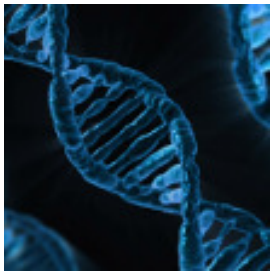

Contribution ID: **70** Type: **Oral presentation**

KEYNOTE 11 - Neutron scattering and drug discovey

Tuesday 5 June 2018 17:10 (40 minutes)

Neutron scattering, when combined with computational science, can aid in the drug discovery process in several ways. We illustrate how precision neutron crystallography can permit the derivation of the thermodynamic driving forces behind the binding of drugs to their targets. Also, we show how computational drug design protocols benefit considerably from a dynamic, rather than just a static, description of the protein to be modulated. We describe how small-angle and dynamic neutron scattering, when combined with computer simulation, provide useful information on the motions involved. We show that motions in single protein molecules are complex, being non-ergodic and non-equilibrium, and exhibit ageing, these properties arising from the fractal nature of the topology and geometry of the energy landscape explored. We describe how taking these motions into account in supercomputer-based virtual high-throughput screening has led to the discovery of lead compounds for a variety of diseases.

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Session Classification: Protein Dynamics and Drug Discovery

Track Classification: Protein dynamics and drug discovery