# Resolving the Longstanding Riddle of pH-Dependent Outcome of Glycine Polymorphic Nucleation

Guangjun Han[a,*], Satyanarayana Thirunahari[a], Pui Shan Chow[a] and Reginald B. H. Tan[a,b,*]

5

PXRD patterns of α- and γ-glycine

The simulated PXRD patterns of α- and γ-glycine (CSD ref. codes 10 gly29 and gly33 respectively) are presented in Figure S1. They are distinct and enable us to determine the polymorphs of glycine crystals formed under various conditions (A. S. Myerson et al., Cryst. Growth Des. 2001, **1**, 5 – 8; R. B. H. Tan et al., Cryst. Growth Des. 2010, **10**, 4883 – 4889).
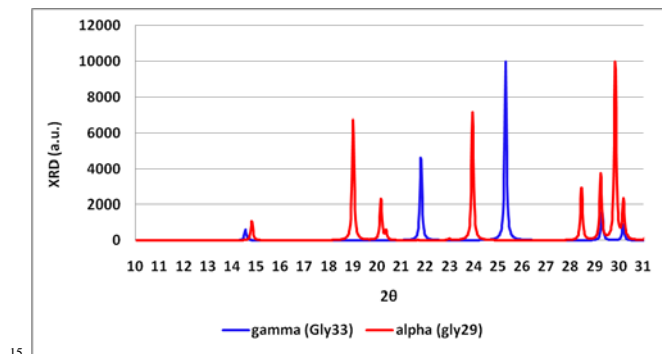
15

Figure S1. Simulated PXRD patterns of α- and γ-glycine.

The measured PXRD pattern of the glycine crystals formed in a pure glycine solution is presented in Figure S2. It is practically the same as 20 the simulated PXRD pattern of α-glycine, showing that the polymorph of these glycine crystals is α form.
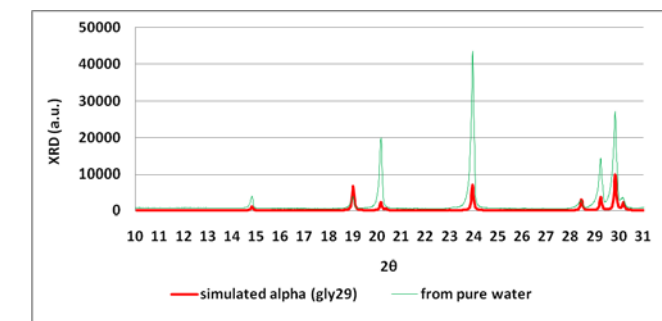

Figure S2. PXRD pattern of glycine crystals formed in a pure aqueous glycine solution.

25

The measured PXRD patterns of the glycine crystals formed in acidic and basic glycine solutions are presented in Figures S3. These 30 measured PXRD patterns are practically the same as the simulated PXRD pattern of γ-glycine, showing that the polymorph of all the glycine crystals formed in acidic and basic environments is γ form.
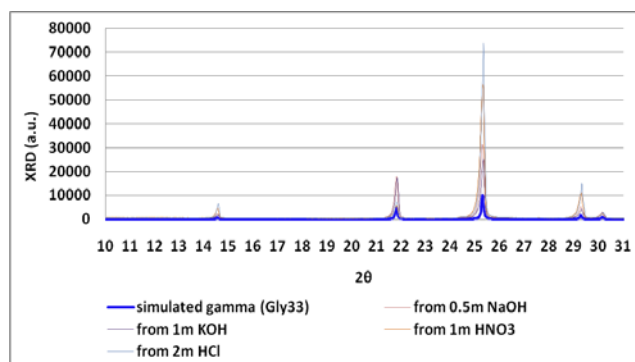

Figure S3. PXRD patterns of glycine crystals formed in acidic and 35 basic aqueous glycine solutions.

Notes and references

[a]Institute of Chemical and Engineering Sciences, A*STAR (Agency for Science, Technology and Research), 1 Pesek Road, Jurong Island, 40 Singapore 627833 Fax: 65 63166183; Tel: 65 67963841 ; E-mail: reginald_tan@ices.a-star.edu.sg; han_guangjun@ices.a-star.edu.sg
[b]Department of Chemical and Biomolecular Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260