Lecture Title:

Computational Chemistry in an Industrial Setting in the 21st Century

Speaker:
Dr Jas Bhachoo (Schrödinger, Germany)

Abstract: How have computational protocols advanced in the last few years to make quantifiable impact in projects for small molecules in drug design?

We will explore a birds-eye view of how state-of-the-art science is being used routinely, to alleviate challenging design questions and enable ideation across different teams. This is with a view to achieving one critical and common goal - speeding up drug discovery cycles.

Discover and the type of questions that Modeling can answer in an industrial setting, and what this means for the role of a Modeler.

Meeting Description: The past five years or so has witnessed a revolution in what in silico tools can offer. Massive advances in available computational power enable us to look at previously hidden properties such as solvation and dynamics. These advances give us unprecedented insights into the factors governing potency, selectivity, solubility and overall structure-property relationships, allowing us control over the key criteria of success.

Capitalising on these insights requires modelling to be fully integrated with the traditional pillars of drug design: biology and chemistry. This is not simply a matter of collating data from various departments into one place; what is required is a continuing mind-set change that will leverage collaborative design.

Discover how Modeling and Modelers can play a crucial role in impacting design projects, in this 40-minute seminar.

About the speaker: Jas is Principal Scientist at Schrodinger, and straddle the role of Applications Scientist and Head of Education in Europe, working with both the Commercial and Academic Community. She has been with Schrodinger for 18 years and headed a number of education initiatives world-wide: Europe, India and the U.S., where her focus has been to make modelling easy to understand thereby helping to bridge the historical gap often seen between Modelers and Chemists.

In a previous role, she was a Computational Chemist at BioFocus for 4 years working on contractual drug design projects for the UK Pharma industry. She continues to work on projects for our Pharmaceutical and Biotech Customers at Schrodinger, specializing in working with Medicinal Chemists.

Jas received her post-graduate in Computational Drug Design and Chemical Research from University College London with Distinction, and studied Mathematics and Chemistry at Sussex. She is co-author of book chapters such as “Modeling Peptide-Protein Interactions”.