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Supporting Information

Incisive Analysis of Hydrogen-Bonded Supramolecular Architectures in designer Polycyclitols: Observation of Some Interesting Self-Assembly Patterns

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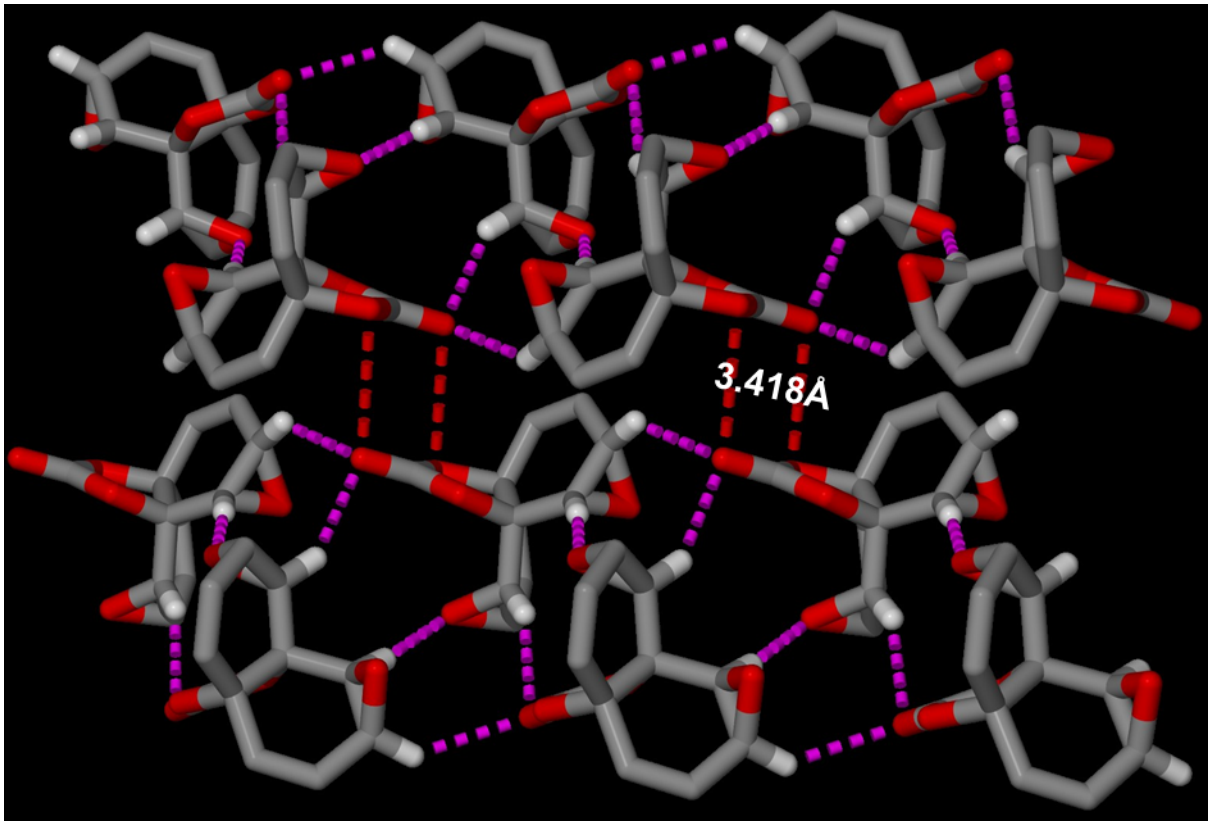

Fig. S1. The C–H···O interactions connecting neighbouring molecules to form 1D chain in the packing diagram of **10**. The 1D chains are further stacks up through cyclic dipolar interactions between the neighbouring symmetry generated molecules of **10**.

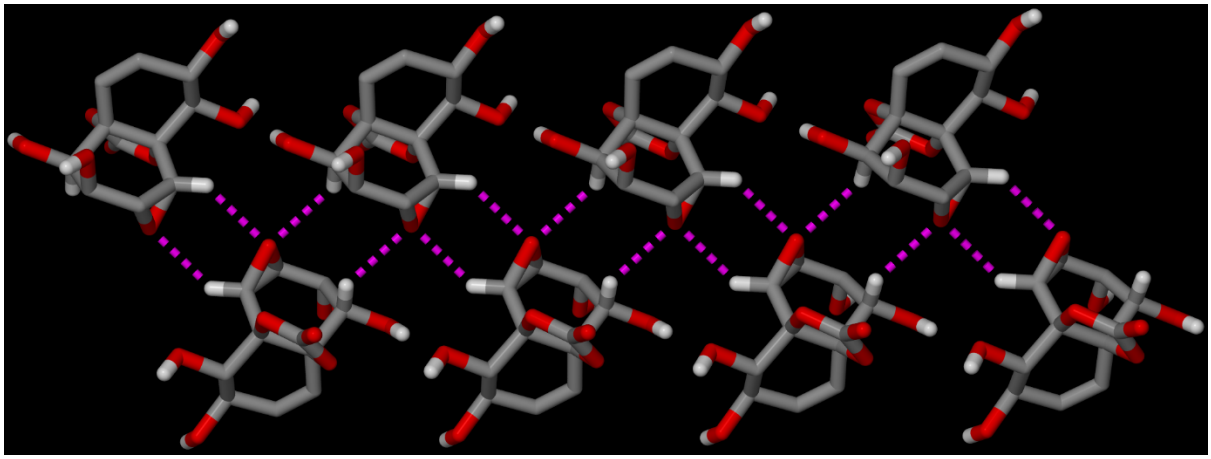

Fig. S2. Packing diagram of **11** displaying involvement of epoxide in C–H···O interactions resulting in the formation of 1D-ribbon.

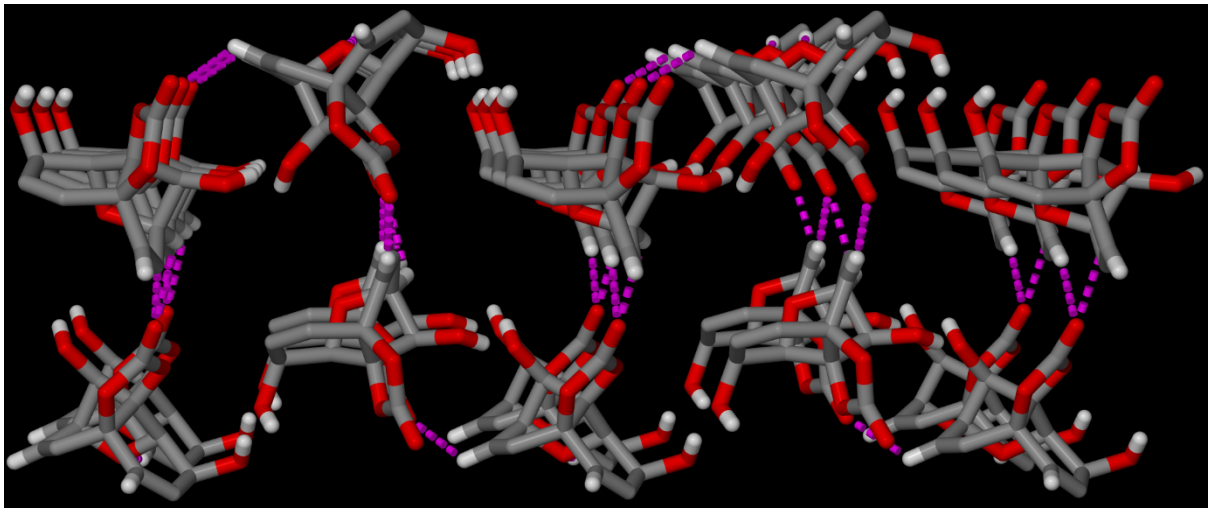

Fig. S3. The C–H···O interactions forming 2D sheets parallel to the *bc*-plane in the packing diagram of **12**.

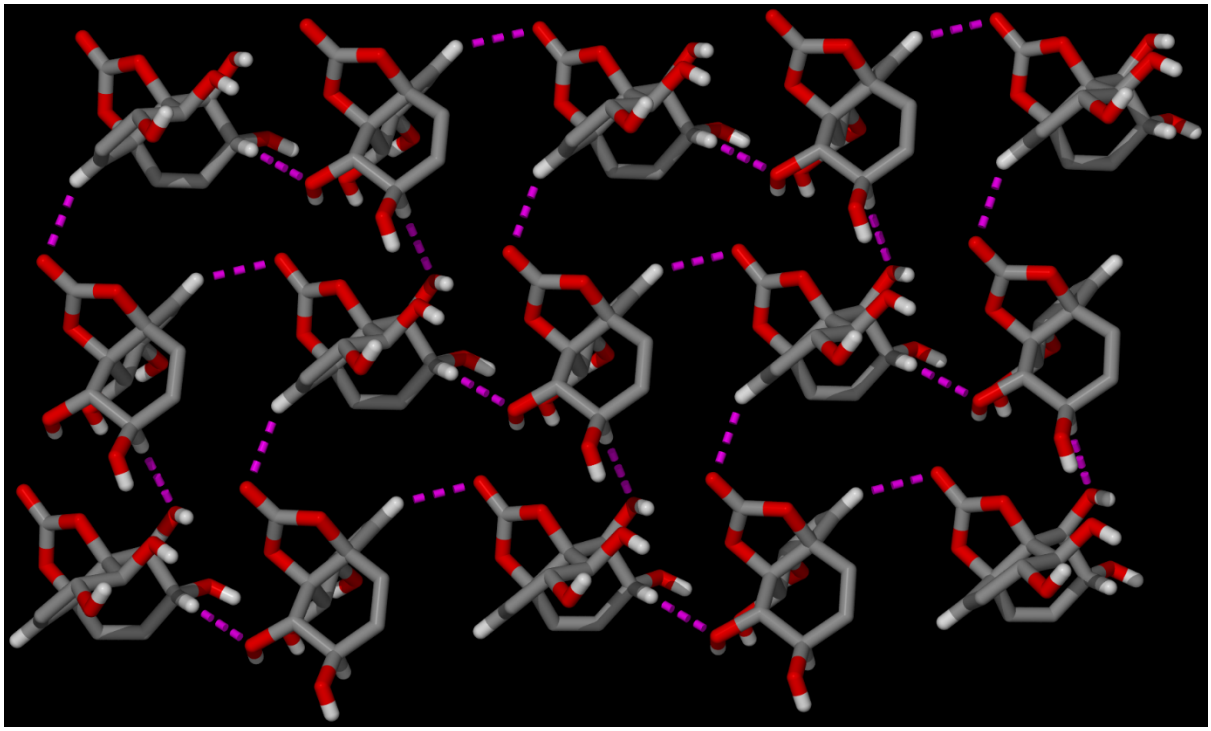

Fig. S4. The C–H···O interactions form 2D sheets viewing down *a*-axis in the packing diagram of **13**.

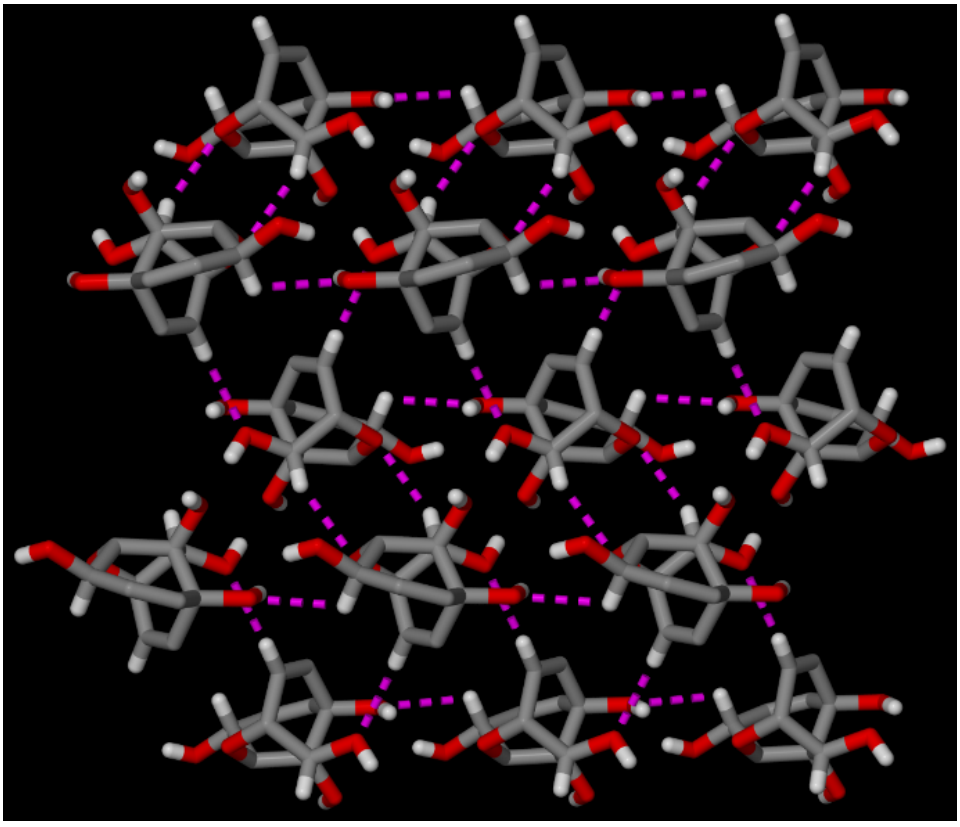

Fig. S5. The C–H···O interactions form 2D sheets viewing down the *a*-axis in the packing diagram of **14**.

Hirshfeld surface analysis

The Hirshfeld surface is unique[1] and facilitates a novel method to visualize the intermolecular interaction of molecular crystals by colour-coding short or long contacts, the colour intensity indicating the relative strength of the interactions. The Hirshfeld surfaces have been mapped over d_{norm} (-1.281 to 1.417Å) and identify the occurrence of different kinds of intermolecular interactions, which were generated using Crystal Explorer 3.0.[2] The function d_{norm} is a ratio encompassing the distances d_i and d_e. The d_e is the distance from the point to the nearest nucleus external to the surface and d_i is the distance to the nearest nucleus internal to the surface.

Table S1. Crystal data and structure refinements for polycyclitols **10-14.**

	10	**11**	**12**	**13**	**14**
CCDC number	1885547	1886483	2164511	2164510	1885526
Empirical formula	$C_{11}H_{10}O_6$	$C_{11}H_{12}O_8$	$C_{11}H_{12}O_7$	$C_{11}H_{12}O_7$	$C_{10}H_{12}O_5$
Formula weight	238.19	272.21	256.21	256.21	212.20
Crystal system	monoclinic	triclinic	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/_n$	$P\bar{1}$	$P2_1/n$	$Pca2_1$	$P2_1/n$
a [Å]	11.1420(14)	7.1276(8)	6.5680(2)	12.0789(3)	10.7437(12)
b [Å]	6.8138(8)	7.5031(8)	27.9778(8)	10.0528(2)	6.9554(7)
c [Å]	13.6024(17)	11.3065(13)	12.4818(4)	8.6569(2)	12.3782(14)
α [Å]	90	98.614(6)	90	90	90
β [Å]	102.714(4)	105.390(7)	92.584(3)	90	92.629(4)
γ [Å]	90	105.364(7)	90	90	90
Volume [Å^3]	1007.4(2)	546.16(11)	2291.30(12)	1051.17(5)	924.01(17)
Z	4	2	8	4	4
ρ_{calc} [g/cm^3]	1.571	1.655	1.485	1.619	1.525
μ [mm^{-1}]	0.130	0.144	0.126	0.138	0.123
F(000)	496	284	1072	536	448
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	Mo K_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	Mo K_α (λ=0.71073 Å)
2θ range [°]	5.34 to 55.93 (0.76 Å)	6.15 to 50.05 (0.84 Å)	4.38 to 54.56 (0.78 Å)	6.75 to 50.04 (0.84 Å)	5.14 to 50.04 (0.84 Å)
Index ranges	-14 ≤ *h* ≤ 14 -8 ≤ *k* ≤ 8 -17 ≤ *l* ≤ 17	-8 ≤ *h* ≤ 8 -8 ≤ *k* ≤ 8 -13 ≤ *l* ≤ 13	-8 ≤ *h* ≤ 8 -35 ≤ *k* ≤ 34 -15 ≤ *l* ≤ 16	-7 ≤ *h* ≤ 14 -11 ≤ *k* ≤ 11 -10 ≤ *l* ≤ 5	-12 ≤ *h* ≤ 12 -8 ≤ *k* ≤ 8 -14 ≤ *l* ≤ 14
Reflections collected	30428	15484	20101	2391	15915
Independent reflections	2409 R_{int} = 0.0888 R_{sigma} = 0.0396	1815 R_{int} = 0.0663 R_{sigma} = 0.0366	4879 R_{int} = 0.0597 R_{sigma} = 0.0523	1329 R_{int} = 0.0159 R_{sigma} = 0.0236	1606 R_{int} = 0.0235 R_{sigma} = 0.0123
Completeness to θ = 25.242°	99.9 %	94.6 %	100.0 %	99.9 %	98.7 %
Data / Restraints / Parameters	2409/0/156	1815/0/176	4879/0/335	1329/1/167	1606/0/140
Goodness-of-fit on F^2	1.067	1.143	1.091	1.092	1.097
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0502 wR_2 = 0.1093	R_1 = 0.0759 wR_2 = 0.1990	R_1 = 0.0504 wR_2 = 0.1278	R_1 = 0.0284 wR_2 = 0.0709	R_1 = 0.0350 wR_2 = 0.0867
Final *R* indexes [all data]	R_1 = 0.0756 wR_2 = 0.1188	R_1 = 0.1028 wR_2 = 0.2219	R_1 = 0.0733 wR_2 = 0.1414	R_1 = 0.0306 wR_2 = 0.0723	R_1 = 0.0365 wR_2 = 0.0878
Largest peak/hole [eÅ^3]	0.24/-0.26	0.95/-0.32	0.22/-0.28	0.13/-0.18	0.28/-0.15

Table S2. Hydrogen bond parameter for **10-14**

D–H···A [Å]	d(H···A) [Å]	d(D···A) [Å]	<(DHA) [°]
	10		
O2–H2···O6$^{\#1}$	2.08	2.829(2)	151
C2–H2A···O6$^{\#2}$	2.53	3.473(2)	161
C2–H2A···O2$^{\#3}$	2.66	3.393(2)	131
C3–H3···O2$^{\#4}$	2.64	3.443(2)	145
O1–H1···O2$^{\#5}$	2.01	2.803(2)	162
Symmetry codes: #1: 1-X, 2-Y, 1-Z; #2: -1/2+X, 3/2-Y, -1/2+Z, #3: -x+1/2, y-1/2, -z+1/2, #4: -x+1/2,+y+1/2,-z+1/2, #5: 1/2-x,-1/2+y,1/2-z.			
	11		
O1–H1···O2$^{\#1}$	1.94	2.732(5)	164
O2–H2···O8$^{\#2}$	1.90	2.700(5)	166
O3–H3···O1$^{\#3}$	2.00	2.815(5)	172
O4–H4···O3$^{\#4}$	1.95	2.762(5)	172
C8–H8···O5$^{\#5}$	2.47	3.261(7)	137
C4–H4A···O8$^{\#6}$	2.635	3.526(7)	161
Symmetry codes: #1: 1-x,2-y,-z; #2: 1+x,1+y,z; #3: x,-1+y,z; #4: 2-x,1-y,1-z; #5: -x+1,-y+2,-z+1; #6: x+1,+y,+z			
	12		
O1–H1···O14$^{\#1}$	1.85	2.664(2)	174
O2–H2···O8	1.91	2.713(2)	168
O7–H7A···O1$^{\#2}$	1.96	2.728(2)	156
O8–H8A···O13$^{\#3}$	1.87	2.674(3)	166
O13–H13A···O2	1.94	2.785(2)	173
O13–H13B···O2$^{\#4}$	2.10	2.925(3)	163
O14–H14A···O9$^{\#5}$	2.13	2.964(2)	168
O14–H14B···O7	2.11	2.949(2)	168
C17–H17···O6	2.59	3.289(3)	132
C16–H16···O9$^{\#6}$	2.66	3.455(3)	143
C5–H5···O3$^{\#6}$	2.41	3.284(2)	157
C15–H15···O6$^{\#7}$	2.51	3.431(2)	169
C1–H1A···O5$^{\#8}$	2.66	3.419(2)	134
C7–H7···O12$^{\#9}$	2.42	3.322(3)	153
Symmetry codes: #1: 1+x,y,-1+z; #2: x,y,1+z; #3: -1+x,y,z; #4: 2-x,1-y,1-z; #5: -1/2+x,3/2-y,1/2+z; #6: x-1,+y,+z; #7: x-1/2,-y+1/2+1,+z+1/2; #8: x+1,+y,+z; #9: -x+1,-y+1,-z+1			
	13		
O1–H1···O4	2.12	2.739(3)	132
O1–H1···O7$^{\#1}$	2.35	3.016(3)	139
O2–H2···O4$^{\#1}$	1.95	2.765(3)	170
O3–H3···O1$^{\#2}$	2.05	2.867(3)	177
O4–H4···O2$^{\#2}$	1.91	2.717(3)	169
C2–H2A···O1$^{\#1}$	2.56	3.538(3)	161
C1–H1A···O2$^{\#3}$	2.65	3.487(3)	144
C7–H7···O3$^{\#4}$	2.65	3.527(4)	149
C5–H5···O7$^{\#5}$	2.56	3.323(3)	140
Symmetry codes: #1: 1-x,2-y,1/2+z; #2: 1/2+x,2-y,z; #3: 1/2-x,y,1/2+z; #4: -x-1/2,+y,+z-1/2; #5: 1-x,1-y, z+1/2.			
	14		
O1–H1···O4$^{\#1}$	1.90	2.717(1)	177
O2–H2···O5$^{\#2}$	2.00	2.748(2)	151
O4–H4···O2$^{\#3}$	1.94	2.708(2)	156
O5–H5···O1	2.09	2.741(2)	136
C1–H1A···O3$^{\#4}$	2.53	3.415(2)	151
C6–H6···O1$^{\#5}$	2.69	3.614(2)	172
C3–H3···O1$^{\#6}$	2.49	3.410(2)	169
Symmetry codes: #1: 1-x,-y,1-z; #2: x,1+y,z; #3: 3/2-x,-1/2+y,3/2-z; #4: -x+1,-y+1,-z+1; #5: x+1/2,-y+1/2,+z+1/2; #6: -x+1/2+1,+y+1/2,-z+1/2.			

References

1. J. J. McKinnon, M. A. Spackman and A. S. Mitchell, Acta Crystallogr., Sect. B: Struct. Sci., 2004, 60, 627–668.
2. S.K. Wolff, D.J. Grimwood, J.J. McKinnon, M.J. Turner, D. Jayatilaka, M.A. Spackman, CrystalExplorer (Version 3.0), University of Western Australia, 2012.