61	0.4E-08
G	1.0655	1.0019
G (su)	0.1186	0.3193
Hooft y . . .	-0.03(6)	0.00(16)

Figure S1. Summary of Bijvoet analyses performed with the program *Platon* [S2] (using IAM models derived with two different radiation energies, see Table S1), assessing the absolute configuration of **1** by anomalous dispersion.

3. Copies of ^{1}H and ^{13}C NMR Spectra of Compound 1.

Figure S2. ^{1}H NMR (400 MHz, CDCl$_3$) Spectrum of Compound **1** (α/β *ca.* 2:3).
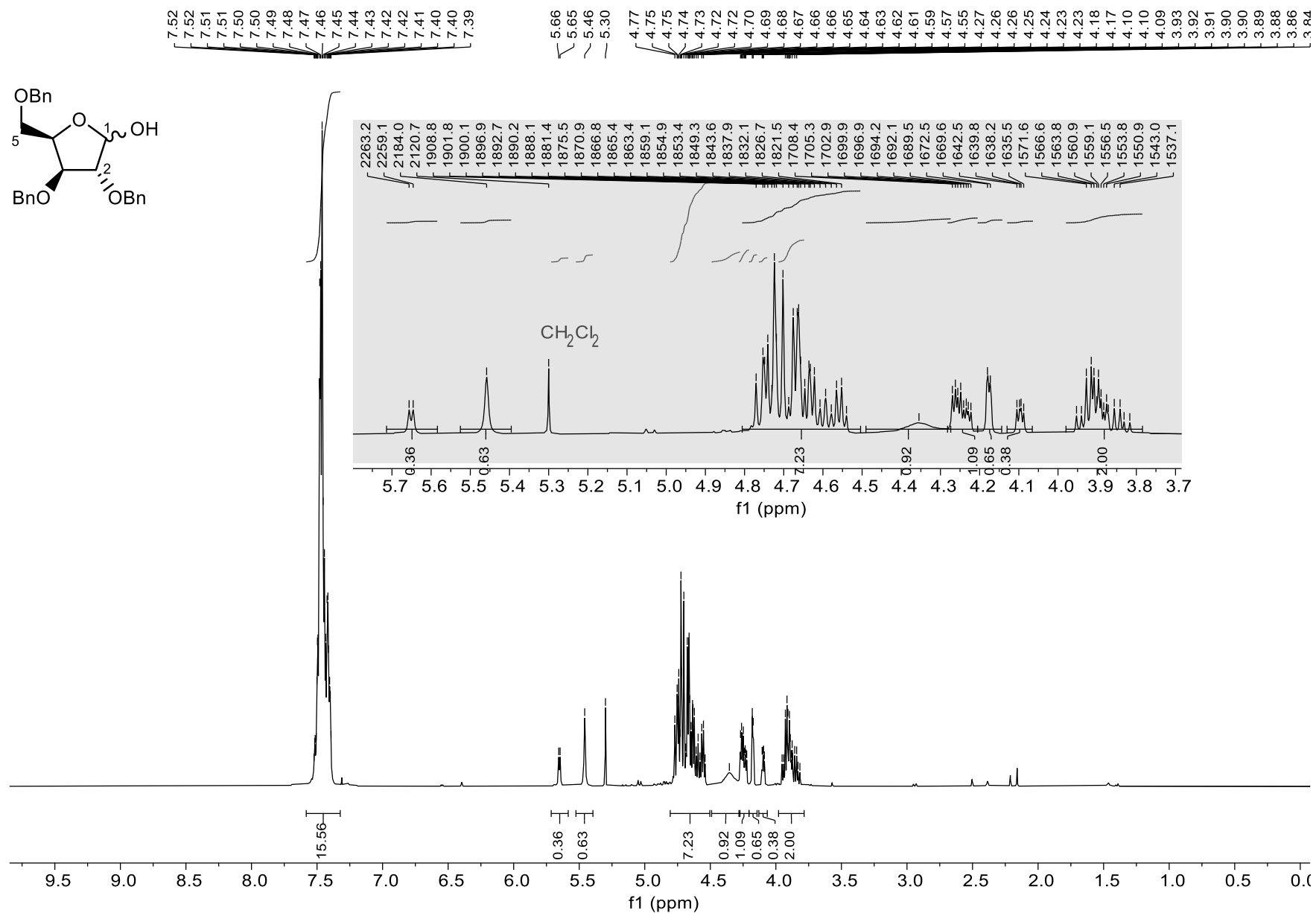
Figure S3. ^{13}C NMR (101 MHz, CDCl$_3$) Spectrum of Compound **1** (α/β *ca.* 2:3).
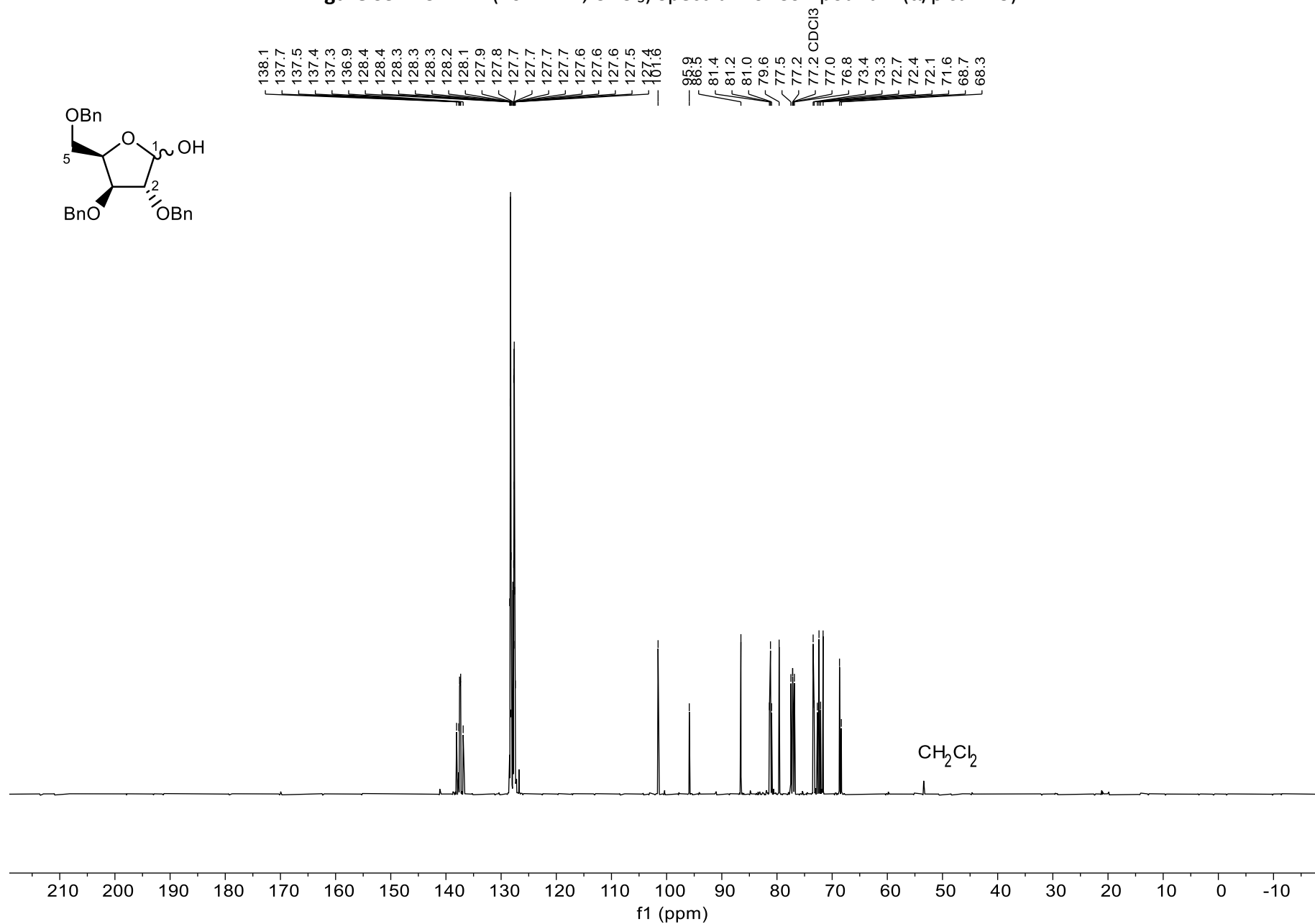
4. References.

S1.   Parsons, S.; Flack, H.D.; Wagner, T. Use of intensity quotients and differences in absolute structure refinement. *Acta Cryst.* **2013**, *B69*, 249–259. doi:10.1107/S2052519213010014

S2.   Spek, A. L. Structure validation in chemical crystallography. *Acta Cryst.* **2009**, *D65*, 148–155. doi:10.1107/S090744490804362X