Supplementary Materials

Mechanochemical synthesis of the catechol-theophylline cocrystal: spectroscopic characterization and molecular structure

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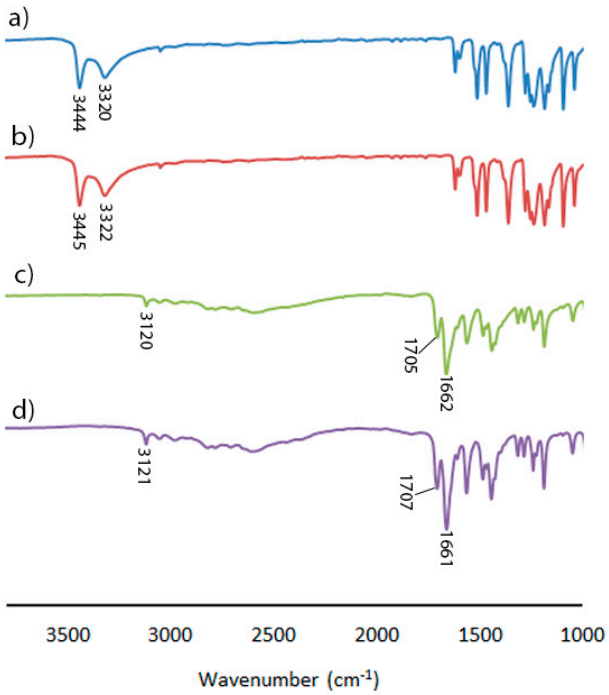

Figure S1. IR spectra of a) bulk catechol; b) catechol ground with dichloromethane after 15 minutes of grinding; c) bulk theophylline; d) theophylline ground with dichloromethane after 15 minutes of grinding.

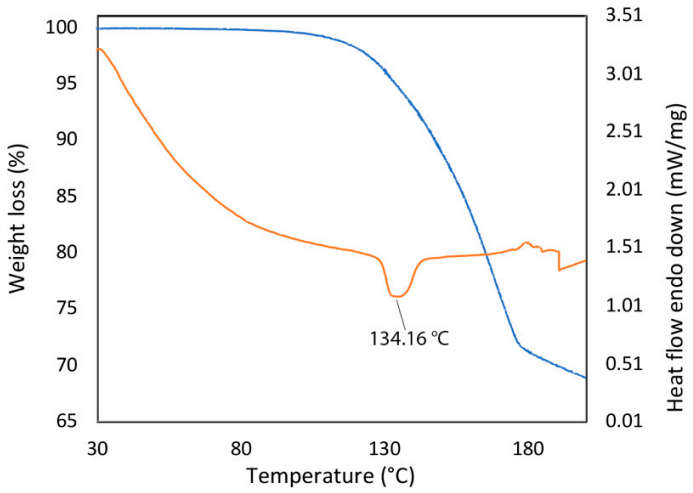

Figure S2. DSC and TGA curves of the CAT-TEO cocrystal.

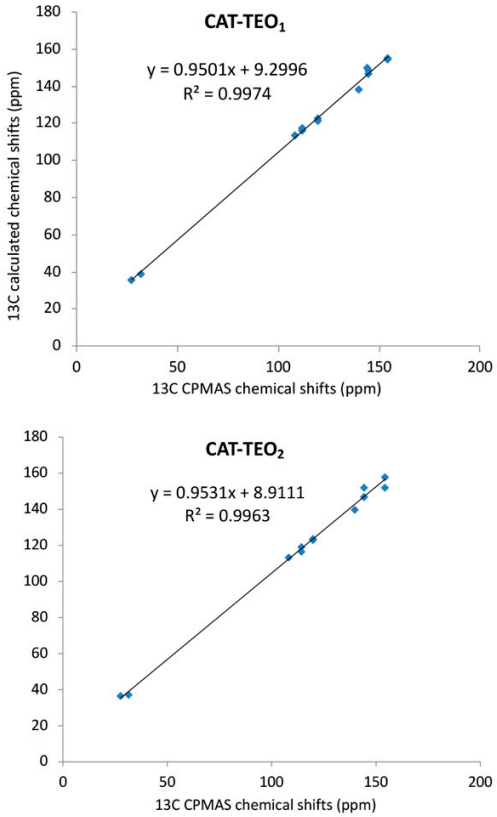

Figure S3. Correlations of the experimental and theoretical shielding parameters for CAT-TEO_1 and CAT-TEO_2 models.

Table S1. Theoretical optimization energy and Second Order Perturbation theory analysis of Fock matrix in NBO basis of the optimized complexes. (a) These values are the estimated strengths of the donor(i)-acceptor(j) interactions the stabilization energy. (b) The energy splitting (in kcal/mol) of the donor and acceptor orbitals. (c) The element of the Fock (or Kohn-Sham) matrix describing the donor-acceptor interaction.

HB model	E (kcal/mol)	Orbital NBO	Distance (Å)	E(2)	E(j)-E(i) kcal/mol	F(i,j)
CAT-TEO$_1$	-642 439. 245	$n_{O2} \rightarrow \sigma_{OH}^*$	1.777	12.00	1.18	0.106
CAT-TEO$_2$	-642 441.649	$n_{O1} \rightarrow \sigma_{OH}^*$	1.770	11.76	1.17	0.105