Prediction of Cocrystal Formation by Thermodynamic Modeling

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Cocrystal (CC) refers to single crystalline phase composed of multi-components. These CCs have received much attention in many fields such as pharmaceutical, agricultural industries, and energetic material engineering due to its ability that can improve the properties of drugs. However, since CC screening requires high-priced chemicals and lot of time for numerical experiments, there has been an increase in the importance of efficient CC screening method.

The purpose of this paper is prediction of CC forming area for evading these problems by thermodynamic modeling. In this paper, COSMO-SAC, one of thermodynamic method assuming molecule as conductor, was used for estimating thermodynamic properties. Furthermore, experimental data were verified by X-ray diffraction method and microscopic analysis to compare with predicted data. Result shows that there was a formation of CC in predicted area. We hope that these results can make a significant contribution to the future cocrystal screening development.