IDPbyNMR Intensive Training Module May 2-3, 2012
Protein Structure Analysis using NMR Chemical Shifts
at Department of Chemistry, University of Cambridge

Organizing Committee
Prof Michele Vendruscolo
Dr Andrea Cavalli

Intrinsically disordered proteins (IDPs) are widespread in nature, as they play a variety of significant biological roles. However, to date, they have not been characterized structurally in much detail. Recent efforts in NMR spectroscopy have started to uncover the breadth of their conformational space. Chemical shifts, which are the most readily and accurately measurable NMR parameters, can be used for detection of transiently formed structure in intrinsically disordered proteins. This strategy, which is widely applicable, enables quantitative structural analysis to be carried out to address a range of complex biological problems.

This course was aimed to develop an understanding of the computational technique of NMR chemical shifts to analyze protein secondary and tertiary structures. After a comprehensive introduction of Molecular Dynamics simulations by Prof Michele Vendruscolo, Dr Andrea Cavalli and Dr Carlo Camilloni gave practical hands-on sessions. Lectures on the first day of the workshop introduced the participants to the theoretical aspects of Molecular Dynamics Simulations, followed by a practical session on the use of Cheshire method, which was developed in the group. Theory and applications of protein structure determination using chemical shifts were covered on the second day of the course in the form of didactic modules, which included a hands-on session on the CamShift method. Handouts were provided for each module. Towards the end of the course, participants developed a basic understanding of the use of these methods, sufficient enough to plan the application of the methods to their respective research projects. The workshop witnessed effective communication in the form of discussions between the IDPbyNMR fellows and course organizers.

University of Cambridge provided the perfect academic setting for the course where the fellows were housed in college accommodation. Informal dinners in the evenings saw the fellows engage in discussions while, also, relaxing after the intensive training during the day.

In future, the UCAM partner of IDPbyNMR ITN aims to hold an extensive workshop where participants will be encouraged to bring their own data for analysis.

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Unilever Centre Training Room, Department of Chemistry, University of
Cambridge, Cambridge CB2 1EW

Day 1, May 2

9:00-10:00 : Introduction to Monte Carlo and Molecular Dynamics
(Michele Vendruscolo)
Coffee Break
10:00-11:00 : How to run a simulation (Andrea Cavalli)
11:00-12:00 : Advanced sampling techniques (Carlo Camilloni)
Lunch
13:00-18:00 : Practicals on Monte Carlo and Molecular Dynamics
18:30   : Dinner at St. Johns Chop House

Day 2, May 3

9:00-10:00 : Introduction to restrained MC and MD
(Michele Vendruscolo)
Coffee Break
10:00-11:00 : How to run a restrained simulation (Andrea Cavalli)
11:00-12:00 : Advanced sampling techniques using restraints
(Carlo Camilloni)
Lunch
13:00-18:00 : Practicals on restrained MC and MD
18:30   : Dinner at The Eagle, Cambridge

Participants

IDPbyNMR Fellows

Name	Institution
Cesyen Cedeño	VIB - Department of Structural Biology (Brussels)
Pallab Bhowmick	VIB - Department of Structural Biology (Brussels)
Jaka Kragelj	CNRS-IBS, Grenoble
Zsófia Sólyom	CNRS-IBS, Grenoble
Tomas Hosek	CERM, Florence, Italy
Eduardo Calçada	CERM, Florence, Italy
Erica Valentini	EMBL Hamburg
Sergio Gil Caballero	Bruker BioSpin AG
Anna Lovrics	Biotalentum Ltd.
Biao Fu	Department of Chemistry, UCAM
Priyanka Joshi	Department of Chemistry, UCAM
Magdalena Korzak	Giotto Biotech, Sesto Fiorentino, Italy

Outside the IDPbyNMR Network

Sara Martos	VIB - Department of Structural Biology (Brussels)