Supporting Information

Nanotubular Non-covalent Macrocycle within Non-covalent Macrocycle Assembly: $(MeOH)_{12}$ Encapsulated in a Molecular Clip Cyclododecamer

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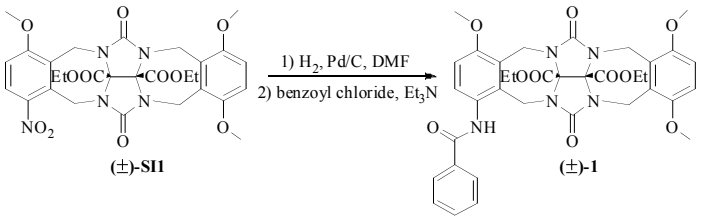
1. Experimental procedure for (±)-1–3:

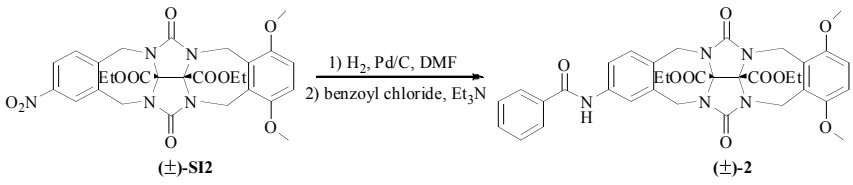
1.1 General.

Compounds **SI1**,[1] **SI2**,[1] **SI3**,[2] and *N*-(4-ethynylphenyl)acetamide[3] were prepared according to the literature procedures. Anhydrous CH_2Cl_2 and DMF were obtained by distillation of the commercial materials from CaH_2 and 4Å molecular sieves, respectively. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (230-400 mesh, 40-63 μm) using eluents in the indicated v:v ratio. IR spectra were recorded on a PE-983 spectrophotometer as KBr pellets and are reported in cm^{-1}. Melting points were determined using XT-4 apparatus and were not corrected. ^1H and ^{13}C-NMR spectra were recorded on a Varian Mercury 400 or 600 spectrometer operating at 400 or 600 MHz and 100 or 150 MHz, respectively. Chemical shifts are reported in ppm, relative to the internal standard of tetramethylsilane (TMS). Electron impact (EI) mass spectra were acquired using a Finnegan Trace MS spectrometer. HRMS were obtained on a Bruker 7-tesla FT-ICR MS equipped with an electrospray source (Billelica, MA, USA). The X-ray crystal-structure determinations of (±)-**1–3** were obtained on a Bruker SMART APEX CCD system.

1.2 Synthetic Procedures and Characterization.

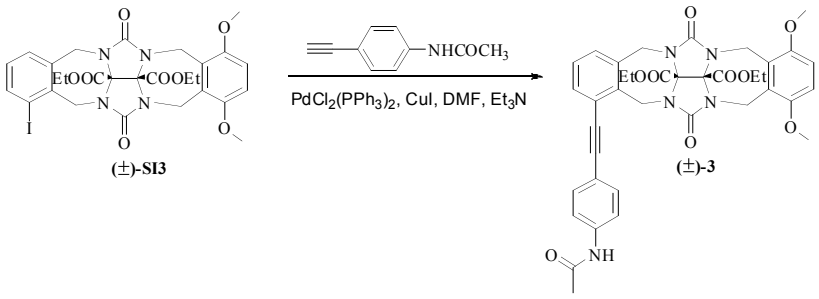


Compound (±)-1: A mixture of (±)-**SI1** (62.5 mg, 0.10 mmol) and 10% Pd/C (20 mg) in anh. DMF (5 mL) was stirred under H_2 (10-20 psi) at RT for 5 h. The reaction mixture was filtered under Ar, and concentrated under high vacuum at RT. The residue was dissolved in a mixture of anh. degassed CH_2Cl_2 (10 mL) and Et_3N (0.05 mL, 0.30 mmol). This solution was added to a solution of benzoyl chloride (14 μL, 0.11 mmol) in anh. degassed CH_2Cl_2 (10 mL) at -78 °C. After 15 min., the cooling bath was removed and stirring was continued at RT for 12 h. The reaction mixture was diluted with $CHCl_3$ (200 mL), washed with sat. aq. $NaHCO_3$, dried over anh. $MgSO_4$, and concentrated. Flash chromatography (SiO_2, $CHCl_3$/MeOH, 50:1) gave slightly impure (±)-**1** (63 mg, 0.090 mmol, 90%). To get highest purity material, the white solid was washed with EtOAc (1.0 mL), centrifuged, the supernatant decanted, and the residual solid dried under high vacuum yielding (±)-**1** (55 mg, 0.080 mmol, 80%). M.p. > 300 °C (dec.). TLC ($CHCl_3$/MeOH 50:1) R_f 0.35. IR (KBr, cm^{-1}): 3443w, 2987w, 2840w, 1751s, 1740s, 1707s, 1660m, 1599w, 1523m, 1472s, 1437s, 1360m, 1307s, 1195w, 1155m, 1136w, 1077s, 1020m, 943m, 913m. ^1H NMR (600 MHz, $CDCl_3$): δ 9.53 (s, 1H), 8.13 (d, J = 7.2 Hz, 2H), 7.61 (d, J = 9.0 Hz, 1H), 7.57-7.52 (m, 3H), 6.85 (d, J = 8.4 Hz, 1H), 6.71 (s, 2H), 5.64 (d, J = 16.8 Hz, 1H), 5.10 (d, J = 15.6 Hz, 1H), 5.06 (d, J = 16.2 Hz, 1H), 4.93 (d, J = 16.2 Hz, 1H), 4.41 (d, J = 15.6 Hz, 1H), 4.36 (d, J = 15.6 Hz, 1H), 4.29 (q, J = 7.2 Hz, 2H), 4.21 (d, J = 16.2 Hz, 1H), 4.09 (q, J = 6.6 Hz, 2H), 4.01 (d, J = 16.2 Hz, 1H), 3.84 (s, 3H), 3.77 (s, 3H), 3.76 (s, 3H), 1.33 (t, J = 7.2 Hz, 3H), 1.22 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.9, 165.8, 165.7, 157.9, 155.9, 154.3, 150.9, 150.5, 133.9, 131.7, 131.4, 129.9, 128.6, 127.4, 126.6, 126.5, 126.0, 125.5, 111.8, 111.7, 111.7, 80.6, 80.4, 63.5, 63.1, 56.5, 56.4, 56.2, 40.4, 37.5, 37.1, 36.7, 13.9, 13.8. HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{36}H_{37}N_5O_{10}Na$: 722.2433; found: 722.2421.



(±)-SI2 (±)-2

Compound (±)-2: A mixture of (±)-**SI2** (59.5 mg, 0.10 mmol) and 10% Pd/C (20 mg) in anh. DMF (5 mL) was stirred under H_2 (10-20 psi) at RT for 5 h. The reaction mixture was filtered under Ar, and concentrated under high vacuum at RT. The residue was dissolved in a mixture of anh. degassed CH_2Cl_2 (10 mL) and Et_3N (0.05 mL, 0.30 mmol). This solution was added to a solution of benzoyl chloride (14 μL, 0.11 mmol) in anh. degassed CH_2Cl_2 (10 mL) at -78 °C. After 15 min., the cooling bath was removed and stirring was continued at RT for 12 h. The reaction mixture was diluted with $CHCl_3$ (200 mL), washed with sat. aq. $NaHCO_3$, dried over anh. $MgSO_4$, and concentrated. Flash chromatography (SiO_2, $CHCl_3$/MeOH, 50:1) gave slightly impure (±)-**2** (52 mg, 0.078 mmol, 78%). To get highest purity material, the white solid was washed with EtOAc (1.0 mL), centrifuged, the supernatant decanted, and the residual solid dried under high vacuum yielding (±)-**2** (47 mg, 0.071 mmol, 71%). M.p. > 300 °C (dec.). TLC ($CHCl_3$/MeOH 50:1) R_f 0.37. IR (KBr, cm^{-1}): 3362m, 2905w, 2838w, 1762s, 1736s, 1708s, 1663m, 1596m, 1538m, 1503w, 1471s, 1428m, 1361w, 1315m, 1259s, 1156m, 1136w, 1081s, 1016w, 976w. ^{1}H NMR (600 MHz, DMSO-d_6): δ 10.25 (s, 1H), 7.91 (d, J = 7.8 Hz, 2H), 7.72 (s, 1H), 7.60-7.57 (m, 2H), 7.51 (t, J = 7.8 Hz, 2H), 7.22 (d, J = 8.4 Hz, 1H), 6.83 (s, 2H), 5.17 (d, J = 5.6 Hz, 2H), 4.57-4.46 (m, 4H), 4.28 (q, J = 7.2 Hz, 2H), 4.20 (q, J = 7.2 Hz, 2H), 4.12 (d, J = 15.0 Hz, 2H), 3.70 (s, 3H), 3.69 (s, 3H), 1.27 (t, J = 7.2 Hz, 3H), 1.23 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, DMSO-d_6): δ 165.6, 165.5, 155.3, 150.5, 138.6, 138.5, 137.6, 137.1, 134.8, 134.7, 132.3, 131.7, 129.9, 128.5, 127.7, 126.6, 126.6, 113.3, 112.4, 112.3, 80.1, 80.0, 63.6, 63.4, 56.6, 56.5, 45.0, 44.3, 36.4, 13.9, 13.8 (only 31 of the 33 expected resonances were observed). HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{35}H_{35}N_5O_9Na$: 692.2327; found: 692.2316.



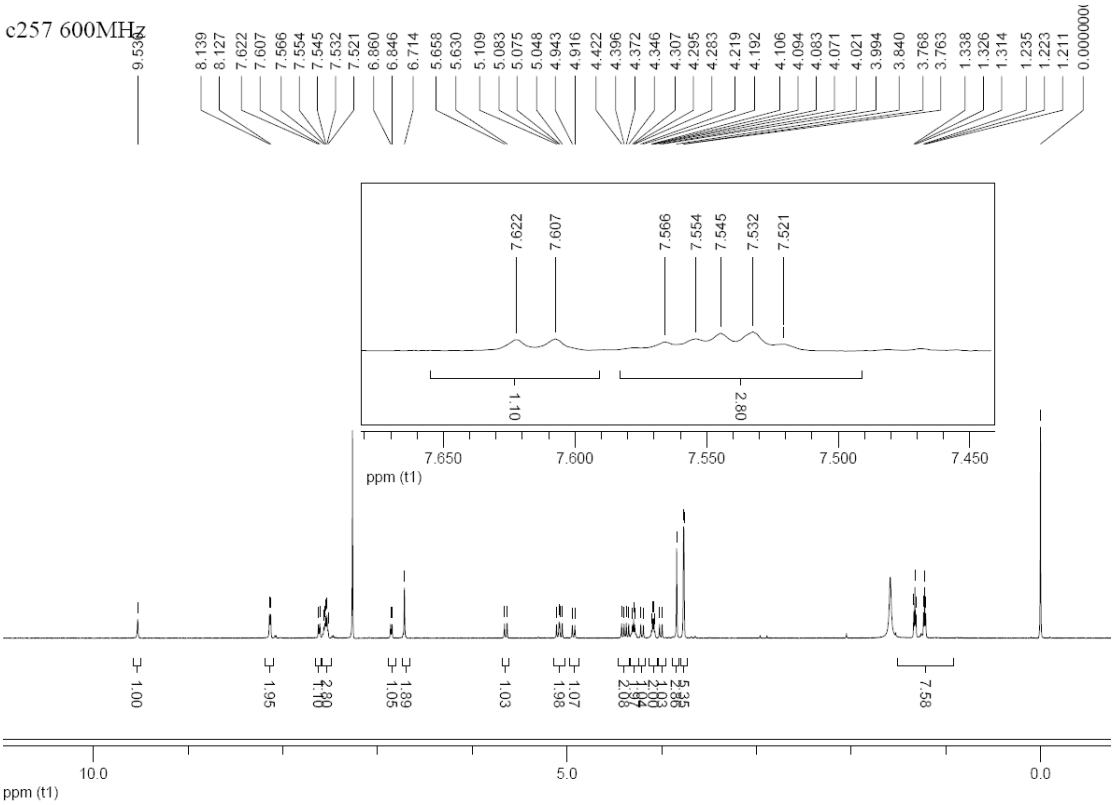
(±)-SI3 (±)-3

Compound (±)-3: To a solution of $PdCl_2(PPh_3)_2$ (18 mg, 0.025 mmol), CuI (9.5 mg, 0.050 mmol) and (±)-**SI3** (135 mg, 0.20 mmol) in freshly distilled Et_3N (10 mL) and DMF (10 mL) under Ar atmosphere at RT, were added *N*-(4-ethynylphenyl)acetamide (40 mg, 0.25 mmol). The mixture was heated at 80 °C for 12 h (monitored by TLC), the solvent was removed under reduced pressure, and the solid residue was purified by flash chromatography (SiO_2, $CHCl_3$/MeOH, 50:1) to give (±)-**2** (123 mg, 0.170 mmol, 87%) as a white solid. To get highest purity material, the white solid was washed with EtOAc (1.0 mL), centrifuged, the supernatant decanted, and the residual solid dried under high vacuum yielding (±)-**3** (111 mg, 0.154 mmol, 79%). M.p. >300 C. TLC ($CHCl_3$/MeOH, 25:1) R_f 0.22. IR (KBr, cm^{-1}): 3443s, 2924w, 1732s, 1713s, 1650m, 1635m, 1521m, 1463s, 1259s, 1083m. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.19 (s, 1H), 7.68 (d, J =8.4 Hz, 2H), 7.53 (d, J =8.4 Hz, 2H), 7.37 (d, J = 7.6 Hz, 1H), 7.29 (d, J = 7.6 Hz, 1H), 7.21 (t, J = 7.6, 1H), 6.83(s, 2H), 5.41 (d, J = 16.0 Hz, 1H), 5.16 (d,

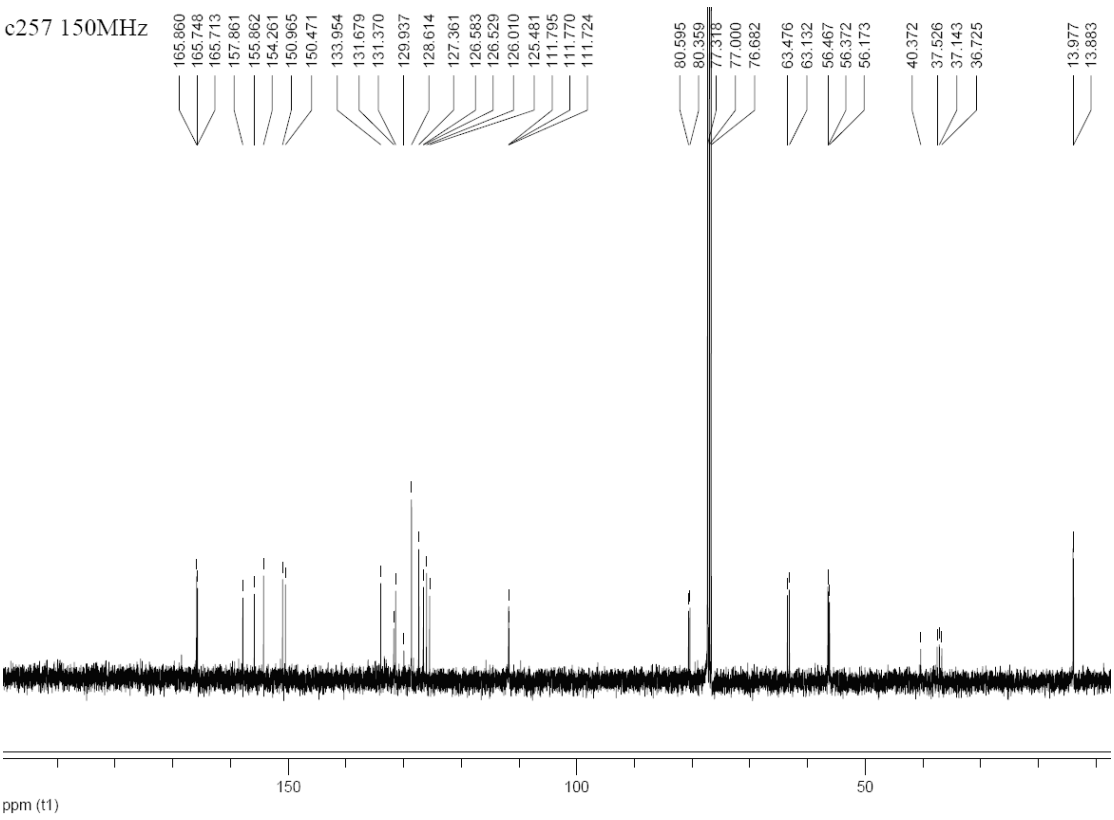
J = 15.6 Hz, 1H), 5.15(d, *J* = 16.4 Hz, 1H), 4.64-4.49 (m, 3H), 4.27-4.11 (m, 6H), 3.70 (s, 3H), 3.69(s, 3H), 2.08(s, 3H), 1.27 (t, *J* = 7.2 Hz, 3H), 1.23 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.7, 165.4, 165.3, 155.3, 155.2, 150.3, 150.2, 139.9, 138.6, 137.9, 132.1, 131.2, 130.0, 127.8, 126.4, 122.6, 118.8, 116.3, 112.2, 112.1, 111.9, 93.8, 86.5, 80.0, 79.8, 63.6, 63.4, 56.4, 56.3, 44.9, 41.6, 36.5, 36.3, 24.2, 13.8, 13.7. EI-MS: *m/z* 708 (M+1, 100).

2. ^{1}H and ^{13}C NMR spectra for (±)-1–3:

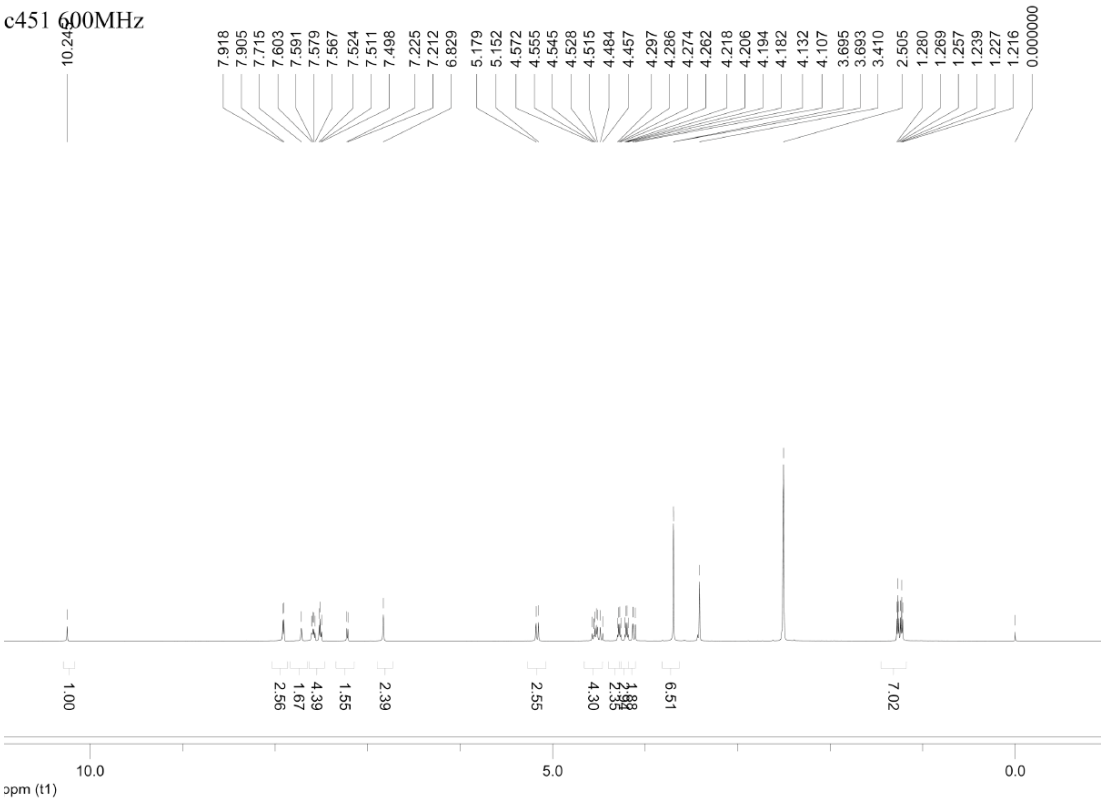
^{1}H NMR of Compound (±)-**1** ($CDCl_3$, 600 MHz)



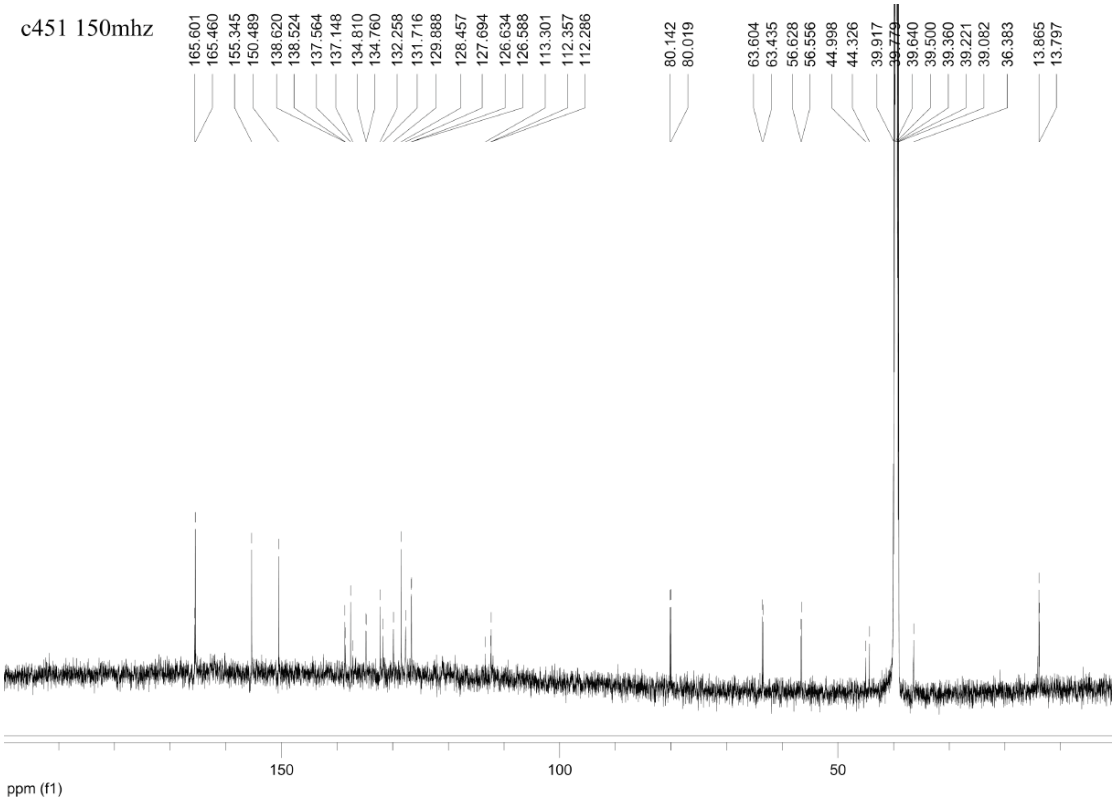
^{13}C NMR of Compound (±)-**1** ($CDCl_3$, 150 MHz)



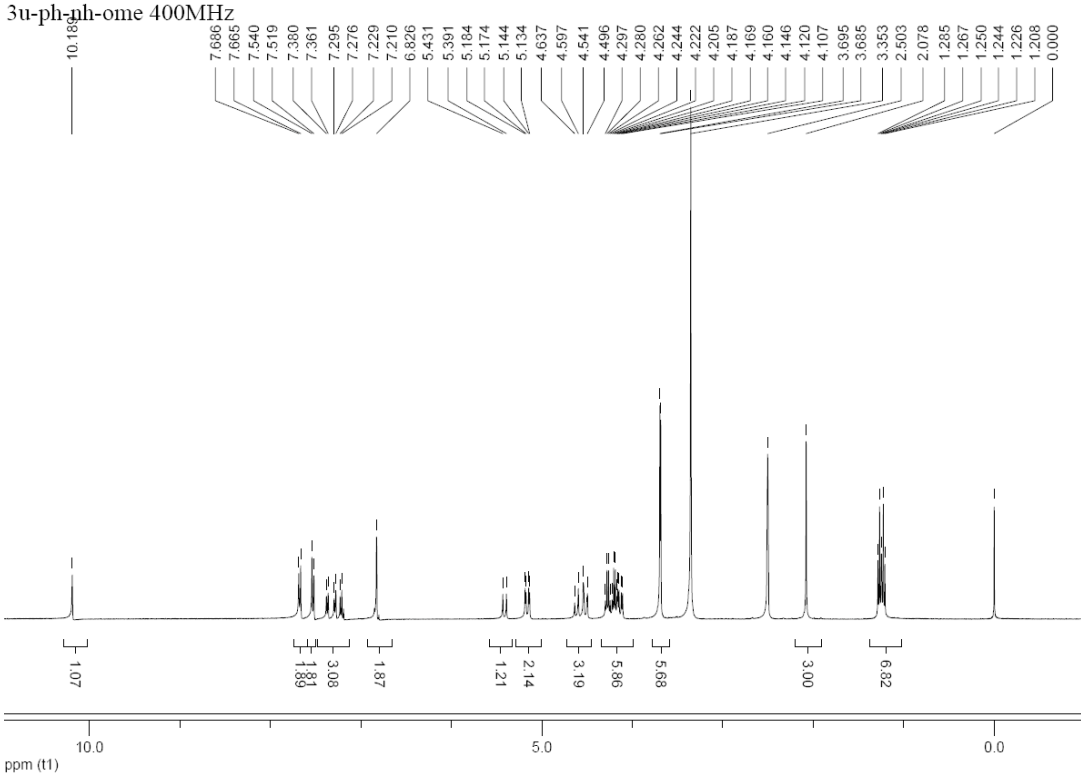
^{1}H NMR of Compound (±)-**2** (DMSO, 600 MHz)



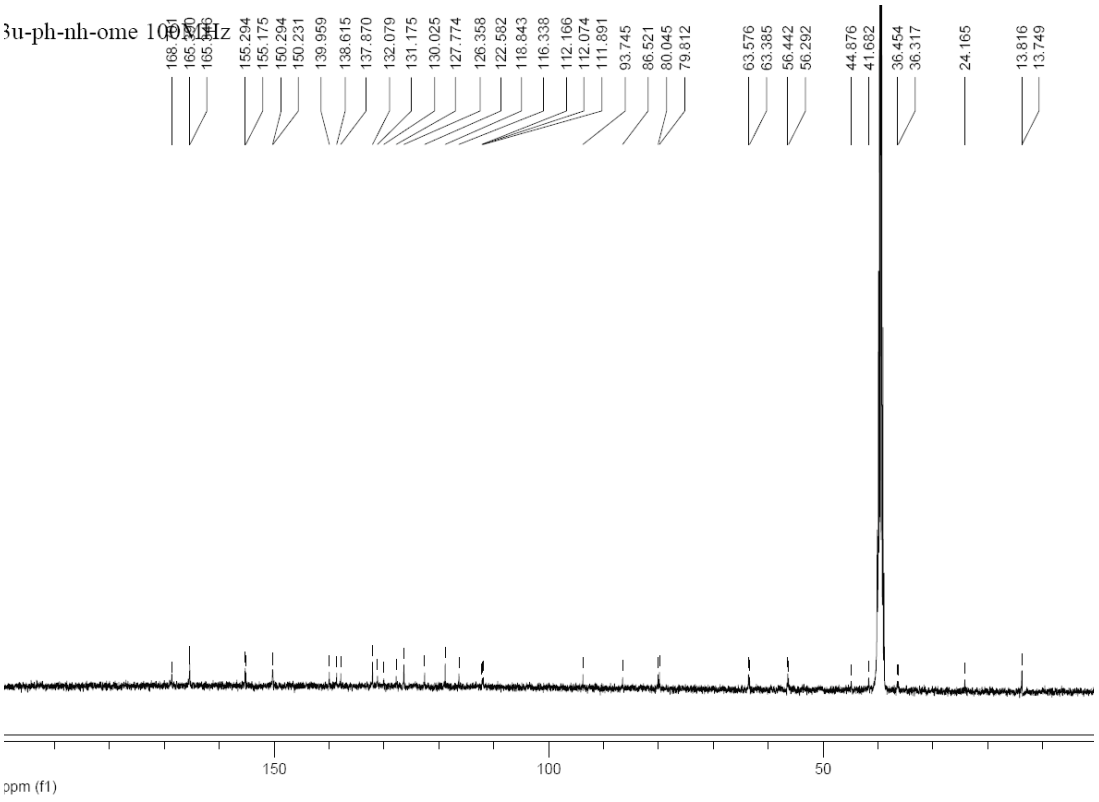
^{13}C NMR of Compound (±)-**2** (DMSO, 150 MHz)



^{1}H NMR of Compound (±)-**3** (DMSO, 600 MHz)



^{13}C NMR of Compound (±)-**3** (DMSO, 150 MHz)



3. Analysis of (±)-1–3 in crystalline state:

3.1 Crystallographic Summary.

Single crystal of (±)-**1** suitable for X-ray diffraction were grown from the CH_2Cl_2, MeOH and a small amount of H_2O. The intensities of 4656 independent reflections with $I > 2\sigma(I)$ were measured on a Bruker Smart Apex CCD area-detector diffractometer with Mo-Kα radiation (λ = 0.71073 Å). The structure was solved by direct methods and refined on F^2 using SHELXL-97. All the non-hydrogen atoms were refined anisotropically. Carbon bound H-atoms were located at the geometrical positions. Hydrogen atoms bonded to nitrogen and oxygen atoms were found from the difference maps with the constraints of N-H = 0.86(1) Å, O-H = 0.82(1) Å and H_{water}-H_{water}=1.35(2) Å, respectively (note: DFIX and SADI commands were used during the refinement). The CH_2Cl_2 solvent molecules were symmetrically disordered by a 6-fold axis. The ethyl group containing C13 and C14 atoms was disordered over two positions with the final satisfactory occupancies being 0.65(1):0.35(1) for the major and minor components, respectively. Calculation by the aid of *Platon 2003* shows that a 362.2 $Å^3$ void existed in the crystal lattice which should be occupied by water solvent molecules. Attempts were made model the missing water solvents, but we are failed owing the weak diffraction of the selected crystal. However, the missing water molecule was included in the formula and some related items as below. In (±)-**3**, the methanol molecules are seriously disordered. During the final refinement, the contribution of the solvent molecules to the crystal structure is treated by using the *Platon/SQUEEZE* procedure. Check using platon shows that there are 458 $Å^3$ volumes in the unit cell (approximately 84 electrons, i.e. ca. 4.66 methanol molecules based on the solvents we have used and each host molecule was distributed 1.16 methanol molecules). So the suitable formula should be $C_{38}H_{37}N_5O_9 \cdot (MeOH)_{1.16}$. Some related items have been corrected in the cif file.

Crystal data for (±)-**1**$\cdot(MeOH)_{3.00}\cdot(CH_2Cl_2)_{0.18}\cdot(H_2O)_2$: $C_{39.17}H_{51.68}Cl_{0.34}N_{5.00}O_{14.17}$, M_r = 828.29. rhombohedral, space group $R\bar{3}$, a = 36.4925(4), b = 36.4925(4), c = 16.5404(3) Å, Z = 3, V = 19075.8(5) $Å^3$, D_c = 1.298 g cm^{-3}, μ = 0.119 mm^{-1}, θ_{max} = 25.00°, F(000) = 8048, reflections collected/unique, 15964/7380 (R_{int} = 0.0938), final R indices [$I > 2\sigma(I)$] R_1 = 0.0769, wR_2 = 0.2046, R indices (all data) R_1 = 0.1128, wR_2 = 0.2262, GOF = 0.978 for all data.

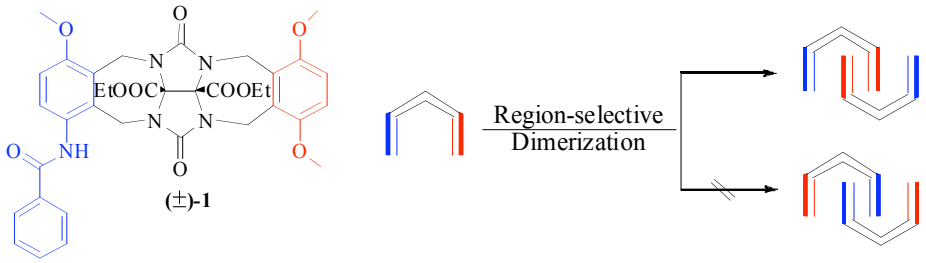
Crystal data for (±)-**2**: $C_{35}H_{35}N_3O_9$, M_r = 669.68. monoclinic, space group $P2_1/n$, a = 10.9776(9), b = 18.8944(16), c = 16.5449(14) Å, Z = 4, V = 3284.5(5) $Å^3$, D_c = 1.354 g cm^{-3}, μ = 0.099 mm^{-1}, θ_{max} = 25.00°, F(000) = 1408, reflections collected/unique, 19350/5766 (R_{int} = 0.0564), final R indices [$I > 2\sigma(I)$] R_1 = 0.0864, wR_2 = 0.1888, R indices (all data) R_1 = 0.1246, wR_2 = 0.2095, GOF = 1.153 for all data.

Crystal data for (±)-**3**$\cdot(MeOH)_{1.16}$: $C_{39.16}H_{41.65}N_5O_{10.16}$, M_r = 744.91. monoclinic, space group $P2_1/c$, a = 9.9808(16), b = 12.1396(19), c = 32.044(5) Å, Z = 4, V =

3852.4(11) Å^3, D_c = 1.284 g cm^{-3}, μ = 0.094 mm^{-1}, θ_{max} = 25.5°, F(000) = 1570, reflections collected/unique, 28041/7122 (R_{int} = 0.0517), final R indices [$I > 2\sigma(I)$] R_1 = 0.0709, wR_2 = 0.1660, R indices (all data) R_1 = 0.1063, wR_2 = 0.1846, GOF = 1.048 for all data.

CCDC 756893–756895 for (±)-**3**·$(MeOH)_{1.16}$, (±)-**2**, and (±)-**1**·$(MeOH)_{3.00}$·$(CH_2Cl_2)_{0.18}$·$(H_2O)_2$, contain the supplementary crystallographic data for this paper, respectively. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request /cif.

3.1 Analysis of (±)-1 in crystalline state.



Scheme S1. Schematic representations of the regio-selective dimerization of clip (±)-**1** in crystallographic state. Color code: red, dimethoxyxylyene wall; blue, amide-substituted xylyene wall.

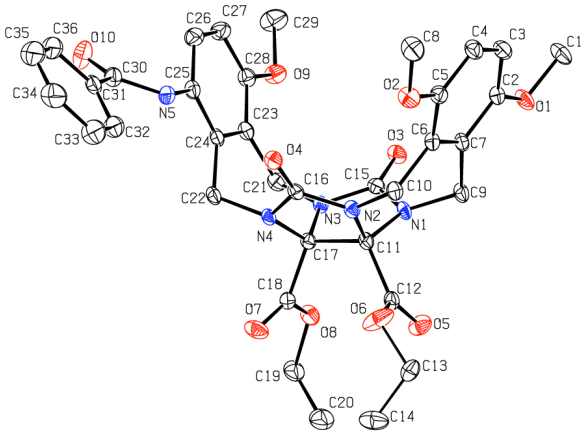


Figure S1. ORTEP drawing and atom numbering for (±)-**1**. Thermal ellipsoids are drawn at the 30% probability level. Solvent molecules and H atoms have been omitted for clarity. Colour code: C, gray; N, blue; O, red.

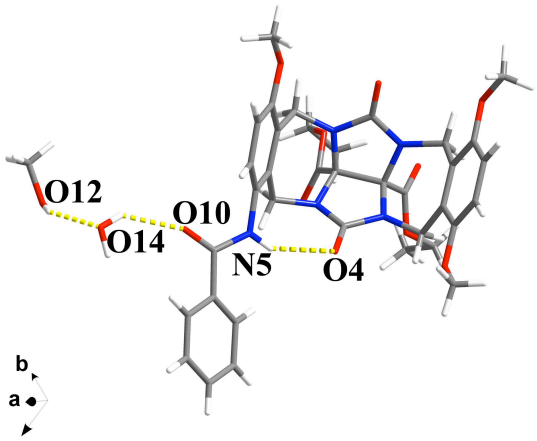


Figure S2. Details of H-bonds among clip, water, and methanol including intermolecular O12–H12•••O14, O14–H14H•••O10 and intramolecular N5–H5•••O4 H-bonds (yellow dotted lines). Colour code: C, gray; H, white; N, blue; O, red.

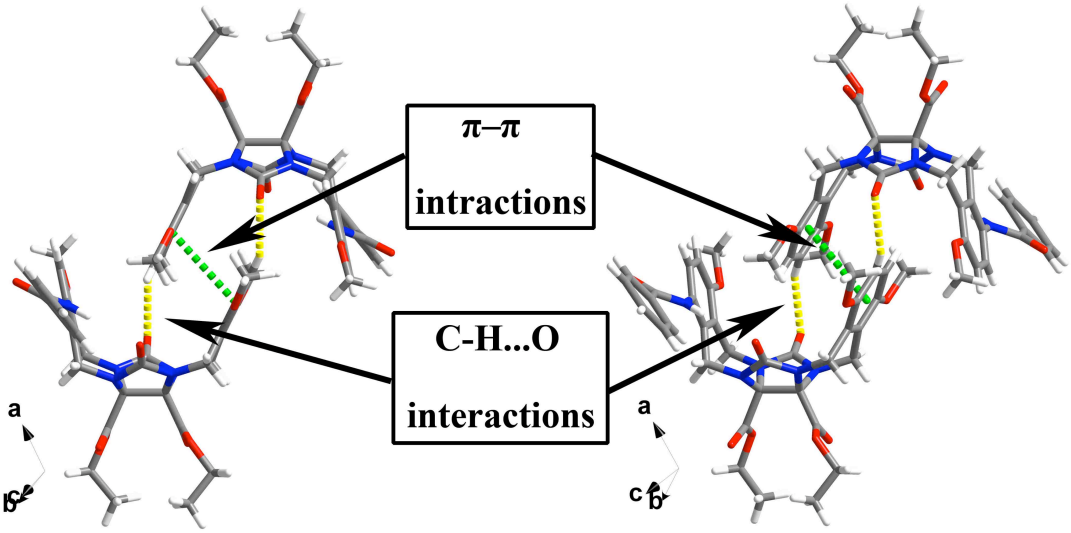


Figure S3. Details of H-bonds of the bimolecular synthon (+)-**1**•(–)-**1** including C4–H4•••O3 and interactions (yellow dotted lines) and π–π interactions (green dotted lines)**.** Colour code: C, gray; H, white; N, blue; O, red.

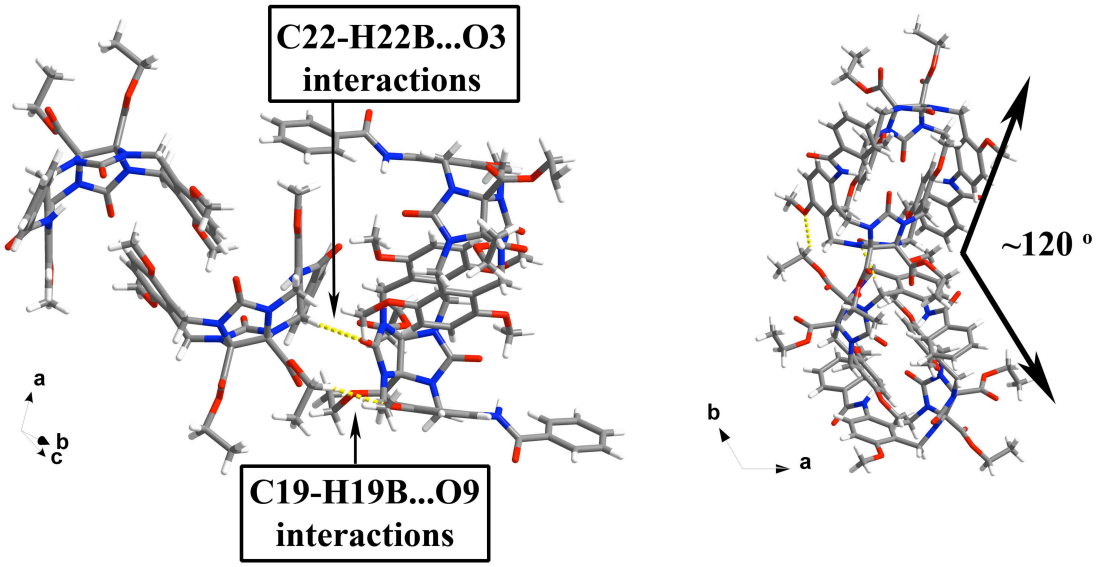


Figure S4. Details of H-bonds between the bimolecular synthons ($Clip_2$) including C22–H22B•••O3 and C19–H19B•••O9 interactions (yellow dotted lines)**.** Colour code: C, gray; H, white; N, blue; O, red.

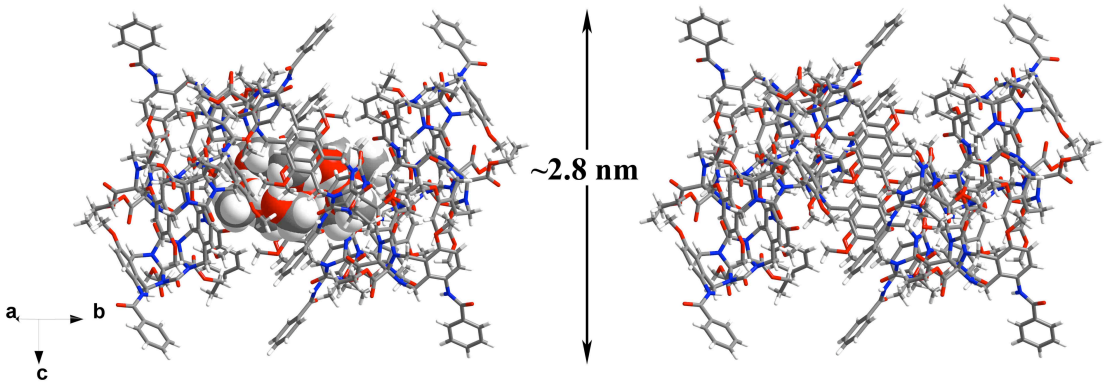


Figure S5. Side view of the packing of the supramolecular ring [$(Clip_2)_6$] assembled by six bimolecular synthons ($Clip_2$) parallel to c axis (right). Space filling model of twelve methanol molecules built in the supramolecular ring (left). Colour code: C, gray; H, white; N, blue; O, red.

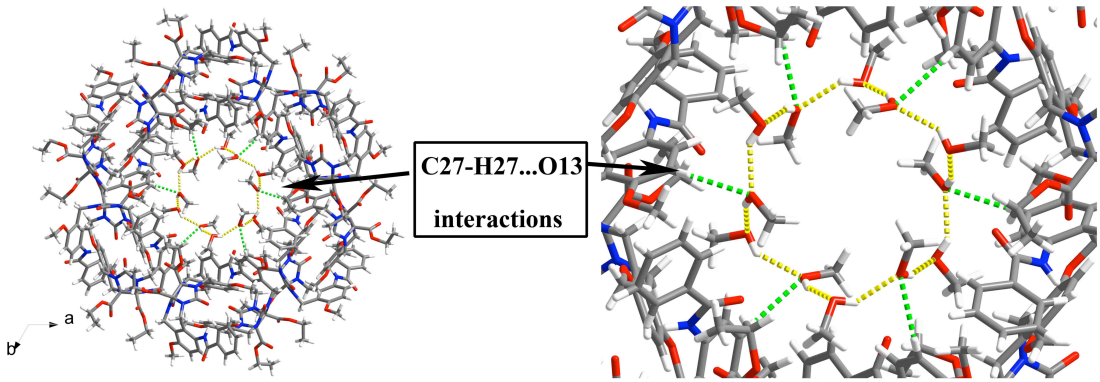


Figure S6. Details of H-bonds between the outer supramolecular rings and the inner methanol cluster in $(MeOH)_{12}@(Clip_2)_6$ including C27–H27•••O13 H-bonds (green dotted lines)**.** H-bonds of the methanol cluster: yellow dotted lines. Colour code: C, gray; H, white; N, blue; O, red.

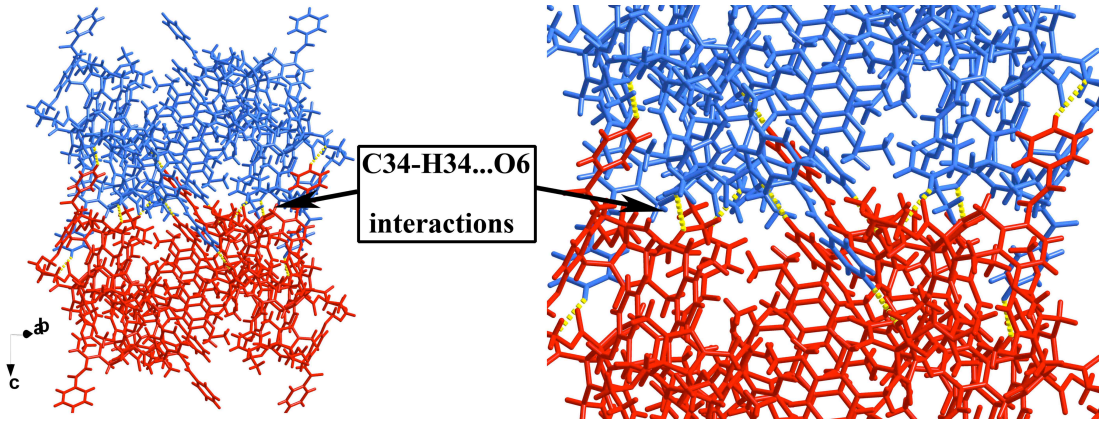


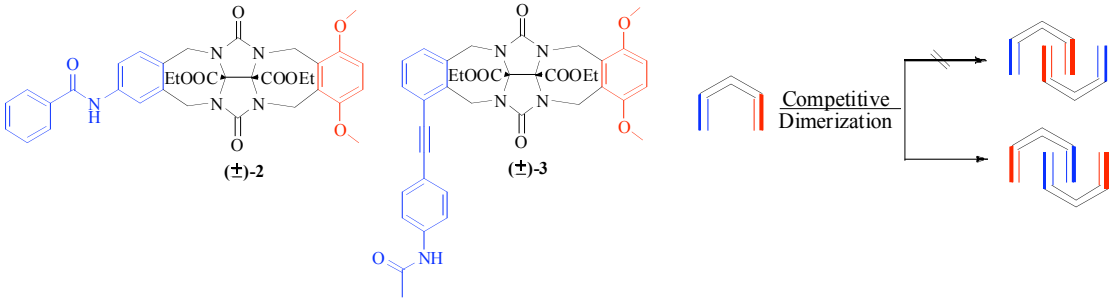
Figure S7. Details of H-bonds between supramolecular rings $(Clip_2)_6$ including twelve C34–H34•••O6 H-bonds (yellow dotted lines). Colour code: C, gray; H, white; N, blue; O, red.

Table S1. Hydrogen bonds for (±)-**1** [Å and °].

D-H...A	d(D-H)	d(H•••A)	d(D•••A)	<(DHA)
O(12)-H(12)...O(14)	0.8(2)	1.80(17)	2.390(19)	126.0
O(14)-H(14H)...O(10)^{i}	0.82(15)	2.11(13)	2.764(8)	135(16)
C(34)-H(34)...O(6)^{ii}	0.95	2.60	3.373(5)	138.8
C(22)-H(22B)...O(3)^{iii}	0.99	2.49	3.481(4)	175.3
C(27)-H(27)...O(13)^{iii}	0.95	2.53	3.383(8)	150.1
C(19)-H(19B)...O(9)^{iii}	0.99	2.50	3.317(4)	139.5
C(4)-H(4)...O(3)^{vi}	0.95	2.45	3.340(4)	155.2
N(5)-H(5)...O(4)	0.86(3)	2.37(2)	3.128(4)	147(3)
O(13)-H(13)...O(11)	0.83(7)	2.01(3)	2.811(13)	161(8)
O(11)-H(11)...O(13)^{v}	0.84	2.09	2.696(11)	128.5

Symmetry transformations used to generate equivalent atoms: i) -x+y+4/3, -x+2/3, z-1/3; ii) -x+5/3, -y+1/3, -z+7/3; iii) -y+2/3, x-y-2/3, z+1/3; vi) -x+5/3, -y+1/3, -z+4/3; v) y+1, -x+y+1, -z+1.

3.2 Analysis of (±)-2–3 in crystalline state.



Scheme S2. Schematic representations of the competitive dimerization of two clips (±)-**2** and (±)-**3** in crystallographic state. Color code: red, dimethoxyxylyene wall; blue, amide-substituted xylyene wall.

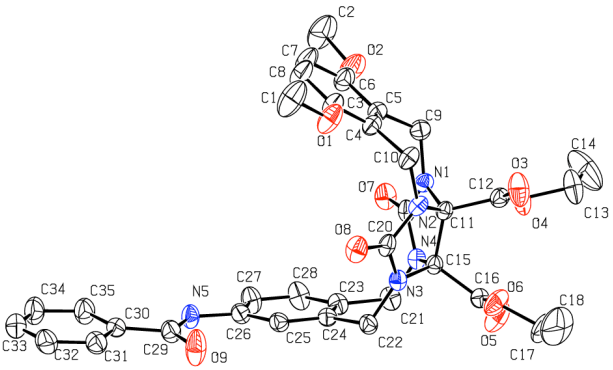


Figure S8. ORTEP drawing and atom numbering for (±)-**2**. Thermal ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. Colour code: C, gray; N, blue; O, red.

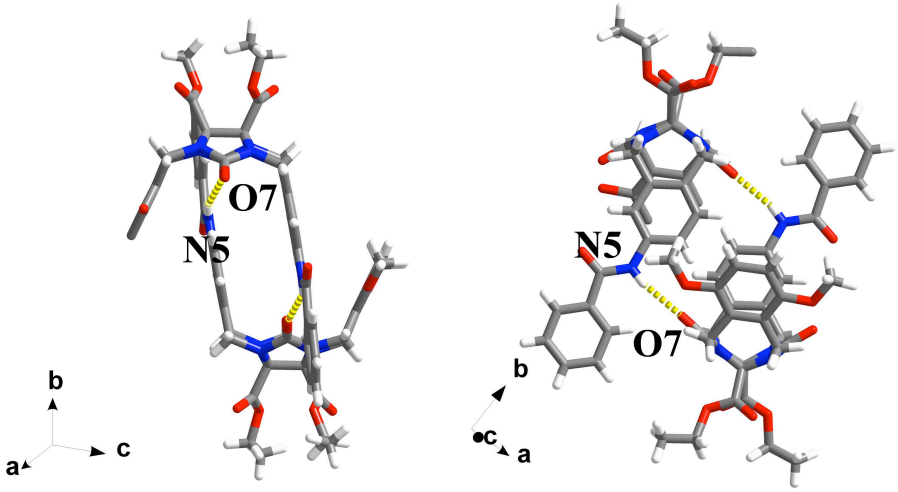


Figure S9. View of the packing of the competitive dimer (+)-**2**•(–)-**2** highlighting N5-H5•••O7 H-bonds (yellow dotted lines). Colour code: C, gray; H, white; N, blue; O, red.

Table S2. Hydrogen bonds for (±)-**2** [Å and °].

D-H...A	d(D-H)	d(H•••A)	d(D•••A)	<(DHA)
N(5)-H(5)...O(4)^{i}	0.83	2.28	3.053(1)	156.0

Symmetry transformations used to generate equivalent atoms: i) -x, 1-y, -z

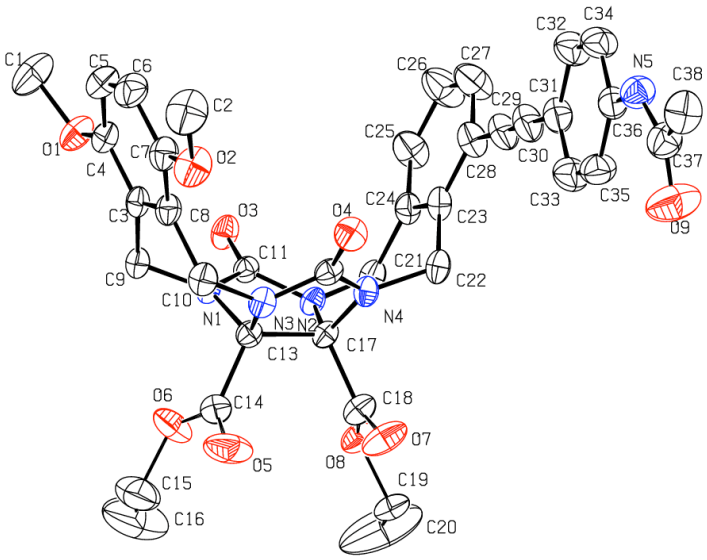


Figure S10. ORTEP drawing and atom numbering for (±)-**1**. Thermal ellipsoids are drawn at the 30% probability level. Solvent molecules and H atoms have been omitted for clarity. Colour code: C, gray; N, blue; O, red.

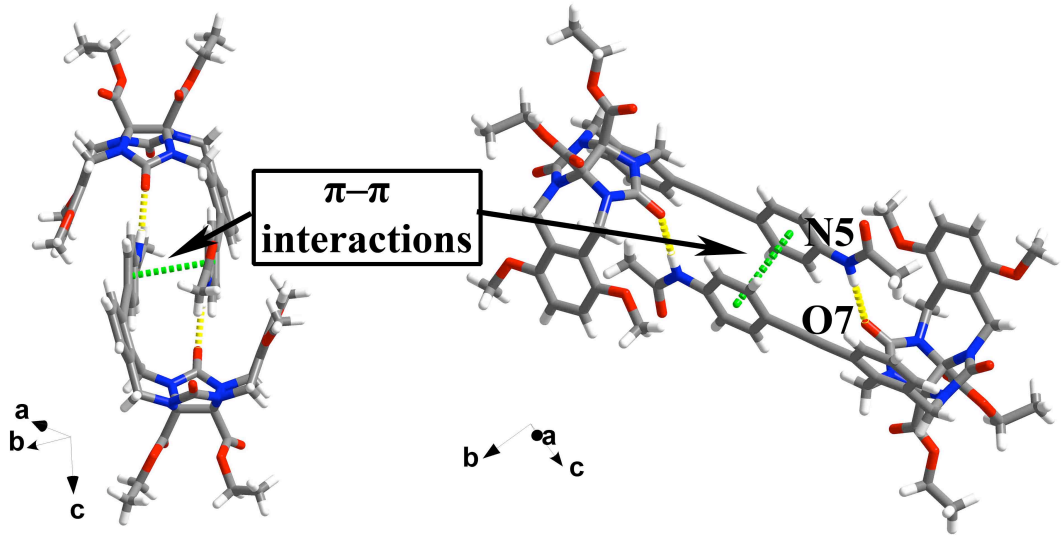


Figure S11. View of the packing of the competitive dimer (+)-**3**·(–)-**3** highlighting N5-H5•••O7 H-bonds (yellow dotted lines) and π–π interactions (green dotted lines). Colour code: C, gray; H, white; N, blue; O, red.

Table S3. Hydrogen bonds for (±)-**3** [Å and °].

D-H...A	d(D-H)	d(H•••A)	d(D•••A)	<(DHA)
N(5)-H(5A)...O(4)^{i}	0.86	2.04	2.897(3)	172.0

Symmetry transformations used to generate equivalent atoms: i) -x, -y+2, -z

4. Analysis of methanol clusters in CSD.

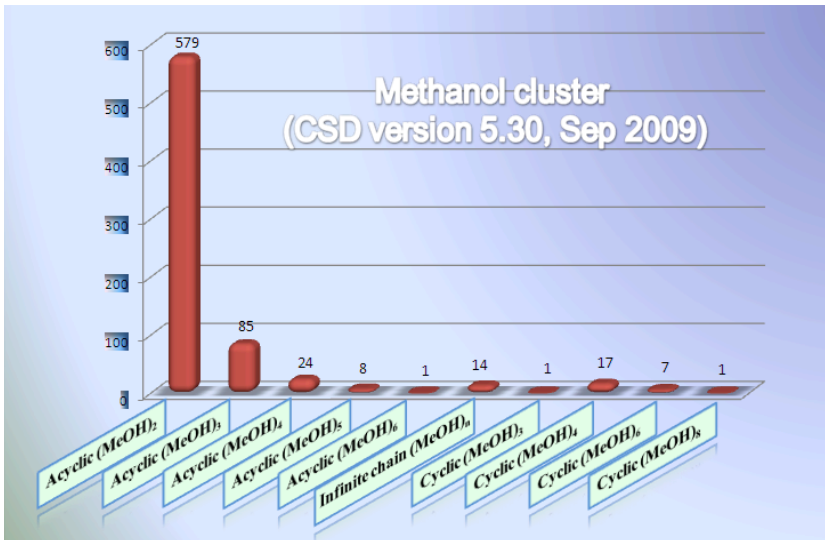


Figure S12. The study was carried out on the V5.30 release of the CSD (Nov 2008, updates including Feb, May, and Sep 2009): the distance of two oxygen atoms of the methanols was defined from 2.0Å to 3.2 Å.

CSD refcodes of acyclic (MeOH)$_2$: ACAREC, ACOZAU, ACUYAZ, AFOGOR, AFOHAE, AGACER, AGAXUB, AGEBUK, AGEYOB, AGODAB, AHABOA, AHIFAY, AJACUJ, AJADAQ, AQOGOC, AREHAG, ASUNEH, ASUNIL, AVAYAX, AVAYEB, AWOHAV, AWOKUS01, AWOKUS, AXUHAC01, BACTEE10, BACTEE20, BAHCAP, BAPCIF, BASKIQ, BEGZUI, BEMHAD, BEQVAU, BETDOU, BICCEW, BICFOJ, BIGWIY, BIQPIA, BIWWUA, BIYYEN, BIYYIR01, BOCQAM, BOCQAM01, BOFWOJ, BOJDUA, BOKCAG, BOTNUU, BOQLOJ, CAKTEN, CANVIX, CAZFIS10, CAZPAV, CAZRAX, CEBTUZ, CEKNOW, CEKNUC, CELGOQ, CENCED, CEVYAE, CEYZUC, CIBPUZ, CIFHIJ, CIFJOR, CIGKUZ01, CIGKUZ, CIHNUD, CIHYUN, CIJGEI, CIKWAV01, CIKWAV, CIKWEZ01, CIKWEZ, CISRUS, CIXHIB, CIYNEE, COBNEN, COJLET, CORHAT, COTBAP, COMGER, CTZICU, CYDSAR, DAGVEN, DAGXUF, DAKJAA, DAMHAB, DEBFOG, DEDYIV, DEDYOB, DEFQAH, DEKHEG, DEKHEG01, DENHOU, DENHUA, DENXIE, DESRAV, DISSED, DISSED10, DITJEV, DITMUP, DITNAW, DIVKOJ, DIYCIY, DORNAA, DOSTIP, DOSVEN, DUGVOQ, EBALID, ECAQIJ, EGEMOT, EGIVAS, EJIZAY, EJUXOW, EQITED, EQUBIB, EQUJUV, EZIYOB, FADFUL01, FAGGUQ, FAGHAX, FAGHEB, FAKTIV, FAPPAN, FAZMID, FEGMIO01, FEQRID, FESWAC, FICGAZ, FIQRUT, GADVEN, GAPLAL, GARMUI, GECZOE, GEFDAX, GERDIR, GIDRER, GIGDAC, GIHQIY, GIHQUK, GIHREV, GIHRIZ, GIJPUL, GIKXUU, GIMDEM, GIQKAS, GIRSOQ, GOQHUP, GUCTON, GUTGUX, GUTSAP, HACYEQ, HAJCAX, HAJCIF, HAJCOL, HAJDOM, HAJFAA, HASFIQ, HASQAF, HAYPUT, HICLIP, HICLUB, HILFUE, HIPYAH, HIVMII, HIYDID, HIZHIH, HIZSUF, HIZTAM, HIZXEU, HOCHOW, HOFGIT, HOHQUR, HOMLEB, HOLGEU, HOPDEV, HUCBUC, HUJVEN, HUKMUV, HYDTML, IBOGAI, IBUJUL, ICEHUU, IDOTUR, IFARUC, IFEYOH, IKEJIR, IKIZOR, IMUXUJ, IMUZAR, IQISUW, ISOPIP, IWEJAV, IWONEN, IYEZER, JADZUK, JAJCAZ, JALFEI, JALREU, JEFJEJ, JEKBOR, JEKPOF, JELZAC, JEPLEW, JEZLIJ, JIFWEB, JITCEV, KAJRAP, KALGUA, KARLAR, KASCOX, KATSAA, KAXGIA, KEDZAV, KEFQES, KEFQIW, KEFQOC, KEJHUD, KEKPUM,

KEMKIX, KEQTOP, KEQTOP, KETRIL, KICVAU, KIGPAS, KIKVOP, KIWCAV, KIZTOD, KOFQAX, KOFYIO, LAHSUJ, LAHTAQ, LAHTEU, LASDEO, LAXPIK, LEBLIN, LEYQOV, LIFWED, LIHJOC, LIRPOR, LIRSEK, LOCYAE, LOFXIN, LOFXUZ, LOPGEC, LOTPUF, LOZHOX, LUWTUS, LUZLEX, MADYEW, MAHGUY, MANLAP, MAPPOJ, MAQFEQ, MATHOF, MATTAD, MAVTOS, MAVTUY, MAXQAE, MAZVAK, MEGRUM, MELLEU, MEVHEA, MEVHIE, MEXNAE, MICKUE, MIDQAS, MIFYIK, MIHFUF, MIHLIY, MIHMOF, MIKLIC, MODQOM, MOLVOY, MOMGEA, MOSNOX, MOTGEI, MOTLOW, MOXSAT, MUJTAM, MURMUH, MUTWED, NABCID, NAFBOM, NAFCIH, NAJPIX, NAKBEH, NAKBIL, NALKIV, NALKOB, NAQBEN, NATCAN, NAVPAC, NAXWEP, NAXWUF, NEBHUX, NEBJAF, NEDHUZ, NEDPIW, NERGOG, NERNIH, NETSAH, NIGBEL, NIGBOV, NIJPAY, NIMGEW, NIMGEW, NIPZAO, NITMEI, NIXNEN, NIXNEN01, NIXSUJ, NOBJOE, NOCHOD, NOCHUJ, NOFFEU, NOHGUN, NUDYAM, NUGNUY, NUSHIS, NUVVIJ, NUVVOP, OBITAV, OCEBUU, OCEDEG, OCEKEN, OCELEO, OCEMIT, OCUFUO, OCUXIZ, ODAKAF, ODAKEJ, ODOTEH, OFIKAQ, OGEHEN, OJITAC, PAGPUJ, PAGTUN, PAHBEF, PAHXAY, PAHXEC, PASWIQ, PATJAW, PATKEB, PATZIU, PAVBUK, PAVBUK01, PAVCAR, PAZMUZ, PENFOE, PETYUJ, PEWBUP, PEWCAW, PEWCEA, PEWCIE, PEWCOK, PEWCUQ, POBLOI, PORLOY, PORLUE, POTVOK, POVVEB, POZRAX, QAJSUQ, QAQPII, QASKAX, QEHBUA, QEHZOT, QEPDUL, QEPMUT, QESFIE, QESNIL, QESNUX, QETMAE, QETMEI, QIBHEP, QIBTEA, QIFHOC, QIMVEN, QITYUN, QIWFIL, QOCLIE, QOCREG, QOCRIK, QOCWOU, QOQHUA, QORFAE, QORWEA, QOXTIG, QOZSIH, QURZIM, RAGPEV, RAMRAZ, RAQZIT, RATTOW, REHBOW, REHVUW, REJPEC, RELSEG, REMGAR, REMVOU, RENCET, RIBRID, RIDTED, RIFRII, RIVZEC, RIWCAC, RIWDOR, ROHWAH, ROKBOJ, ROKZAT, RUXGIA, SAJWEG, SAJWUW, SAVRAJ, SELXOX, SIJMEE, SIKYER, SIKYIV, SIKYOB, SIKYUH, SIPHOP, SIRLEL, SIXROH, SIYVIF, SODROT, SODVOX, SONGUY, SOTBUZ, SOTHIT, SOTXOP, SOVQAV, TAGLUJ, TAHFOY, TARXAL, TATGIF, TATWUH, TAWJEG, TAYLOU, TAYLOU01, TEBTEA, TEFKEV, TEKWAH, TETMEL, TEVCED, TEVRIW, TEYFOT, TEYNIV, TEZVAV, TIDBUE, TIJBEU, TIJBEU01, TIMNOT, TIQTES, TOKKOU, TOJMIO, TOMHUZ, TULNUJ, TUSYUB, UCEKAO, UDAZAB, UDEYIM, UDEYOS, UDEYUY, UDEZOT, UDIBAL, UDIBEO, UDIBIT, UFEJUK, UKECOC, ULORUI, UMAHAR, UMICIC, UMIPIP, UMIQAI, UNIKUX, VAMPAB, VEBNEW, VEMPUZ, VEQXOE, VEYQUL, VIBQUT, VICROP, VIFNIH, VIGSUA, VINHUW, VIWJEQ, VIZFEQ, VOFLEF, VOFRAK, VOHVOE, VOLBUU, WAJPON, WASCOJ, WATYIZ, WEMNUY, WEPLEI, WERGEF, WEWTEX, WEZQIB, WEZZUX, WIDQUW, WIGZOB, WIWNEW, WOFFUT, WOJZIF, WONNOD, WOKFIM, WOTWIL, WOWCEQ, WUCHOR, WUFXOK, WUFXUQ, WUHGEL, WUHGEL01, WUHJOY, WULXAC, WULXEG, WURWEL, WUXSIR, WUXTAK, WUYFUR, XAFYUZ, XAGWIL, XOFMUB, XOFSOB, XOMFUB, XOMGEM, XOKDIL, XAJTAE, XAPROW, XAPYOC, XAZBEF, XAZBOP, XAZMIU, XILQUF, XIRJIS, XIVKUJ, XOVBAL, XUCBUS, XUCVAS, XUCVOG, XUMRUS, XUSYAL, YAGBOX, YAJYEO, YALBES02, YALROT, YASLOU, YAWCOP, YAXYOM, YAZGEM, YECKUN, YEGHIC, YENGOO, YENKIM, YENQEO, YEQGIL, YERNEO, YIBNIH, YICKIF, YIHTUF, YITJOA, YIVTUT, YIWMOH, YIZWOU, YOMTAW, YUDMUF, ZAGMAV, ZAGMAV10, ZAPCOI, ZAPCOI10, ZIGTEO, ZIGTEO01, ZIGTIS, ZIGTOY, ZIJJEH, ZIPCEG, ZITTIF, ZOJYOM, and ZOSDUG. (579 examples)

CSD refcodes of acyclic $(MeOH)_3$: ACIVAK, BEHXOC, BEKFUT, BOCQEP, CEQLUF, CIGTAO, CIVVEJ, CIXGEW, DAGYEQ, DEWWIM, EQISUS, FASWIG, FEMSUM, FENRIA, GIBYEW, GIQGOD, HILWEE, HOMKOK, HUNKIK, IFAVIV, IKEKUE, JAWQEE, JITCOF, KAWWIO, KOJJUP, LAMNOD, LEYPAH, LIMCAM, LODBAH, LODYUZ, LODZAG, LOSWIZ, LOYVOK, MARSAA, MOGTOR, NAFBUS, NAFCAZ, NAQLAT, NEBZEZ, NODSEF, NOFSUX, ODIYIJ, PASLUR, PASMAY, PEPKUR, QAXYOD, QIRYEV, QITWIA, QIWFAD, QIXQAQ, QOLFUT, QOSDIM, RAKVUV, RAPXIQ, ROLLIO, SAJBAH, SEMFAS, SIKFOI, SILMAC, TEQGOM, UCISEF, UDOQOU, UFIXIR, UFOPIP, UMIPOV, UNEMEP, UNEMIJ, VILCEZ, VIMJUX, WEWXIG, WIMBEA, WIYTII, WIZFER, XAXYIF, XIFBIY, XOMHIQ, XUPHUL, YALBES01, YATVEV, YAYHEM, YINFUW, YINXEZ, YIWQAX, YOMTIE, and ZOJZAZ. (85 examples)

CSD refcodes of acyclic $(MeOH)_4$: BILGEJ, CENCIH, COKYIL, DIRFAL, ELAWOD, EZIROU, IGAVOB, IKIZIL, KOCPOI, KOCPUO, LUBLUP, MUZLIC, PEHLAP, PEHLAP10, PEJWUX, QESNOR, QOJQUB, QOPPEQ, SIJDIZ, SINCEY, UNEMOP, VACQAS, WAWMOW, and WUXSOX. (24 examples)

CSD refcodes of acyclic $(MeOH)_5$: FISXUB, HICLUB, JADVAM, KEVXUF, TOJMOU, VACREX, VACROH, and VIZFIU. (8 examples)

CSD refcodes of acyclic $(MeOH)_6$: CIGYIB. (1 example)

CSD refcodes of infinite chain $(MeOH)_n$: ADUXED, CIYYEP, FIVYUF, HAJVOE01, HAJVOE, HATMEV, METHOL04, MEWQOU, PAVREK, SEDVIH, TUQPUQ, UGAQIC, UGAQOI, and UGENAV. (14 examples) [4]

CSD refcodes of cyclic $(MeOH)_3$: QEKJUM. (1 example)

CSD refcodes of cyclic $(MeOH)_4$: AHIHII, COHXON, DIHCON, FISXOV, HIKJUG, IPASUN, LECMOW, MAZVEO, QEFDAG, QIRYIZ, RECTAU01, RECTAU, REHBIQ, REKFOD, RETQUD, RIRMUB, and VIQHOS. (17 examples) [5]

CSD refcodes of cyclic $(MeOH)_6$: BOGXOL, FEZTUA, KENGIU, LEYNIN, NILCUG, XERDOO, and YAHYIQ. (7 examples) [6]

CSD refcodes of cyclic $(MeOH)_8$: OFOREH. (1 example)

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