Parvathi KRISHNAKUMAR

Technology Centre: Pharmaceutical Manufacturing Technology Centre (PMTC), UL, Limerick
Academic Mentor: Prof. Damien Thompson
Company Partner: Eli Lilly Kinsale Ltd.
Company Mentor: Dr. Salvador Garcia Munoz

Parvathi received her bachelor's degree in chemistry from University of Calicut, India, and master's degree from Cochin University of Science and Technology, India. She obtained her PhD from Homi Bhabha National Institute, India. Her doctoral work involved the in-silico study of structure, properties and interactions of molecular hydrated acid clusters.

Prof. Damien Thompson

Prof. Damien Thompson is an expert on modelling and designing of nanostructured materials for technology applications. He leads a group of PhD and postdoc researchers at the Bernal Institute in University of Limerick and collaborates with leading experimental and industry partners in European Framework, Science Foundation Ireland and Enterprise Ireland funded projects.

Dr. Salvador Garcia Munoz

Dr. Salvador Garcia Munoz senior engineer advisor for Eli Lilly and Co. He leads the efforts in building Digital Design capabilities in the small molecule design and development organization at Eli Lilly.He teaches a course on Process Analytics using Multivariate Latent Variable Techniques at Ghent University,Carnegie Mellon University and Imperial College of London. Dr. Garcia Munoz has been extensively involved in academic-industry collaborations and haschampioned the foundation of two major research programs.

Eli Lilly Kinsale Ltd

Eli Lilly Kinsale Ltd aims to support the development, manufacture and supply of many of the medicines in Lilly's portfolio. The site uses advanced chemical and biological processes to produce a range of pharmaceutical ingredients that produce a medical benefit; these are further processed at various facilities to supply medicines to patients worldwide. Eli Lilly Kinsale Ltd is engaged in four main business activities: small molecule API manufacture and supply, small molecule commercialization, bio-pharmaceutical manufacture and supply and bio-pharmaceutical commercialization.

Pharmaceutical Manufacturing Technology Centre (PMTC)

The PMTC was established in December 2013 and is led by an industry steering board with an active research program, in leading Irish RPOs, driven by its industry members. Companies access PMTC to create projects & execute world-beating industry-relevant research in advanced technology solutions which address contemporary manufacturing issues.

Parvathi's project

"Determination of SAFT-gamma-mie parameters for pharmaceutical compounds using experimental data from starting materials and computational chemistry tools"

Understanding molecular-scale properties of materials is crucial for their successful and safe manufacturing. In many cases, manufacturing processes are built around properties of the materials (solubility, strength, etc.). Prediction of physico-chemical properties of molecules and materials has been a major field of research for decades. This has led to the development of established computer-based models for property prediction. But they have drawbacks in terms of either low accuracy, not fit for process design or excessively long time to solution. The computationally simple, group-contribution "building block" method is based on the assumption that the properties of a compound can be determined from the chemically distinct functional groups that comprise it. Recently developed SAFT-gamma-mie methodology is an exciting new group approach to the estimation of physico-chemical properties. This group-contribution methodology has proven to be successful in predicting a wide range of properties, including phase equilibrium, solubilities and chemical equilibrium.

This project aims at exploring a hybrid solution to the application of SAFT-gamma-mie method for a new molecule. In this approach, parameters for available groups could be estimated from starting materials; and augmented with Quantum-Mechanical calculations. In this way, we combine the accuracy of quantum mechanics calculations with the computational simplicity of group contribution methods, and the goal of our project is to make a method that is transferable and can be applied to make predictions across many types of molecules that have not yet been experimentally tested.

If successful, this approach could be used in R&D to create a powerful predictive platform. This would enable in-silico process related decisions making, early in the development timelines, without the need to do any work with bulk amounts of materials. Our project applies state of the art computational modelling techniques and informatics tools to speedup material's discovery, selection and optimization, using high-performance computing-enabled predictive modelling.