

## GABBA AND MCBIOL PHD PROGRAMMES

### STRUCTURAL BIOLOGY COURSE SCHEDULE

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#### Monday (April 23<sup>th</sup>) Meeting Room A

- 10:00-10:20 Welcome address (S. M. R.)
- 10:20-12:00 Structural Biology and Protein Crystallography Overview (P. P.)
- LUNCH
- 14:00-15:00 Biological Small Angle X-ray Scattering: principles and applications (J.A.M.)
- 15:30-16:30 Natural anticoagulants (P.P.)
- 17:00-18:00 Polyglutamine disorders: more than simple repeats (S. M. R.)

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#### Tuesday (April 24<sup>th</sup>) Meeting Room B

- 9:00-10:30 Structural and functional studies of membrane proteins (J. M. C.)
- 11:00-13:00 Computational Approaches to Predict and Refine the Structure of Proteins (J.C.)
- LUNCH
- 14:30-16:00 **PRACTICAL 1:** MODEL BUILDING (Groups I, II) – 115S2  
**PRACTICAL 2:** How to read a Structural Biology paper; PDB AND PYMOL (Groups III, IV) – Room B
- 16:00-17:30 **PRACTICAL 1:** MODEL BUILDING (Group III, IV) – 115S2  
**PRACTICAL 2:** How to read a Structural Biology paper; PDB AND PYMOL (Groups I, II) – Room B

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#### Course Tutors:

Sandra de Macedo Ribeiro (Biomolecular Structure and Function Group, IBMC/i3S, Porto)  
Pedro J. B. Pereira (Macromolecular Structure Group, IBMC/i3S, Porto)  
José António Manso (Macromolecular Structure Group, IBMC/i3S, Porto)  
João Morais Cabral (Structural Biochemistry Group, IBMC/i3S, Porto)  
João Coimbra (Dept. Química e Bioquímica, Fac. Ciências, Universidade do Porto)

#### Suggested Bibliography:

##### Protein crystallography and structure analysis

- 1 – A. L. Lamb, T. J. Kappock and N. R. Silvaggi (2015). You are lost without a map: Navigating the sea of protein structures. *Biochim Biophys Acta* 1854: 258–268. (<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5051661/>)
- 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 Biol* 18:617-22. (<http://www.ncbi.nlm.nih.gov/pubmed/18755272>)

5 – Lander, G.C., Saibil, H.R., 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>)

5 – S. A. Adcock, and J. A. McCammon (2006). Molecular Dynamics: Survey of Methods for Simulating the Activity of Proteins. *Chem. Rev.* 106: 1589-1615. (<https://pubs.acs.org/doi/abs/10.1021/cr040426m>)

#### **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>

Protein crystallography for aspiring crystallographers or how to avoid pitfalls and traps in macromolecular structure determination  
: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4080831/>