

CP5 sponsored a UK visit by Dr Xavier Daura from the Autonomous University of Barcelona from 10-15 October 2010.

Monday 11 October- Daresbury Laboratory.

Title: "Protein-ligand binding: exploiting structural conservation to identify binding sites and MD simulations of binding".

Local contact: Dr. Bill Smith. [bill.smith@stfc.ac.uk]

Meetings held: with Bill Smith and Ilian Todorov, on current developments in DL_POLY and other simulation-related topics such as calculation of free energy differences; with other members of the Computational Chemistry group, on current research projects and possible common interests.

Wednesday 13 October - Nottingham University, School of Chemistry.

Title: "Polypeptide folding on a conformational-space network: thermodynamics and kinetics".

Local contact: Prof. Anthony Stace. [Anthony.Stace@nottingham.ac.uk]

Meetings held: with Jonathan Hirst and members of his group and with Charlie Laughton (School of Pharmacy), on current research projects and possible common interests; with Tony Stace, who gave an overview of the research in Physical and Theoretical Chemistry at the School of Chemistry.

Thursday 14 October - Bradford University, Institute of Pharmaceutical Innovation

Title: "Polypeptide folding on a conformational-space network: thermodynamics and kinetics".

Local contact: Dr. John Kendrick. [j.kendrick@bradford.ac.uk]

Meetings held: with Jamshed Anwar, John Kendrick and members of their groups, on current research projects and possible common interests; exploring possibilities for a collaborative project.

Friday 15 October - University of Leeds, Centre for Molecular Nanoscience - School of Chemistry

Title: "Polypeptide folding on a conformational-space network: thermodynamics and kinetics".

Local contact: Dr. Stefan Auer. [S.Auer@leeds.ac.uk]

Meetings held: with Stefan Auer, Emanuele Paci (Institute of Molecular and Cellular Biology) and Sarah Harris (School of Physics and Astronomy) on current research projects and possible common interests; discussions with Stefan Auer on the potential application of the methods presented in the lecture to the study of polypeptide aggregation.