Effective Co-crystal Separation by Thermodynamic Modeling

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Co-crystal is a technology, which improves the stability of the drug, drawing attention from pharmaceutical industries. Many researchers have carried out several methods to separate the co-crystal efficiently. One of the most commercially used methods is cooling crystalization using phase equilibrium data. It is usually widely used due to its high yield and high purity of the product. However, many experimental efforts are inevitable in that they require phase equilibrium data.
In this work, we will use predicted value to separate co-crystal instead of the experimental value. COSMO-SAC(**CO**nductor like **S**creening **MO**del for **R**eal **S**olvents-Segment Activity Coefficient.), which predicting chemical potentials μ in liquids, is introduced to reduce experimental efforts. For validation, literature values and prediction values were compared. The cooling crystallization experiments were carried out to show that co-crystals can be separated from predicted data. XRD(X-ray diffraction) and microscopy were used, and saturation solutions were prepared by the isothermal method. As a result, the co-crystal separation was successfully achieved.