Electronic Supplementary Information

for

Weak becomes strong: Remarkable strength of C-H···π hydrogen bond in the presence of O-H···O hydrogen bonds in the crystal stabilization

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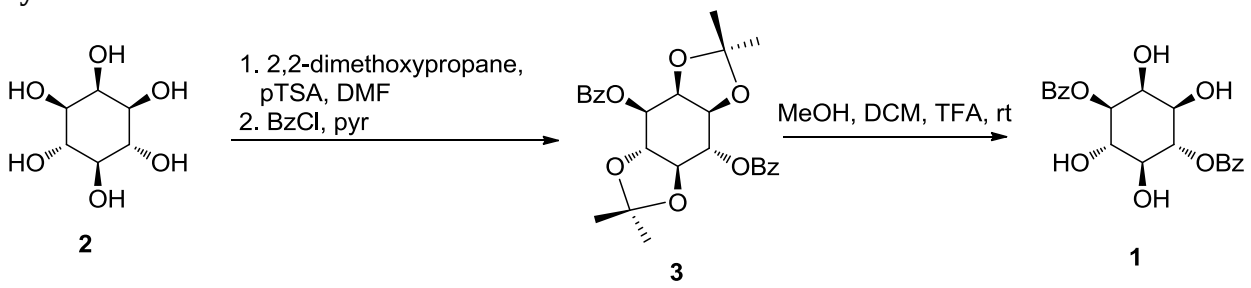
Synthesis of 1:



Myo-inositol (**2**) was converted to the dibenzoate **3** in two straightforward steps adopting the reported procedure.[1] 500 mg (1.07 mmol) of **3** was suspended in a mixture of dichloromethane and methanol (20 mL, 1:1 v/v) and 1 ml of TFA was added to this. The mixture was stirred at rt for 24 h. The solvents were evaporated under reduced pressure and the solid thus obtained was crystallized from its hot ethyl acetate solution to get colorless crystals of **1** (350 mg, 85%).

X-ray data collection and Refinement:

X-ray intensity data measurements of the compound kms_bz was carried out on a Bruker SMART APEX CCD diffractometer with graphite-monochromatized (MoK_α= 0.71073Å) radiation at room temperature [297(2) K]. The X-ray generator was operated at 50 kV and 30 mA. Data were collected with ω scan width of 0.3° at three different settings of φ (0°, 90° and 180°) keeping the sample-to-detector distance fixed at 6.145 cm and the detector position (2θ) fixed at -28°. The X-ray data collection was monitored by SMART program (Bruker, 2003).[2]

Molecular formula: $C_{20}H_{20}O_8$, M = 388.36, colorless plate, 0.18 x 0.12 x 0.08 mm^3, monoclinic, space group $P2_1/c$, a = 14.385(4), b = 11.708(4), c = 10.799(3) Å, β = 98.286(6)°, V = 1799.8(10) $Å^3$, Z = 4, T = 297 (2) K, $2\theta_{max}$=50.00°, D_{calc} (g cm^{-3}) = 1.433, $F(000)$ = 816, μ (mm^{-1}) = 0.112, 8816 reflections collected, 3150 unique reflections (R_{int}=0.0301), 2370 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.981, T_{max} = 0.991,

257 refined parameters, S = 1.031, $R1$=0.0376, $wR2$=0.0883 (all data R = 0.0560, $wR2$ = 0.0967), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.212, $\Delta\rho_{min}$= -0.125 (eÅ^{-3}).

All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2003). SHELX-97 was used for structure solution and full matrix least-squares refinement on F^2.[3] All the hydroxy H atoms were constrained to an ideal geometry [O-H = 0.82 Å and U_{iso}(H) = 1.5 U_{eq}(O)] using the AFIX 147 command integrated in SHELX-97 program. Other H atoms were placed in idealized positions (C-H = 0.98 Å for the inositol ring H atoms, C-H = 0.93 Å for the phenyl H atoms) and constrained to ride on their parent atoms [U_{iso}(H) = 1.2 U_{eq}(C)].

Molecular and packing diagrams were generated using Mercury 3.0.[4] Geometrical calculations were performed using SHELXTL (Bruker, 2003)[2] and PLATON.[5]

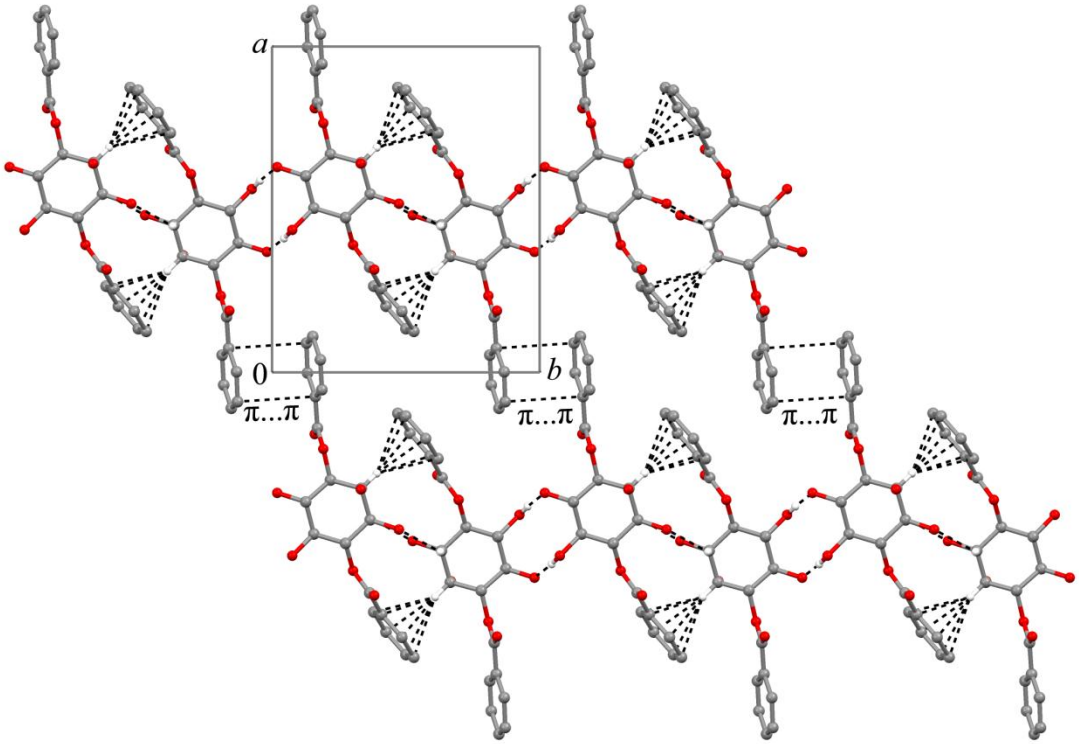


Figure S1. Packing of the spindle shaped dimers along the *a*-axis *via* aromatic π…π interactions.

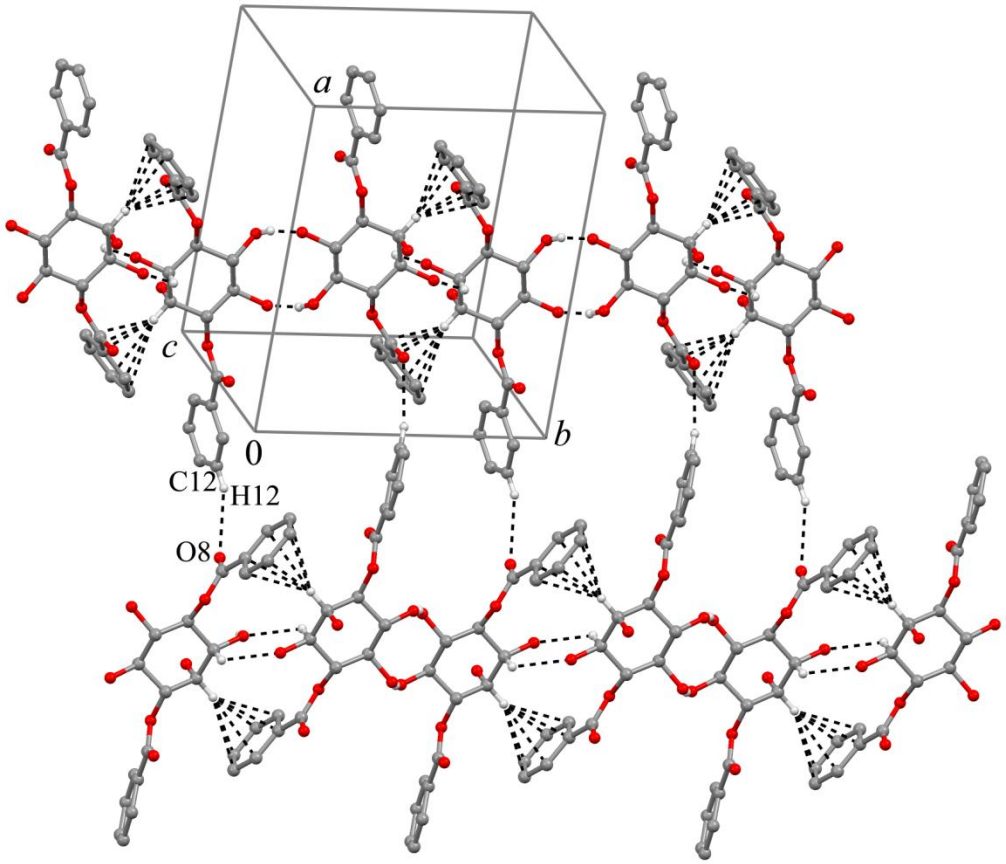


Figure S2. Packing of the spindle shaped dimers along the *a*-axis *via* aromatic C12-H12…O8 contact.

References:

[1] S. K. Chung and Y. Ryu, *Carbohydr. Res*., 1994, **258**, 145.

[2] Bruker (2003). *SADABS* (Version 2.05), *SMART* (Version 5.631), *SAINT* (Version 6.45) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.

[3] G. M. Sheldrick, *Acta Crystallogr*., 2008, A**64**, 112.

[4] F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler and J. van de Streek, *J. Appl. Crystallogr*., 2006, **39**, 453.

[5] A. L. Spek, PLATON – a multipurpose crystallographic tool, Utrecht University, The Netherlands, 2002, *Acta Crystallogr. Sect. A*, 1990, **46**, C34.