Electronic Supplementary Information (ESI†)

Polymorphism in anti-hyperammonemic agent N-carbamoyl-L-glutamic acid†

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Table S1 Shows that difference in the torsion angle in both the forms (Form-I and Form-II).

Torsion angles (τ)	CGA-Form-I	CGA-Form-II molecule A/molecule B
C2-C3-C4-C5 (τ_1)	79.72°	177.35°/ 178.73°
C6-N1-C2-C1 (τ_2)	81.26°	–55.77°/ –57.59°
N1-C2-C3-C4 (τ_3)	176.89°	–175.87°/ –168.49°

Table S2 Summary of FT-IR stretching frequencies of CGA polymorphs.

Drug forms	1° and 2° N–H stretch (cm^{-1})	C–H Stretch (cm^{-1})	Carboxylic C=O stretch (cm^{-1})	Amide C=O stretch (cm^{-1})	O–H stretch (cm^{-1})
CGA-Form-I	3439.9 3344.3 3295.4	2952.1	1728.5	1697.3	3169.2
CGA-Form-II	3454.3 3315.3 3247.3	2957.7	1709.9	1666.9	3112.5

Table S3 ^{13}C ss-NMR chemical shift values (δ, ppm) of CGA Polymorphs

Carbon No.	CGA-Form-I	CGA-Form-II
C1	175.43	175.36, 177.33
C2	55.85	55.83

C3	25.62	25.56
C4	30.35	30.31
C5	179.47	179.44, 181.67
C6	160.19	160.18

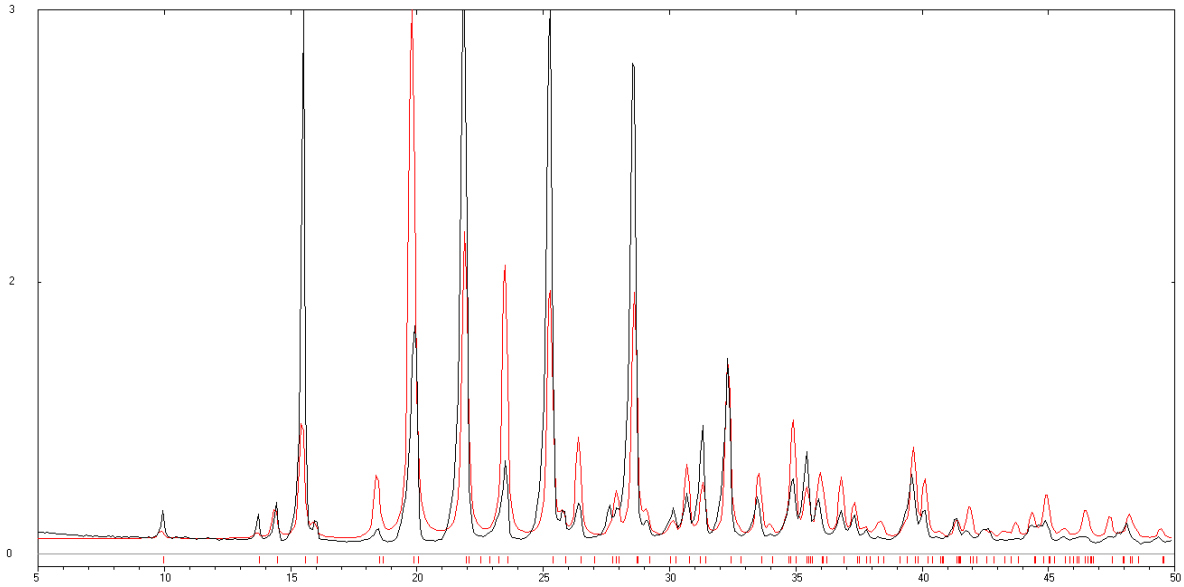
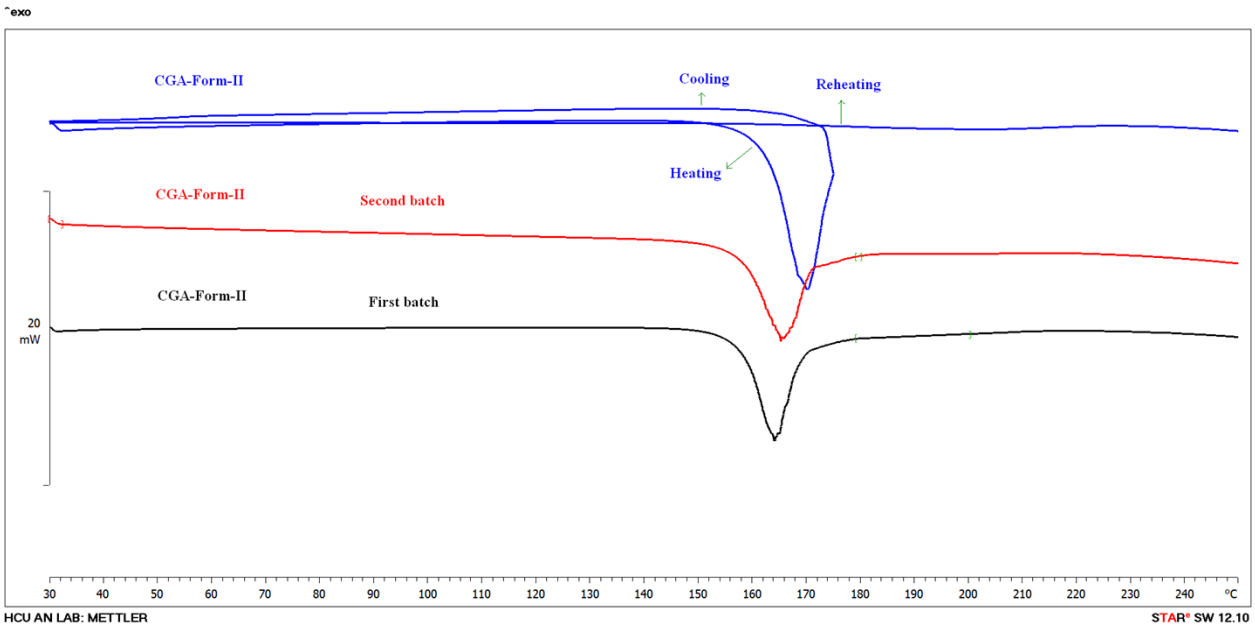
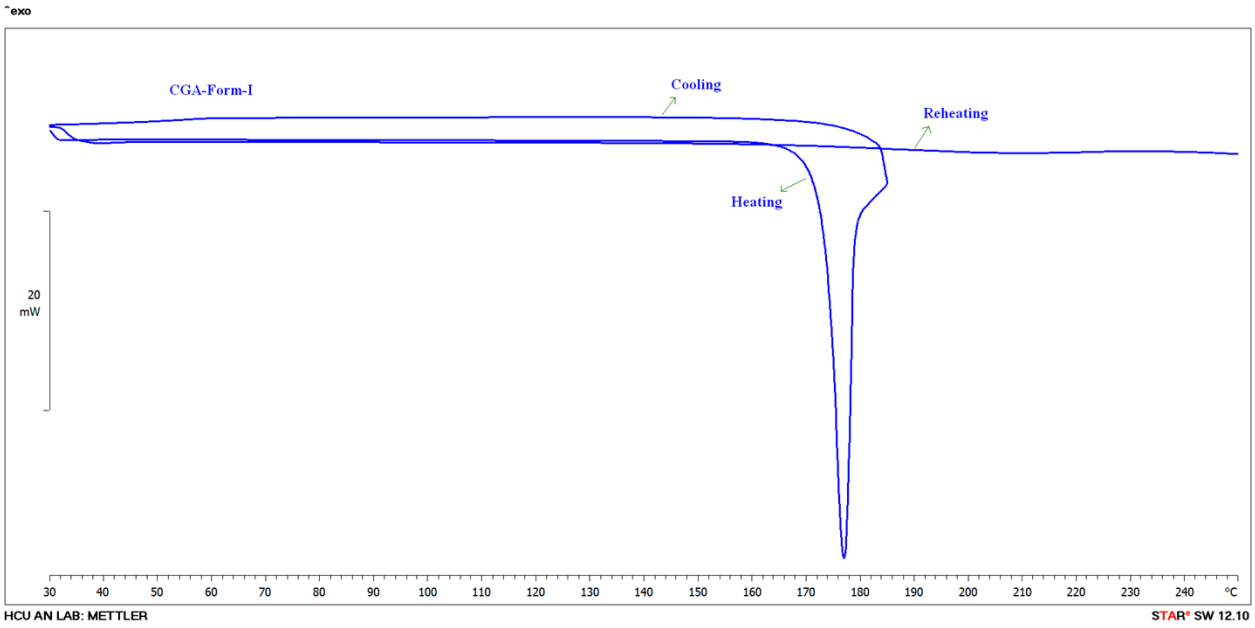


Figure S1 Overlay of experimental PXRD pattern (black) of CGA-Form-I matches with the calculated powder lines from the crystal structure (red).



(a)



(b)

Figure S2 (a) The broad peak for endotherm of Form-II is reproducible. A heat-cool-heat experiment on Form-II (a) as well as Form-I (b) showed no phase transition events at the melting temperature suggesting some kind of decomposition of CGA takes place upon heating to the melting temperature.

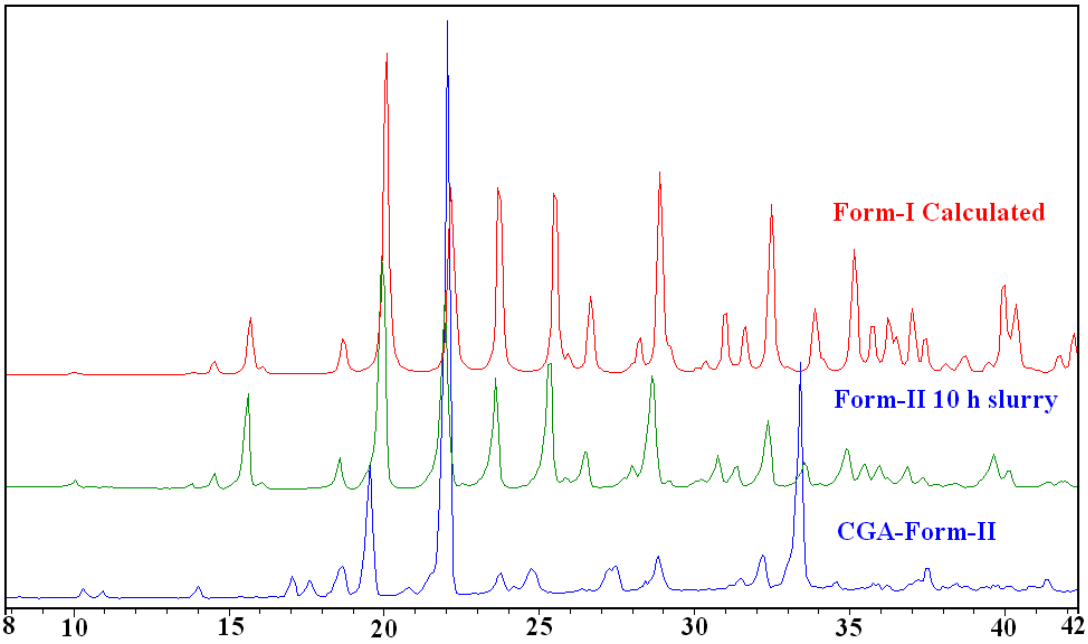


Figure S3 Overlay of experimental PXRD pattern of CGA-Form-II (blue) with the PXRD pattern after slurry experiment in which Form-II was found to convert into Form-I after 10 h slurry in EtOH. The calculated pattern of Form-I is shown for comparison (red).

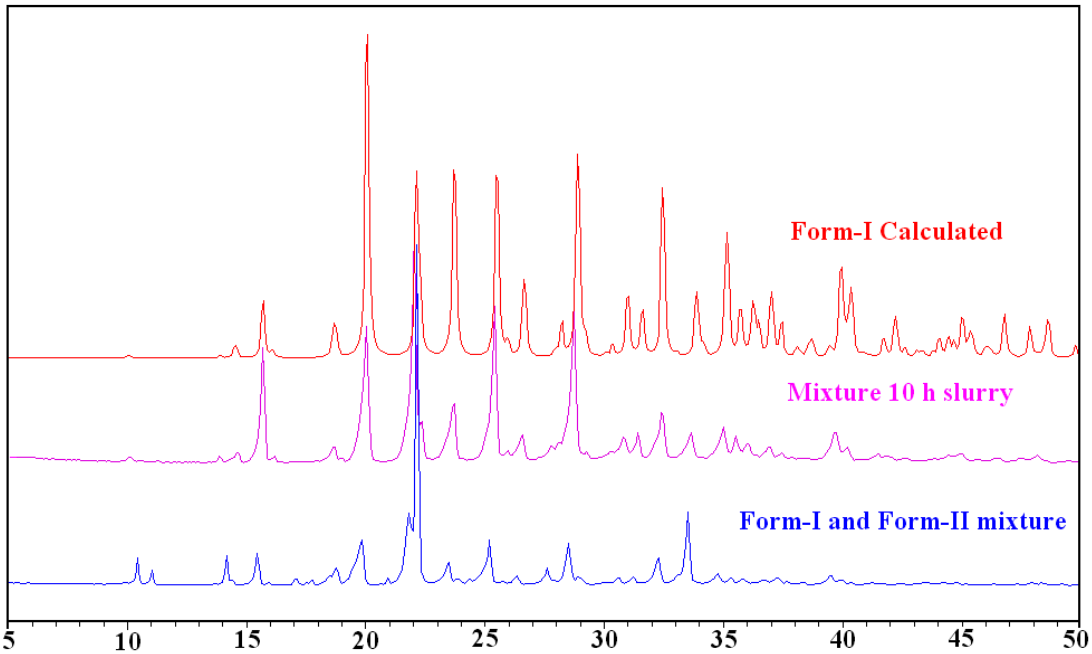


Figure S4 The mixture of Form-I and II (blue) was found to convert into Form-I (magenta) after slurry in pentane solvent. The calculated PXRD pattern of Form-I (red) was shown for comparison.