Keywords: Blind test, Powder X-ray diffraction, Stoichiometry

Computational techniques for crystal structure prediction (CSP) of organic molecules have received much attention as a useful theoretical tool for designing new materials with desirable properties in pharmaceutical and functional material industries and have been steadily established by many efforts. The Cambridge Crystallographic Data Center has periodically organized international scientific workshop on predicting crystal structures of organic molecules that is known as CSP blind test for promoting development and improvement of the computational techniques [1-6]. According to the reports of blind tests, there are some successful predictions, although given information is two-dimensional chemical diagrams. Obata and Goto have attempted CSP of three targets (XXII, XXIII, and XXV) in the 6th blind test by using own methods [7,8] and have successfully predicted the crystal structures of XXII and XXIII polymorphs [6].

Recently, we have attempted improvement of accuracy in stability estimation between polymorphs, which is one of the challenging subjects in CSP research, by using fragment molecular orbital (FMO) method at the MP2 level of theory. The MP2 method can estimate dispersion interactions non-empirically by correcting for electron correlations, and we have confirmed that our approach can evaluate the stability between polymorphs with high accuracy [9]. Furthermore, Obata and Goto reported a new method related to the CSP technique with powder X-ray diffraction (PXRD) data [8]. The method can assist determination of crystal structure from the observed PXRD data, which is often difficult, by using CSP technique and similarity calculation between PXRD patterns. In this work, we will present our recent CSP research using force field, density functional theory with D3 dispersion correction (DFT-D3), and FMO techniques as well as PXRD data, including the 7th blind test case.