Chemistry Innovation
Knowledge Transfer Network

Molecular Modelling for Solvent Optimization

Modelling for Chemistry of one of Chemistry Innovation's seven key priority areas. Through consultation with industry and academia, the Modelling for Chemistry priority is focused on the modelling of chemical behaviour, material interactions and process performance to increase the productivity and value of research and innovation to industry.

Priority Manager, Dr Adrian Toland is driving a programme of activity that seeks to exploit the UK's expertise and knowledge base in modelling techniques and systems to deliver product and process innovation for industry.

Bioniqs is working with Chemistry Innovation as part an Advisory Group on Modelling for Chemistry that is seeking to address the important challenges of applying modelling systematically to chemistry and the chemistry-related challenges facing industry.

Solvent Database

Bioniqs has data on over 12 million solvent permutations which are evaluated to assess and identify ideal materials for each customer's application.

Bioniqs Service

This evaluation takes the form of the 'solventS' service which has two stages. The first is a small solvent screening study which evaluates about 450 commercially available green solvents, including Bioniqs protic ionic liquids. If a suitable solvent is not available a larger design study can be undertaken to create a new unique solvent that meets the all of the customer's requirements.

Technical Solution

To be able to screen such large numbers of solvents Bioniqs utilize their proprietary solvent modelling software. This software combines advanced structure-property alignment tools with a series of databases to evaluate the performance and properties of solvents along with other requirements such as cost and toxicity/environmental impact. The molecular modelling is based on pharmaceutical industry techniques and is refined using solubility parameter algorithms such as Hilderbrand and Hanson.

Benefits

This high throughput screening technology means that lab-bench testing can be focused on the small selection of candidate solvents identified in the modelling. The software can be used for both ionic and molecular solvents and by combining modelling with empirical data a highly accurate assessment of overall performance can be carried out leading to the identification of the ideal green solvent.

Further details can be found at **www.bioniqs.com**