

Electronic Supplementary Information

Selective Guest Retention in Thermal Guest-release Process in Sandwich-type Inclusion Crystal of Cholic Acid

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Crystallographic data

| CA·(G1·G2) | |
|-------------------------------------|--|
| Formula moiety | C ₂₄ H ₄₀ O ₅ , C ₉ H ₈ , C ₆ H ₆ FN |
| Empirical formula | C ₃₉ H ₅₄ FNO ₅ |
| Molecular weight | 635.83 |
| Color, Habit | Colorless platelet |
| Crystal system | Monoclinic |
| Space group | P2 ₁ (No. 4) |
| Z | 2 |
| a/Å | 14.8259(5) |
| b/Å | 7.8389(2) |
| c/Å | 16.1032(5) |
| α/° | 90 |
| β/° | 108.6510(16) |
| γ/° | 90 |
| Volume/Å ³ | 1773.21(9) |
| Density/g cm ⁻³ | 1.191 |
| Temperature/K | 273 |
| X-Ray | 1.54187 |
| wavelength/Å | |
| μ/mm ⁻¹ | 0.6477 |
| 2θ _{max} /° | 136.5 |
| No. of reflections/ | |
| Total | 20060 |
| No. of reflections/ | 5641 |
| unique | |
| R _{int} | 0.060 |
| R ₁ ($I < 2\sigma(I)$) | 0.0623 |
| wR ₂ (all) | 0.1922 |