STRUCTURAL BIOLOGY COURSE SCHEDULE

Tuesday (Feb 16th) **Auditório Corino de Andrade**

10:00-10:20	Welcome address (S. M. R.)
10:20-12:00	Structural Biology: Overview (S. M. R.)
LUNCH	
14:00-15:00	Protein Crystallography: Overview (P.P.)
15:30-17:00	Recombinant protein expression and purification (F. F. S.)

Wednesday (Feb 17th) **Meeting Room A**

9:30-10:30	Electron Microscopy: Overview (J. M. C.)
10:30-11:30	How to read a Structural Biology paper (S.M.R.)
11:45-13:00	Natural anticoagulants (P. P.)
LUNCH	
14:30-16:00	**PRACTICAL 1:** MODEL BUILDING (Groups I, II) **PRACTICAL 2:** PDB AND PYMOL (Groups III, IV)
16:00-17:30	**PRACTICAL 1:** MODEL BUILDING (Group III, IV) **PRACTICAL 2:** PDB AND PYMOL (Groups I, II)

Thursday (Feb 18th) **Meeting Room A**

10:00-11:15	Biological SAXS: principles and applications (B. C.)
11:30-12:30	An integrated structural study on pathogenicity factors of the human pathogen *Mycoplasma genitalium* (B. C.)
LUNCH	
14:00-15:00	Polyglutamine disorders: more than simple repeats (S. M. R.)
15:00-17:00	JOURNAL CLUB PREPARATION

Friday (Feb 19th) **Meeting Room A**

9:30-10:30	Structural and functional studies of a protein involved in osmotic adaptation (J.M.C.)
10:45-12:00	Computational Approaches to Predict and Refine the Structure of Proteins (P.A.F)
LUNCH	
14:30-17:00	Journal club

Course Tutors:

Sandra de Macedo Ribeiro (Protein Crystallography Group, IBMC/i3S, Porto)
Pedro J. B. Pereira (Biomolecular Structure Group, IBMC/i3S, Porto)
João Morais Cabral (Structural Biochemistry Group, IBMC/i3S, Porto)
Frederico Ferreira da Silva (B2Tech - BIOCHEMICAL AND BIOPHYSICAL TECHNOLOGIES, IBMC/i3S, Porto)
Pedro Alexandrino Fernandes (Dept. Química e Bioquímica, Fac. Ciências, Porto)
Bárbara Calisto (ESRF, Grenoble, France)

Suggested Bibliography:

Protein crystallography and structure analysis

1 - *International Tables for Crystallography (2006). Vol. F, Chapter 1.1, pp. 1–63*

2 - G. Rhodes (2006). Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models. Academic Press, Burlington. ISBN 9780125870733.

3 - Minor Jr., D.L. (2007). The Neurobiologist's Guide to Structural Biology: A Primer on Why Macromolecular Structure Matters and How to Evaluate Structural Data. Neuron 54: 511–533 (http://www.ncbi.nlm.nih.gov/pubmed/17521566)

4 - Cowieson, N.P., Kobe, B., Martin, J.L. (2008). United we stand: combining structural methods. Curr Opin Struct Biol18:617-22. (http://www.ncbi.nlm.nih.gov/pubmed/18755272)

5 – Lander, G.C., Saibil, HR., Nogales. E. (2012). Go hybrid: EM, crystallography, and beyond. Curr Opin Struct Biol. 22:627-35. (http://www.ncbi.nlm.nih.gov/pubmed/22835744)

6 – Dyer, K.N., Hammel, M., Rambo, R.P., Tsutakawa, S.E., Rodic, I., Classen, S., Tainer, J.A., Hura, G.L. (2014). High-throughput SAXS for the characterization of biomolecules in solution: a practical approach. Methods Mol Biol. 1091:245-58. (http://www.ncbi.nlm.nih.gov/pubmed/24203338).

7 – Petoukhov, M.V., Svergun, D.I. (2013). Applications of small-angle X-ray scattering to biomacromolecular solutions. Int J Biochem Cell Biol. 45:429-37. (http://www.ncbi.nlm.nih.gov/pubmed/23235262)

Protein Interactions and Computational Biology:

1 – Kastritis, P.L., Bonvin, A.M. (2013). On the binding affinity of macromolecular interactions: daring to ask why proteins interact. J R Soc Interface. 10:20120835. (http://www.ncbi.nlm.nih.gov/pubmed/23235262)

2 - Moreira, IS; Fernandes, PA; Ramos, MJ (2010). Protein-Protein Docking: Dealing with the Unknown, J. Comput. Chem. 31: 317 (http://www.ncbi.nlm.nih.gov/pubmed/19462412)

3 - Sousa, SF; Ribeiro AJM; Coimbra JTS; Neves, RPP; Martins, SA; Moorthy, NSHN; Fernandes, PA; Ramos, MJ (2013). Protein-Ligand Docking in the New Millennium - A Retrospective of 10 Years in the Field, CURRENT MEDICINAL CHEMISTRY 20: 2296-2314 (http://www.ncbi.nlm.nih.gov/pubmed/23531220)

4 - Sousa, SF; Fernandes, PA; Ramos, MJ (2006). Protein-ligand docking: Current status and future challenges. Proteins 65: 15. (http://www.ncbi.nlm.nih.gov/pubmed/16862531)

Journal Club:

1- Moreira IS, Martins JM, Coimbra JTS, Ramos MJ, Fernandes PA
A new scoring function for protein–protein docking that identifies native structures with unprecedented accuracy, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 2015, 17, 2378. (http://www.ncbi.nlm.nih.gov/pubmed/25490550).

2 – Cao, E., Liao, M., Cheng, Y., Julius, D. (2013). TRPV1 structures in distinct conformations reveal activation mechanisms. Nature 504:113-8. (http://www.ncbi.nlm.nih.gov/pubmed/24305161)

3- Krukenberg, K.A., Förster, F., Rice, L.M., Sali, A., Agard, D.A. (2008). Multiple conformations of E. coli Hsp90 in solution: insights into the conformational dynamics of Hsp90. Structure 16:755-65. (http://www.ncbi.nlm.nih.gov/pubmed/18462680)

4- Santos, J.A., Alonso-García, N., Macedo-Ribeiro, S., Pereira, P.J. (2014). The unique regulation of iron-sulfur cluster biogenesis in a Gram-positive bacterium. Proc Natl Acad Sci U S A. 111:E2251-60. (http://www.ncbi.nlm.nih.gov/pubmed/24847070).

Additional Reading:

History of Crystallography:
http://onlinelibrary.wiley.com/doi/10.1111/febs.12796/full

Protein Crystallography for non-crystallographers:
http://www.ncbi.nlm.nih.gov/pubmed/18034855