MS31 Unconventional interactions or symmetries for optimized and new properties, including chirality

MS31-03
Solid solutions as a mean to investigate and exploit the structure-property relationships in molecular crystals
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Abstract
Current strategies for the rational design of crystal structure and the optimization of their properties rely on the exploitation of known supramolecular interactions and the application of rough practical experimental rules on thumbs. This approach enable the prediction of general structural features but does not allow for fine tuning and properties optimization. On the contrary the continuous stoichiometry variation that is typical of substitutional solid solutions offers a better control of structures and properties.
Here a series of solid solutions are presented to control solubility and thermal stability in multidrug solid forms. At the same time, stoichiometry variation in these phases give insight into the relative strength of different supramolecular interactions. In particular, a cocrystals that combines enantiomers of a chiral drug and a multiple chiral conformer exemplifies the potential of these materials to synthetic crystallography and crystal engineering.