GRC Lecture Series

Simulation of Biomolecular Recognition Process in Atomic Precision and at Real-time

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At Seminar Hall, SLS, UoH
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Underlying the drug discovery, there exists the critical process of molecular recognition of ligand by the target protein. However, the computational approach of molecular recognition mostly relies on docking based techniques whose accuracies are limited by sampling issues. We have undertaken a novel approach where we capture the entire process of ligand diffusing to the protein cavity at atomistic resolution and in real-time. We have successfully applied this approach to T4 Lysozyme/benzene and cytochrome P450/camphor systems. In both cases, we simulated the binding process at crystallographic accuracy and correct kinetics. The ligand-binding pathways that emerge from these simulations unravel the complete mechanism of biomolecular recognition.