SUPPORTING INFORMATION

for

RING SIZE EFFECT ON THE SOLID STATE ASSEMBLY AND INCLUSION PROPERTIES OF PROPARGYL SUBSTITUTED HEXA AND OCTA CYCLIC PEPTOIDS

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LIST OF ABBREVIATIONS

**DMSO**  dimethylsulfoxide

**Npa**  \(N\)-(propargyl)glycine
Figure S1. (a) ORTEP with numbering scheme for the cyclopeptoid molecule Cyclo-(Npa)$_6$ 1 (a) in crystal form 1A and (b) in crystal form 1B.
Figure S2. (a) Superposition of the backbone atoms of cyclopeptoid molecules in crystal form 1A with idealized type III beta-turn peptide (magenta), rmsd 0.344 Å; (b) superposition of the backbone atoms of cyclopeptoid molecules in crystal form 1B with idealized type III beta-turn peptide (magenta), rmsd 0.369 Å.
Figure S3. Rectangular shape of cyclic peptoid backbone in crystal form 1B. Four cis amide bonds reside at each corner, trans amide bonds are located on two opposing sides.
Figure S4. Hirshfeld surface for the cyclopeptoid molecule mapped with $d_{\text{norm}}$ (a) in crystal form 1A and (b) in crystal form 1B as viewed along the $c$ axis. $a$ and $b$ cell axes are, respectively, red and green.
Figure S5. (a) Intralayer CO···HC (green dotted lines), CH-pi (light blue dotted lines) and π-π interactions (blue dotted lines) in 1A; (b) Intralayer CO···HC (green dotted lines) and CH-pi interactions (light blue dotted lines) in 1B.
Figure S6. Void space available for guest molecules in crystal forms 1A (left) and 1B (right) as viewed along the $b$ axis.
Figure S7. (a) Superposition of the backbone atoms of cyclopeptoid molecules in crystal form 2A with idealized type III beta-turn peptide (magenta), rmsd 0.359 Å.

Figure S8. Guest accessible voids in crystal form 2A as viewed along the b axis (perspective view).
Figure S9. (a) Molecular overlay between crystal forms 2A (blue) and 2B (green), rmsd 0.1325 Å; (b) molecular overlay between crystal forms 2A (blue) and 2C (magenta), rmsd 0.1956 Å; (c) molecular overlay between crystal forms 2A (blue) and 2D (orange), rmsd 0.0563 Å.
Figure S10. Crystal packing of forms 2A (a), 2B (b), 2C (c), and 2D (d) as viewed along the b axis. Guest molecules are depicted as ball-and-sticks, methanol molecules in blue and water molecules in red.