CMAC
FUTURE MANUFACTURING
RESEARCH HUB

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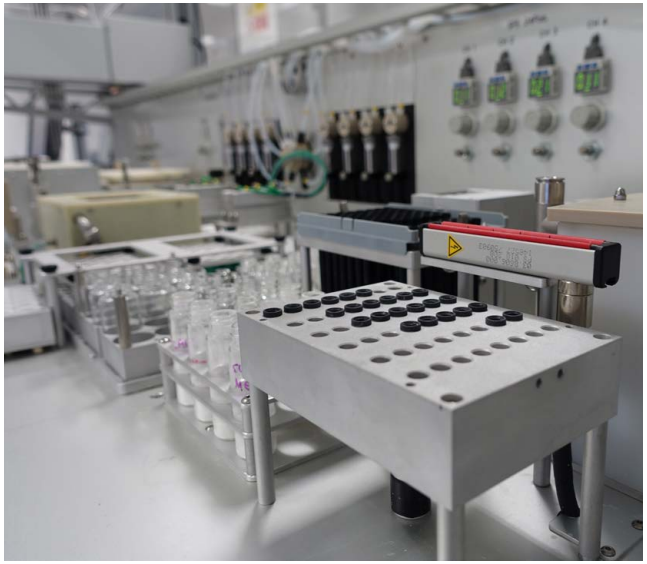
Solvent Selection

Towards predictive solvent selection for crystallisation and beyond

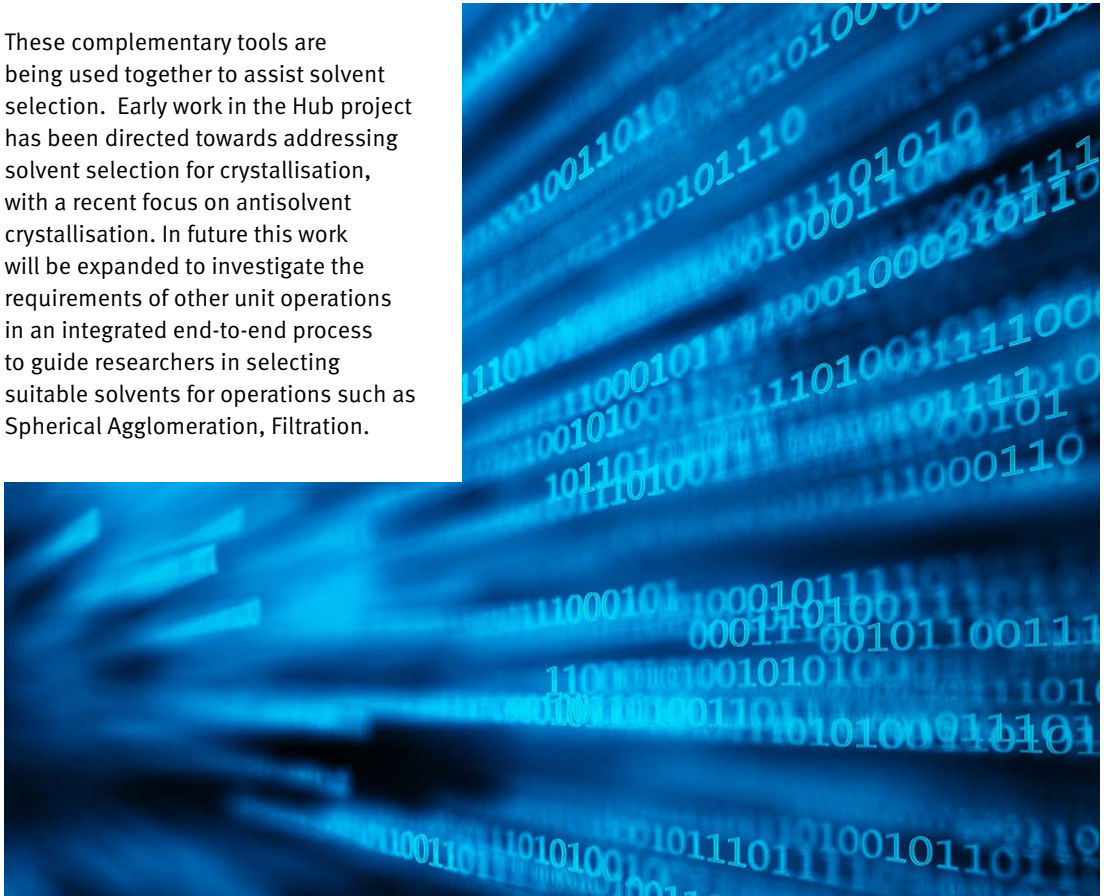
EPSRC
Engineering and Physical Sciences
Research Council

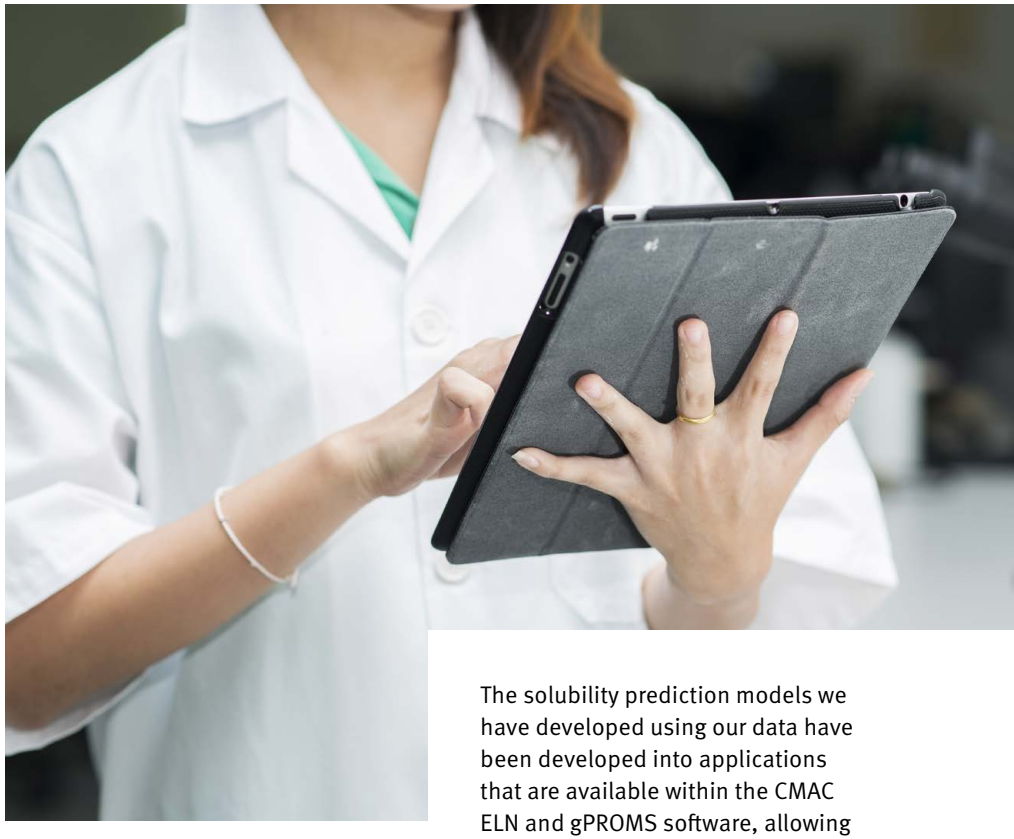
Solvent Selection



CMAC has the capability to undertake solvent selection for crystallisation process design through experimental and increasingly via predictive modelling approaches. The academic partners in CMAC have expertise in three key areas: (i) solubility measurement, (ii) solubility prediction using two approaches – COSMOtherm combined with Machine Learning (Strathclyde) and the group-contribution Statistical Associating Fluid Theory (SAFT) (Imperial), (iii) rational model-based solvent design.

These complementary tools are being used together to assist solvent selection. Early work in the Hub project has been directed towards addressing solvent selection for crystallisation, with a recent focus on antisolvent crystallisation. In future this work will be expanded to investigate the requirements of other unit operations in an integrated end-to-end process to guide researchers in selecting suitable solvents for operations such as Spherical Agglomeration, Filtration.





The CMAC Electronic Laboratory Notebook (ELN) and Data Management Policy have been a critical part of this effort. Together these tools ensure the collection, contextualisation and dissemination of data collected in solvent screening experiments by researchers so that it can be used to build and validate the predictive models being developed.

The solubility prediction models we have developed using our data have been developed into applications that are available within the CMAC ELN and gPROMS software, allowing researchers who are not specifically experts in predictive modelling to automatically generate predictions for Active Pharmaceutical ingredients (APIs) that are within model scope, comparing predictions to their experimental results or providing predictions that can help to plan experimental campaigns.

Our long term goal is to build a large enough library of data for a variety of APIs that will permit more general solvent selection predictions to become possible.