

Supporting Information

Six novel multicomponent systems of theobromine with carboxylic acids: crystallographic structures, solubility determination and DFT calculations

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Table S1. Detailed Information of the Chemicals

chemicals	CAS	molar mass (g·mol ⁻¹)	source	mass fraction purity (%)	analysis method
Theobromine	83-67-0	180.16	Shanghai Aladdin Biochemical Technology Co., Ltd.	≥99	HPLC ^a
<i>p</i> -Coumaric	7400-08-0	164.16	Shanghai Macklin Biochemical Co., Ltd.	≥99	HPLC ^a
1-Hydroxy-2-naphthoic acid	86-48-6	188.18	Shanghai Macklin Biochemical Co., Ltd.	≥98	HPLC ^a
2,4,6-Trihydroxybenzoic acid monohydrate	71989-93-0	188.13	Shanghai Macklin Biochemical Co., Ltd.	≥98	HPLC ^a
Citric acid monohydrate	5949-29-1	210.1388	Sinopharm Chemical Reagent Co., Ltd.	≥99.5	HPLC ^a
Gallic acid monohydrate	5995-86-8	188.14	Tianjin Kermel Chemical Reagent Co., Ltd	≥99	HPLC ^a
methanol	67-56-1	32.04	Sinopharm Chemical Reagent Co., Ltd., China.	≥99.7	GC ^b
ethanol	64-17-5	46.07	Sinopharm Chemical Reagent Co., Ltd., China.	≥99.7	GC ^b
acetone	67-64-1	58.08	Sinopharm Chemical Reagent Co., Ltd., China.	≥99.7	GC ^b
Acetonitrile	75-05-8	41.05	Tianjin Fuyu Fine Chemical Co., Ltd.	≥99.5	GC ^b

^a High-performance liquid chromatography. ^b Gas chromatography.

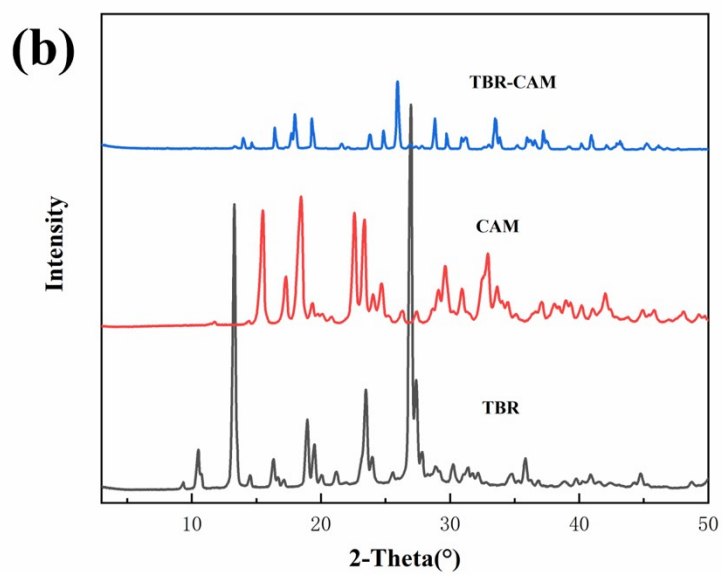
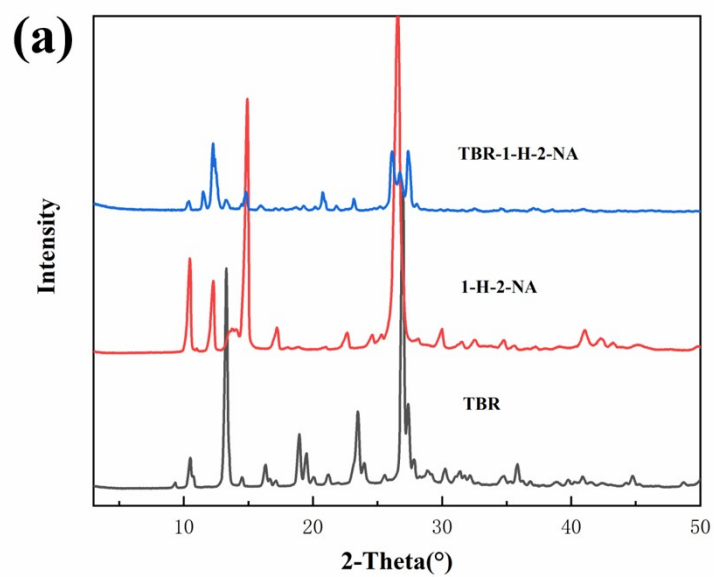
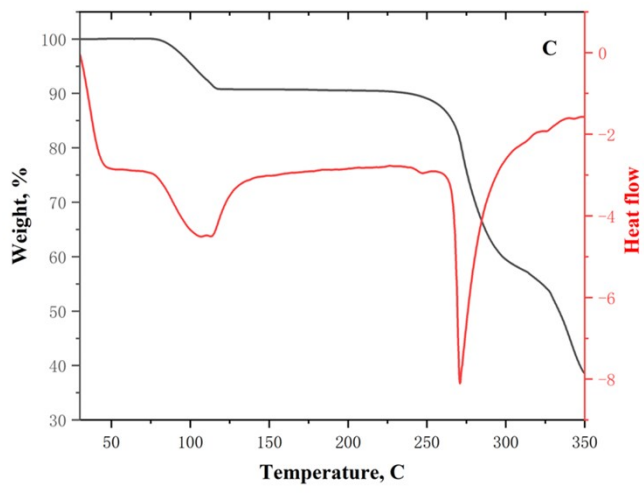
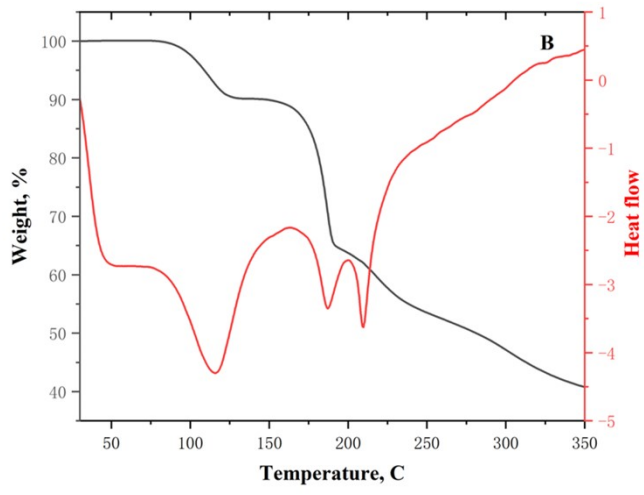
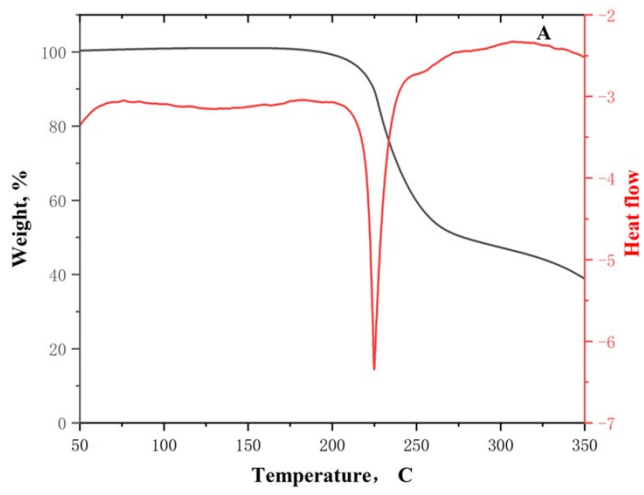


Fig. S1. Powder XRD patterns of the new cocrystals a) TBR-1-H-2-NA, b) TBR-CAM and their corresponding reactants.



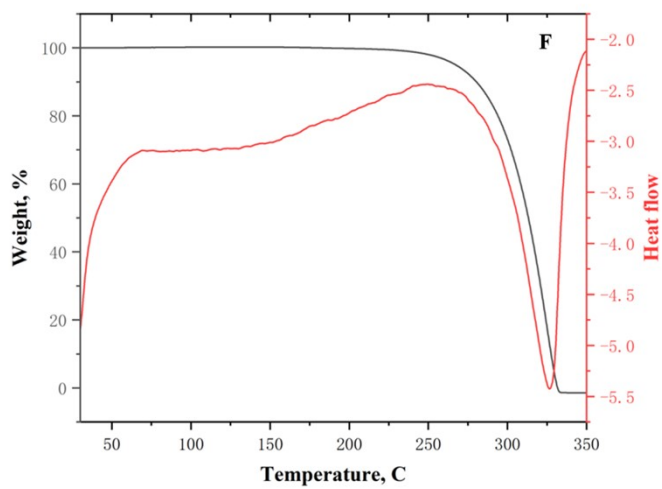
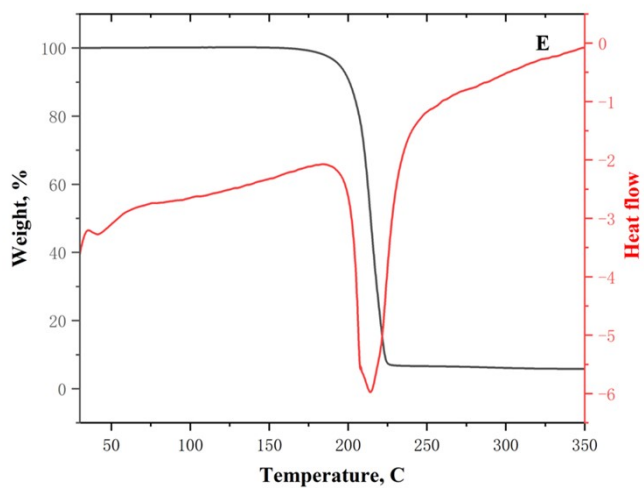
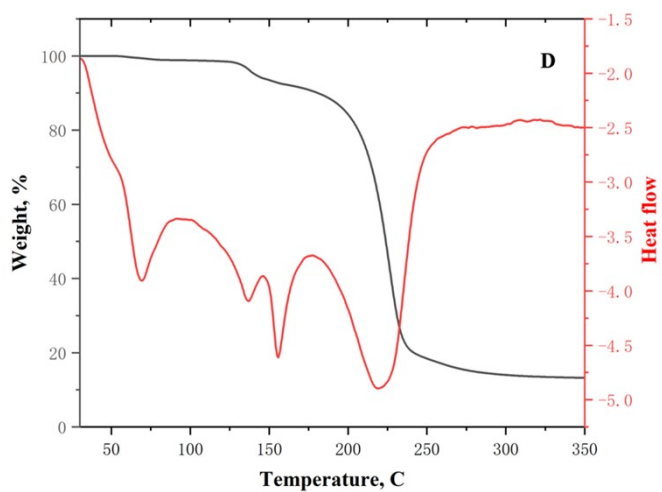


Fig. S2. DSC-TGA curves of (A) *p*-COA, (B) 2,4,6-TRM, (C) GAL, (D) CAM, (E) 1-H-2-NA, (F) TBR.

The TGA and DSC curves are shown in black and red, respectively.