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Chemistry : Physical Chemistry

Bhardwaj, Rajni Miglani, Eli Lilly and Company, , Indianapolis, , USA

Control and Prediction of Solid-State of Pharmaceuticals

Experimental and Computational Approaches

- Nominated as an outstanding PhD thesis by the University of Strathclyde
- Demonstrates the value of combined experimental and computational approaches for a better understanding of the key factors underpinning solid-state structures and diversity in four pharmaceutical compounds
- Details an effective methodology for high-throughput crystallization and analysis for solid-state form screening using 48/96 multi-well plates and Raman spectroscopy
- Reports for the first time on the prediction of crystallizability using the random forest statistical modelling technique

This thesis investigates a range of experimental and computational approaches for the discovery of solid forms. Furthermore, we gain, as readers, a better understanding of the key factors underpinning solid-structure and diversity. A major part of this thesis highlights experimental work carried out on two structurally very similar compounds. Another important section involves looking at the influence of small changes in structure and substituents on solid-structure and diversity using computational tools including crystal structure prediction, PIXEL calculations, Xpac, Mercury and statistical modeling tools. In addition, the author presents a fast validated method for solid-state form screening using Raman microscopy on multi-well plates to explore the experimental crystallization space. This thesis illustrates an inexpensive, practical and accurate way to predict the crystallizability of organic compounds based on molecular structure alone, and additionally highlights the molecular factors that inhibit or promote crystallization.

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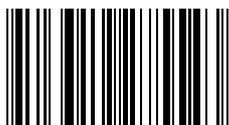
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