

Harnessing the Power of Structural Data for Solid Form Assessment - in partnership with The Crystal Form Consortium

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The selection of the solid form for development is a key milestone in the conversion of a new chemical entity into a drug product. An understanding of the crystallisation process and associated material attributes is crucial to help select the right molecule, design the right product and transfer manufacturing process into production. As the pace of pharmaceutical development accelerates decisions made in solid form selection can have consequences on the whole lifecycle of a crystalline product.

We at the Cambridge Crystallographic Data Centre have been working with industrial partners, through our Crystal Form Consortium, to build software tools that quickly exploit a deeper understanding of the solid state. Central to this work is the Cambridge Structural Database (CSD), the world's most comprehensive database of small molecule crystal structures. With over 1.2 million entries, the information contained in the CSD can provide key links between structural features and potential development issues in the pharmaceutical arena using a knowledge-based approach known as solid form informatics.

A key use of solid form informatics is in crystal form assessment. Here we will describe how using the range of software tools available in the CSD Materials suite, alongside the application of new bespoke tools developed with the CFC members, crystal structures of drug molecules can be evaluated to help navigate the solid form landscape, also known as a 'solid form health check 1.,

References

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