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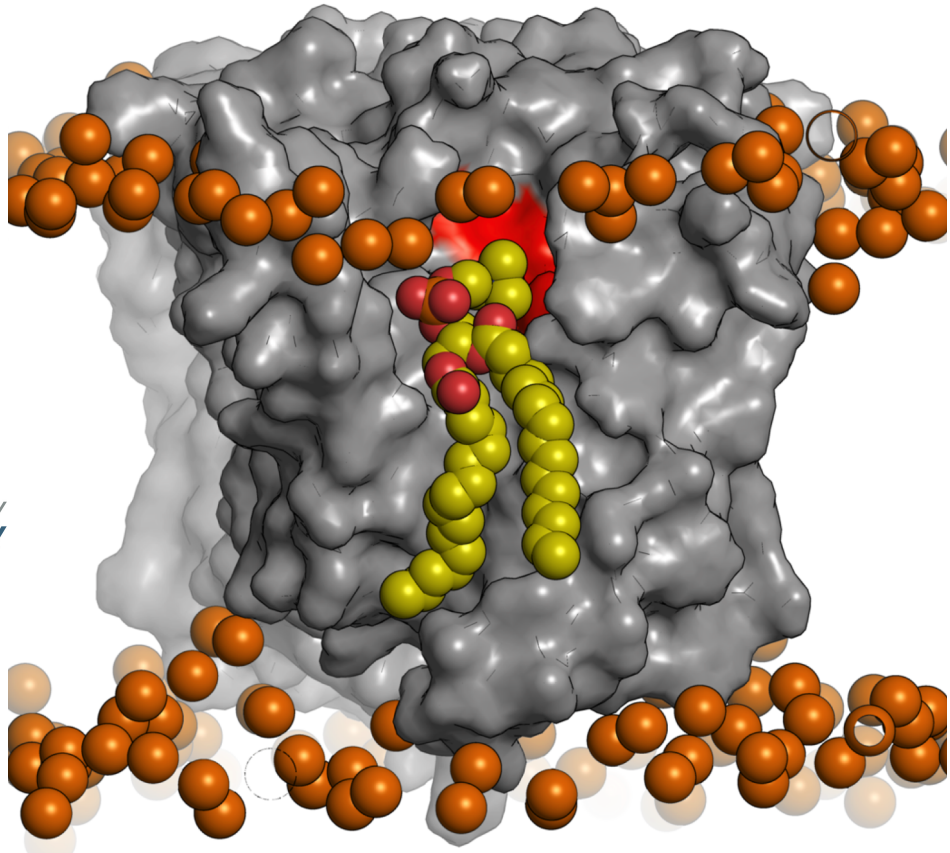

ROYAL SOCIETY OF CHEMISTRY

FRONTIERS OF BIOMOLECULAR SIMULATION

University of Southampton

1pm - 5.30pm, building 27, room 2003

UNIVERSITY OF Southampton

Schedule:

13.00 Welcome

13.05 Prof Jon Essex (Southampton) The computational modelling of protein-ligand structure, affinity & kinetics

13.50 Dr Carlo Camilloni (Cambridge) Enhancing simulations using NMR data

14.20 Prof Bert de Groot (MPI, Groningen) The molecular dynamics of permeation, inhibition & recognition

15.05 Tea break

15.25 Prof Charlie Laughton (Nottingham) Ensemble simulation strategies for the detection & validation of ligand-induced conformational change

16.10 Dr Phillip Stansfeld (Oxford) MemProtMD: Biomolecular simulations of integral membrane proteins

16.40 Prof Adrian Mulholland (Bristol) Enzyme mechanism, specificity & dynamics: insights into biological catalysts from modelling

17.30. Drinks reception

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