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Supplementary Information

Multiple intermolecular interactions in guest inclusion by acyclic host compounds

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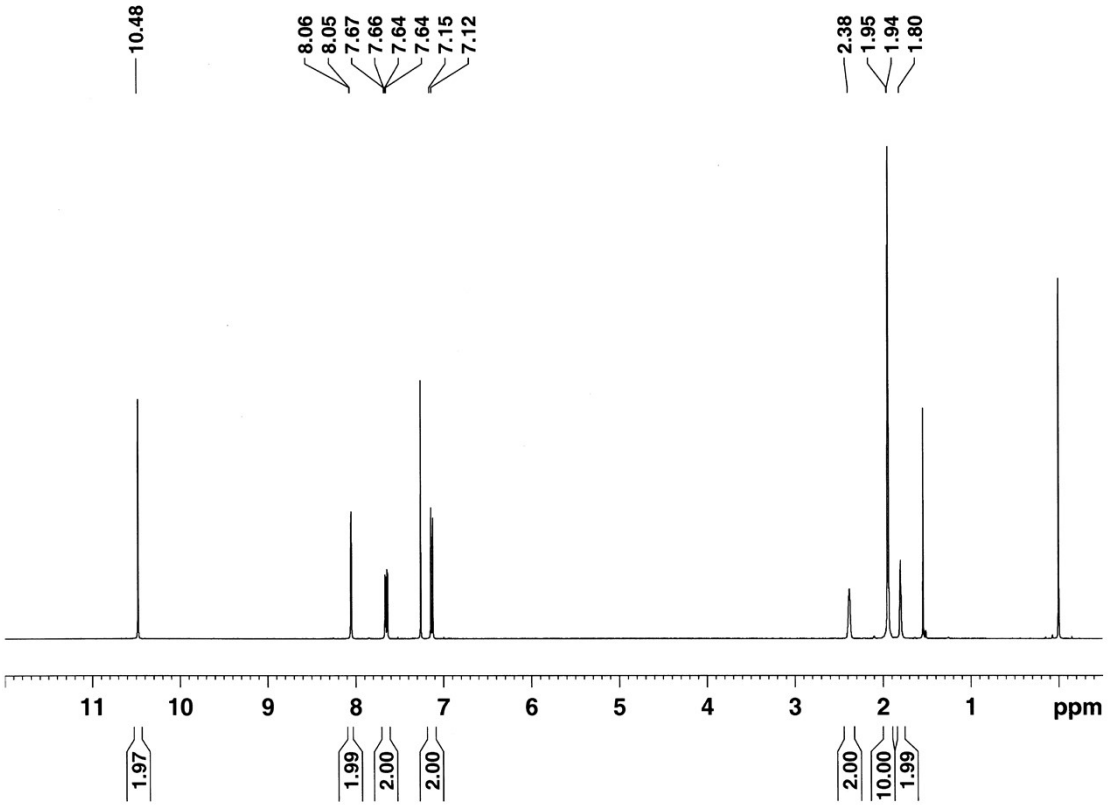
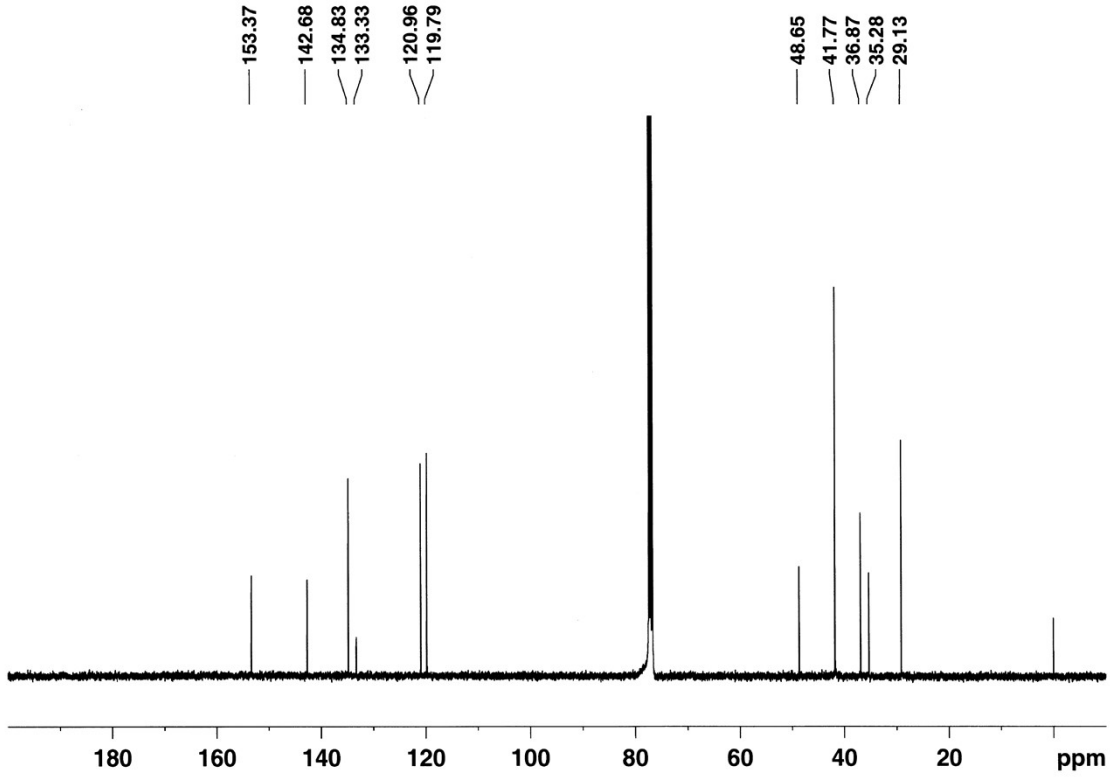
^{1}H NMR spectrum of **2** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **2** (100 MHz, $CDCl_3$)



General procedure of single crystal X-ray diffraction experiment

A single crystal was immersed in Paratone-N oil and placed in the N_2 cold stream at 100 K. Data were collected using diffractometer with PHOTON II 14 CPAD detector (Bruker D8 VENTURE, CuKα: λ = 1.54178 Å). Absorption correction was performed by an empirical method implemented in SADABS.[1] Structure solution and refinement were performed by using SHELXT-2018/2[2] and SHELXL-2018/3[3].

Single crystal X-ray diffraction experiment for crystal 1a

The low diffracting yellow plate crystal (0.100 × 0.100 × 0.050 mm^3) was obtained from slow evaporation of an acetone solution of **1**.

$C_{25}H_{28}N_2O_7$, *M*r = 468.49; triclinic, space group *P*-1, $Z = 2$, $D_{calc} = 1.387$ g·cm^{-3}, a = 6.9004(7), b = 10.5029(11), c = 15.8453(17) Å, α = 95.066(4), β = 92.516(4), γ = 100.761(3)°, V = 1121.6(2) $Å^3$, 16169 observed and 3983 [$I > 2\sigma(I)$], 4439 [all data] independent reflections, 315 parameters, final $R_1 = 0.0375$, $wR_2 = 0.1040$, $S = 1.058$ [$I > 2\sigma(I)$] and $R_1 = 0.0414$, $wR_2 = 0.1075$, $S = 1.058$ [all data]. CCDC 2267699.

All non-hydrogen atoms were refined anisotropically. The O-H hydrogen atoms were assigned from the difference Fourier map and refined isotropically. Another hydrogen atoms were refined isotropically on the calculated positions using a riding model (AFIX 13, 137, 23 and 43) with U_{iso} values constrained to 1.2/1.5 U_{eq} of their parent atoms.

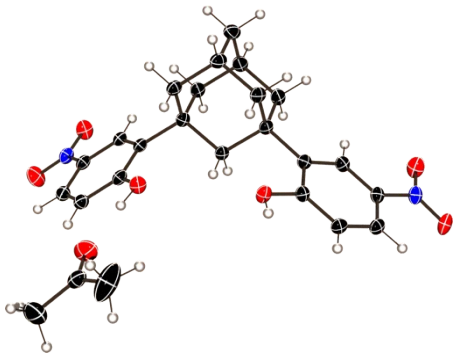


Fig. S1 ORTEP drawing of **1** and acetone in crystal **1a** (asymmetric unit, 50% probability).

Single crystal X-ray diffraction experiment for crystal 1b

The low diffracting colorless prismatic crystal (0.150 × 0.100 × 0.100 mm^3) was obtained from vapor diffusion of hexane into a 2-butanone solution of **1**.

$C_{26}H_{30}N_2O_7$, *M*r = 482.52; triclinic, space group *P*-1, *Z* = 2, D_{calc} = 1.387 $g \cdot cm^{-3}$, *a* = 7.0766(14), *b* = 10.505(2), *c* = 15.939(3) Å, *α* = 95.513(6), *β* = 93.850(6), *γ* = 100.486(5)°, *V* = 1155.4(4) $Å^3$, 15824 observed and 4385 [$I > 2\sigma(I)$], 4522 [all data] independent reflections, 372 parameters, 24 restraints, final R_1 = 0.0381, wR_2 = 0.1028, *S* = 1.057 [$I > 2\sigma(I)$] and R_1 = 0.0389, wR_2 = 0.1040, *S* = 1.058 [all data]. CCDC 2267700.

All non-hydrogen atoms were refined anisotropically. The O-H hydrogen atoms were assigned from the difference Fourier map and refined isotropically. Another hydrogen atoms were refined isotropically on the calculated positions using a riding model (AFIX 13, 137, 23 and 43) with U_{iso} values constrained to 1.2/1.5 U_{eq} of their parent atoms.

A pair of disordered 2-butanone molecules were refined with PART n and each free variable (21/−21). Occupancy ratio was 81/19. The minor 2-butanone molecule (C23B, C24B, C25B, C26B and O7B) was also applied to SIMU.

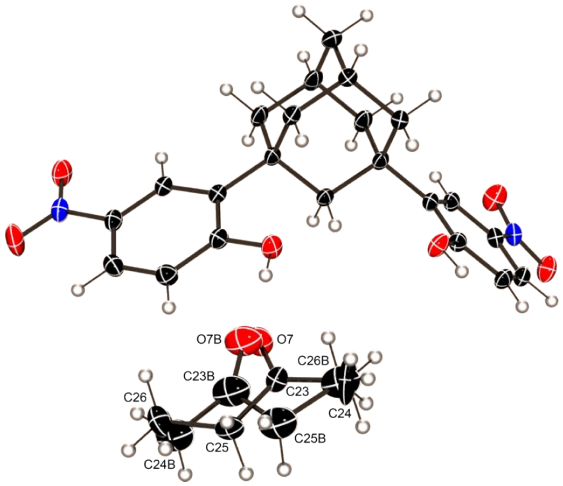


Fig. S2 ORTEP drawing of **1** and 2-butanone in crystal **1b** (asymmetric unit, 50% probability).

Single crystal X-ray diffraction experiment for 1c

The low diffracting colorless prismatic crystal (0.120 × 0.120 × 0.100 mm^3) was obtained from vapor diffusion of hexane into a methyl acetate solution of **1**.

$C_{25}H_{28}N_2O_8$, *M*r = 484.49; triclinic, space group *P*-1, *Z* = 2, D_{calc} = 1.416 $g \cdot cm^{-3}$, *a* = 7.0715(10), *b* = 10.4603(14), *c* = 15.710(2) Å, *α* = 95.120(4), *β* = 94.102(5), *γ* = 99.743(4)°, *V* = 1136.3(3) $Å^3$, 14281 observed and 3956 [$I > 2\sigma(I)$], 4426 [all data] independent reflections, 372 parameters, 24 restraints, final R_1 = 0.0462, wR_2 = 0.1347, *S* = 1.131 [$I > 2\sigma(I)$] and R_1 = 0.0501, wR_2 = 0.1389, *S* = 1.134 [all data]. CCDC 2267701.

All non-hydrogen atoms were refined anisotropically. The O-H hydrogen atoms were assigned from the difference Fourier map and refined isotropically. Another hydrogen atoms were refined isotropically on the calculated positions using a riding model (AFIX 13, 137, 23 and 43) with U_{iso} values constrained to 1.2/1.5 U_{eq} of their parent atoms.

A pair of disordered methyl acetate molecules were refined with PART n and each free variable (21/−21). Occupancy ratio was 70/30. The minor methyl acetate molecule (C23B, C24B, C25B, O7B and O8B) was also applied to SIMU.

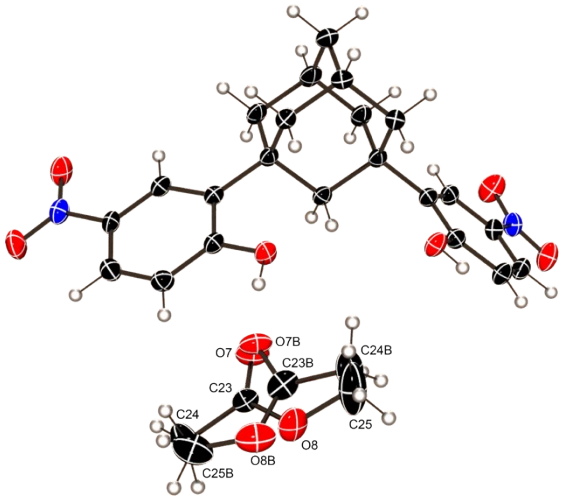


Fig. S3 ORTEP drawing of **1** and methyl acetate in crystal **1c** (asymmetric unit, 50% probability).

Single crystal X-ray diffraction experiment for 1d

The colorless prismatic crystal (0.200 × 0.200 × 0.200 mm^3) was obtained from vapor diffusion of hexane into a bromoform solution of **1**.

$C_{22}H_{22}N_2O_6$, *M*r = 410.41; monoclinic, space group $P2_1/n$, $Z = 4$, $D_{calc} = 1.463$ $g \cdot cm^{-3}$, $a = 10.8801(12)$, $b = 12.8327(14)$, $c = 13.3727(14)$ Å, $\beta = 93.490(4)°$, $V = 1863.6(3)$ $Å^3$, 22303 observed and 3827 [$I > 2\sigma(I)$], 3832 [all data] independent reflections, 278 parameters, final $R_1 = 0.0350$, $wR_2 = 0.0874$, $S = 1.039$ [$I > 2\sigma(I)$] and $R_1 = 0.0350$, $wR_2 = 0.0874$, $S = 1.039$ [all data]. CCDC 2267702.

All non-hydrogen atoms were refined anisotropically. The O-H hydrogen atoms were assigned from the difference Fourier map and refined isotropically. Another hydrogen atoms were refined isotropically on the calculated positions using a riding model (AFIX 13, 23 and 43) with U_{iso} values constrained to 1.2 U_{eq} of their parent atoms.

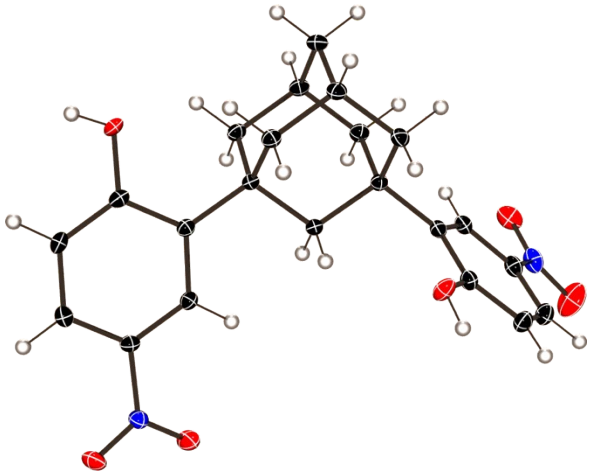


Fig. S4 ORTEP drawing of **1** in crystal **1d** (50% probability).

Single crystal X-ray diffraction experiment for crystal 2a

The yellow prismatic crystal (0.100 × 0.100 × 0.080 mm^3) was obtained from slow evaporation of an acetone solution of **2**.

$C_{22}H_{22}N_2O_6$, *Mr* = 410.41; orthorhombic, space group *Cmcm*, *Z* = 4, D_{calc} = 1.489 $g \cdot cm^{-3}$, *a* = 6.6173(6), *b* = 13.6049(11), *c* = 20.3294(17) Å, *V* = 1830.2(3) $Å^3$, 11088 observed and 1028 [$I > 2\sigma(I)$], 1079 [all data] independent reflections, 92 parameters, final R_1 = 0.0389, wR_2 = 0.1129, *S* = 1.101 [$I > 2\sigma(I)$] and R_1 = 0.0403, wR_2 = 0.1149, *S* = 1.101 [all data]. CCDC 2267703.

All non-hydrogen atoms were refined anisotropically. The O-H hydrogen atom was assigned from the difference Fourier map and refined isotropically. Another hydrogen atoms were refined isotropically on the calculated positions using a riding model (AFIX 13, 23 and 43) with U_{iso} values constrained to 1.2 U_{eq} of their parent atoms.

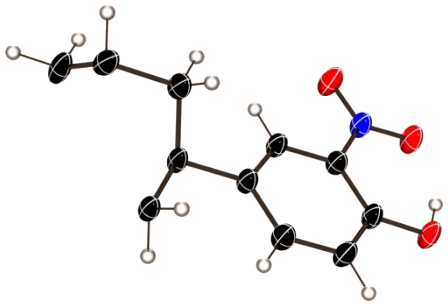


Fig. S5 ORTEP drawing of **2** in crystal **2a** (asymmetric unit, 50% probability).

Single crystal X-ray diffraction experiment for crystal 3a

The colourless prismatic crystal (0.140 × 0.100 × 0.080 mm^3) was obtained from slow evaporation of an acetone solution of **3**.

$C_{26}H_{30}N_2O_6$, *M*r = 466.52; triclinic, space group *P*-1, *Z* = 2, D_{calc} = 1.356 $g \cdot cm^{-3}$, *a* = 7.1643(12), *b* = 9.8755(16), *c* = 17.073(3) Å, *α* = 84.131(5), *β* = 85.474(5), *γ* = 72.254(5)°, *V* = 1142.9(3) $Å^3$, 16106 observed and 4225 [$I > 2\sigma(I)$], 4521 [all data] independent reflections, 309 parameters, final R_1 = 0.0342, wR_2 = 0.0905, *S* = 1.055 [$I > 2\sigma(I)$] and R_1 = 0.0362, wR_2 = 0.0920, *S* = 1.055 [all data]. CCDC 2267704.

All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically on the calculated positions using a riding model (AFIX 13, 137, 23 and 43) with U_{iso} values constrained to 1.2/1.5 U_{eq} of their parent atoms.

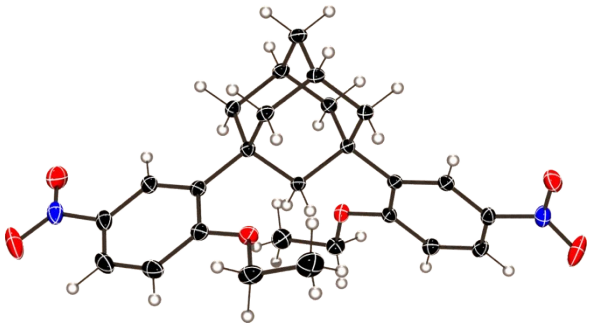


Fig. S6 ORTEP drawing of **3** in crystal **3a** (50% probability).

References

(1) G. M. Sheldrick, *SADABS*. University of Göttingen, Germany, 1996.

(2) G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv.*, 2015, **71**, 3–8.

(3) G. M. Sheldrick, *Acta Crystallogr., Sect. C: Struct. Chem.*, 2015, **71**, 3–8.