MS34-P02 | USE OF CRYSTAL STRUCTURE PREDICTION TO DESIGN TEMPLATE CRYSTALLIZATION EXPERIMENTS OF NITROBENZOIC ACID DERIVATIVES

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Crystal structure prediction of ansolvates and monohydrates of three 2-substiituted 4-nitrobenzoic acids were used to obtain information about the theoretical crystal structure energy landscape. Substituents included in the study were chlorine (2C4NBA), methyl (2Me4NBA) and hydroxyl (2OH4NBA). The obtained structure landscapes were analysed by searching for structures isostructural to the experimental crystal structures of the studied derivatives. This analysis for ansolvates clearly showed that most of such isostructural structures are present in the generated landscapes with part of the structures being energetically competitive or even more stable than the experimentally obtained polymorphs of the respective compound. In monohydrate landscape of 2Me4NBA isostructural phase to the only experimentally obtained monohydrate (2C4NBA monohydrate) was present, while the obtained landscape of 2OH4NBA monohydrates suggested that the obtained landscape is incomplete and doesn't contain all relevant structures. Crystallization experiments in the presence of seed crystals of the other compounds have been initiated to evaluate whether the predicted structures are experimentally accessible. The attempts to crystallize monohydrates of 2Me4NBA and 2OH4NBA in absence and presence of seeds of 2C4NBA monohydrate were unsuccessful.

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