

Two crystal growth stories: deracemization and co-crystal formation

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Story 1. There are several routes to produce compounds of single chirality, i.e. enantiopure molecules. Ever since the days of Pasteur, crystallisation has been a very important route. Here we discuss recent, crystallisation-based methods that allow complete deracemization, thus methods in which the unwanted compound is converted to the desired one and that can lead to 100% chiral purity and 100% yield.

Story 2. A significant amount of attention has been given to the design and synthesis of cocrystals by both industry and academia because of its potential to change a molecule's physicochemical properties. Here a data-driven cocrystal prediction method will be presented, based on two types of artificial neural network models and cocrystal data present in the Cambridge Structural Database.