HADDOCK workshop on Information-driven modelling of biomolecular complexes

Coimbra University – December 18-19th, 2019

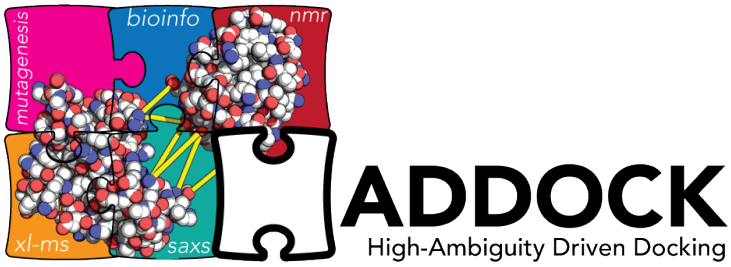
The prediction of the quaternary structure of biomolecular macromolecules is of paramount importance for fundamental understanding of cellular processes and drug design. In the era of integrative structural biology, one way of increasing the accuracy of modelling methods used to predict the structure of biomolecular complexes is to include as much experimental or predictive information as possible in the process.

We have developed for this purpose a versatile flexible information-driven docking approach HADDOCK (http://www.bonvinlab.org/software/haddock2.2) [1,2]. HADDOCK can integrate information derived from biochemical, biophysical or bioinformatics methods to enhance sampling, scoring, or both [3]. The information that can be integrated is quite diverse: among others interface restraints from NMR, mutagenesis experiments, or bioinformatics predictions and, recently, cryo-electron microscopy experiments [4].

The workshop given by Prof. Alexandre Bonvin from Utrecht University, the Netherlands, will consist of lectures and hands-on session on computers during which participants will learn to use HADDOCK and other related tools for the modelling for biomolecular complexes.

References

1. G.C.P van Zundert, J.P.G.L.M. Rodrigues, M. Trellet, C. Schmitz, P.L. Kastritis, E. Karaca, A.S.J. Melquiond, M. van Dijk, S.J. de Vries and A.M.J.J. Bonvin. The HADDOCK2.2 webserver: User-friendly integrative modeling of biomolecular complexes. J. Mol. Biol., 428, 720-725 (2015).
2. S.J. de Vries, M. van Dijk and A.M.J.J. Bonvin The HADDOCK web server for data-driven biomolecular docking. Nature Protocols, 5, 883-897 (2010).
3. J.P.G.L.M Rodrigues and A.M.J.J. Bonvin Integrative computational modeling of protein interactions. FEBS J., 281, 1988-2003 (2014).
4. G.C.P. van Zundert, A.S.J. Melquiond and A.M.J.J. Bonvin. Integrative modeling of biomolecular complexes: HADDOCKing with Cryo-EM data. *Structure*. **23**, 949-960 (2015).



Workshop on Modelling of Biomolecular Interactions with HADDOCK

Where : Coimbra University
When : December 18-19th, 2018
Training : Alexandre Bonvin and Panos Koukos from Utrecht University, the Netherlands

Agenda

November 18th:

- 15:30 - 17:00: Lecture
    - *General introduction to integrative modelling and HADDOCK*
- 17:00 - 17:15: Short break
- 17:15 - 19:00: Computer practical I
    - *Basic protein-protein docking with HADDOCK*

November 19th:

- 09:00 – 10:30: Lecture
    - *HADDOCK advanced topics*
- 10:30 - 11:00: Coffee break
- 11:00 - 13:00: Computer practical II
    - *Integrative modelling of a large macromolecular assembly using cross-linking and cryo-EM data*
- 13:00 - 14:00: Lunch
- 14:00 - 15:30: Computer practical III
    - *Integrative modelling of a large macromolecular assembly using cross-linking and cryo-EM data - continued*
- 15:30 - 16:00: Coffee break
- 16:00 – 17:30: Computer practical IV
    - *Integrative modelling of a large macromolecular assembly using cross-linking and cryo-EM data - continued*
- 17:30 – 18:30: Question and answer session and wrap up

Online tutorials:

- **HADDOCK basic protein-protein docking tutorial**: A tutorial demonstrating the use of the HADDOCK web server to model a protein-protein complex using interface information derived from NMR chemical shift perturbation data. This tutorial does not require any Linux expertise and only makes use of our web server and PyMol for visualisation/analysis

  http://www.bonvinlab.org/education/HADDOCK24/HADDOCK24-protein-protein-basic

- **Integrative modelling of the RNA polymerase III apo complex:** A combination of our DISVIS, POWERFIT and HADDOCK2.4 portals using cross-links and cryo-EM data to model a large macromolecular assembly.

  http://www.bonvinlab.org/education/HADDOCK24/RNA-Pol-III/

Registration deadline: 30th of November 2019

Registration: email to irina.moreira@cnc.uc.pt

Note: There is a limit of 20 participants in this workshop.

Training: Prof. Dr. A.M.J.J. Bonvin

Contact Address

Bijvoet Center for Biomolecular Research
Science Faculty/Chemistry, Utrecht University
Padualaan 8, 3584 CH Utrecht, the Netherlands
Email: a.m.j.j.bonvin@uu.nl
Web: http://www.uu.nl/staff/AMJJBonvin / http://bonvinlab.org

Short CV (A full CV can be downloaded here.)
Alexandre Bonvin (1964) studied Chemistry at Lausanne University, Switzerland and obtained his PhD at Utrecht University in the Netherlands (1993). After two post-doc periods at Yale University (USA) and the ETHZ (CH) he joined Utrecht University in 1998 where he was appointed full professor of computational structural biology in 2009. In 2006, he received a prestigious VICI grant from the Dutch Research Council. He was director of chemical education from February 2009 until February 2012, vice head of the Chemistry Department from 2010 until April 2012 and since September 2019 Scientific Director of the Bijvoet Centre for Biomolecular Research. He is participating to several EU projects including the BioExcel Center of Excellence in Biomolecular Simulations and the European Open Science Cloud Hub project. His work has resulted in over 225 peer-reviewed publications.

- ISI Web of Science, author ID: A-5420-2009
- Google Scholar Citations
- ORCID: http://orcid.org/0000-0001-7369-1322

Research

Research within the computational structural biology group focuses on the development of reliable bioinformatics and computational approaches to predict, model and dissect biomolecular interactions at atomic level. For this, bioinformatics data, structural information and available biochemical or biophysical experimental data are combined to drive the modelling process. This is implemented and further developed in the widely used HADDOCK software for the modelling of biomolecular complexes (http://bonvinlab.org/software).

By following a holistic approach integrating various experimental information sources with computational structural biology methods we aim at obtaining a comprehensive description of the structural and dynamic landscape of complex biomolecular machines, adding the structural dimension to interaction networks and opening the route to systematic and genome-wide studies of biomolecular interactions.

Selected peer-reviewed publications

1. E. Karaca, J.P.G.L.M. Rodrigues, A. Graziadei, **A.M.J.J. Bonvin** and T. Carlomagno. An Integrative Framework for Structure Determination of Molecular Machines. *Nature Methods 14*, 897-902 (2017).
2. G.C.P. van Zundert, M. Trellet, J. Schaarschmidt, Z. Kurkcuoglu, M. David, M. Verlato, A. Rosato and **A.M.J.J. Bonvin**. The DisVis and PowerFit web servers: Explorative and Integrative Modeling of Biomolecular Complexes. *J. Mol. Biol.*, *429*, 399-407 (2017).
3. A Vangone and **A.M.J.J. Bonvin**. Contacts-based prediction of binding affinity in protein-protein complexes. *eLife*, *4*, e07454 (2015).
4. G.C.P. van Zundert, A.S.J. Melquiond and **A.M.J.J. Bonvin** (2015). Integrative modeling of biomolecular complexes: HADDOCKing with Cryo-EM data. *Structure*. **23**, 949-960.
5. P.L. Kastritis, J.P.G.L.M Rodrigues, G.E. Folkers, R. Boelens and **A.M.J.J. Bonvin** (2014). Proteins feel more than they see: Fine-tuning of binding affinity by properties of the non-interacting surface.*J. Mol. Biol.* **426**, 2632-2652.
6. E. Karaca and **A.M.J.J. Bonvin** (2011). A multi-domain flexible docking approach to deal with large conformational changes in the modeling of biomolecular complexes. ***Structure***, **18,** 555-565.
7. T. Schneider, Th. Kruse, R. Wimmer, I. Wiedemann, V. Sass, U. Pag, A. Jansen, A.K. Nielsen, P.H. Mygind, D.S. Raventós, S. Neve, B. Ravn, **A.M.J.J. Bonvin**, L. De Maria, L. Kamenova, H.-G. Sahl and H.-H. Kristensen (2010). Plectasin, a fungal defensin antibiotic peptide, targets the bacterial cell wall precursor Lipid II. ***Science***, **328**, 1168-1172.
8. P.L. Kastritis and **A.M.J.J. Bonvin** (2010). Are scoring functions in protein-protein docking ready to predict interactomes? Clues from a novel binding affinity benchmark. ***J. Proteome Res.***, **9**, 2216-2225.
9. S.J. de Vries, M. van Dijk and **A.M.J.J. Bonvin** (2010). The HADDOCK web server for data-driven biomolecular docking. ***Nature Protocols***, **5**, 883-897.
10. C. Dominguez, R. Boelens and **A.M.J.J. Bonvin** (2003). HADDOCK: A protein-protein docking approach based on biochemical or biophysical information. ***J. Am. Chem. Soc.*** **125**, 1731-1737.