Curriculum vitae — *Dr. A. M. J. J. Bonvin*

January 17th, 2024

Personal

Name: Alexandre M.J.J. Bonvin
Born : November 7, 1964
Place of birth: Sion, Switzerland
Nationalities: Swiss, Dutch
Married to K.N. Bonvin-Witteveen, two daughters

Languages

Fluent in French, English and Dutch, very good knowledge of German.

Education

High school:

maturité B (classical division). Collège des Creusets, Sion, Switzerland (1984)

Undergraduate:

Master's degree Chemistry, University of Lausanne, Switzerland (1989) with specialization in NMR Spectroscopy (Prof. Dr. G. Bodenhausen)

Graduate:

PhD in Chemistry "cum laude" under the supervision of Prof. Dr. R. Kaptein and Dr. R. Boelens, Utrecht University, the Netherlands (Dec. 1993). "Determination of biomolecular structure by NMR. Use of relaxation matrix Calculations"

Present position

Professor of Computational Structural Biology, Faculty of Science/Chemistry, Utrecht University
Scientific Director Bijvoet Centre from Biomolecular Research
Vice head of the Chemistry Department

Previous work

August 2003-August 2009

Associate Professor, NMR Research group, Department of Chemistry, Utrecht University

April 1998-July2003

Assistant Professor, NMR Research group, Department of Chemistry, Utrecht University

June 1996-March 1998

Research assistant with Prof. W.F. van Gunsteren, Physical Chemistry, Swiss Federal Institute of Technology, Zürich, Switzerland

April 1994-May 1996

Research Associate with Prof. A. T. Brünger, the Howard Hughes Medical Institute and Department of Molecular Biophysics and Biochemistry, Yale University, New Haven CT, USA

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https://www.uu.nl/staff/AMJJBonvin
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the Netherlands

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Email : alexandre.bonvin@gmail.com

Major research interests

Biomolecular interactions; protein structure and dynamics; biomolecular modeling; docking; molecular dynamics; NMR spectroscopy; structural molecular biology

Table of Content

Teaching activities

- Programme Director of the PhD programme Molecular Life Sciences of the Graduate School of Life Sciences, UU 09-2019 - 12-2023
- Chairman of the education advisory commission for the Chemistry Department 2015 – 09-2019
- Utrecht University, member of the education advisory commission, May 2012 – Sept 2019
- Utrecht University, Director of Chemical Education and vice-head of the Chemistry Department, Feb. 2009 – Feb. 2012
- Member of the education commission of the lifescience master of Utrecht University (until 2009)
- University Senior Teaching Certificate, Utrecht University, Jan. 2003
- University Basic Teaching Certificate, Utrecht University, Sept. 2000
- Utrecht University College (2000-2014): lecturer in the Advanced Chemistry Course

Teaching Utrecht University (1998-present)

- Lecturer and coordinator of the second year Molecular Modelling and Mathematics course 2005-2013
- Lecturer and coordinator of the second year NMR & Molecular Modelling course 2014-present
- Lecturer in the third year Structural Biology course "Computational aspects of NMR structure determination". 1999-2016
- Lecturer and coordinator of the MCLS master course on Structural Bioinformatics and Modelling. 2017-present
- Lecturer in various courses of the "Biomolecular and Cellular LifeScience" master
- Lecturer in the Advanced Chemistry course at University College Utrecht (UCU) 1999-2013
- Supervisor of the second year NMR project practical
- Supervisor of the bachelor thesis and master research projects
- Tutor for first year chemistry students. 2007-present
- Guest lecturer at high schools to promote chemistry in Utrecht

Teaching – PhD courses

- Co-Organiser and lecturer of the Bijvoet (UU) / IMM (Radboud Universiteit) BNRA PhD cursus (1998-2008, every second year)
- Co-Organizer EMBO Global Exchange Lecture Course "Structural And Biophysical Methods For Biological Macromolecules In Solution", Bejing April 2011, Hyderabad December 2012, Sao Paolo, January 2014, Taipei, May 2015, Suwon, South Korea, June 2016.
- (Co-)Organizer of the EMBO practical course on "Integrative Modelling of Biomolecular Interactions", Barcelona, July 2016 and 2018, Izmir 2021 and 2023
- (Co-)Organizer of the BioExcel summerschool on Biomolecular Simulations, Pula Sardinia, 2018-2023

Memberships

- Netherlands Royal Society for Chemistry (KNCV)
- Netherlands Society for Biochemistry and Molecular Biology (NVBMB)
- Biophysical Society

Other activities

- Member of the UU Faculty of Science Impact group
- Member of the Chemistry Department Advisory Committee Faculty
- Member of the European Open Science Cloud (EOSC) Association Task Force on "Researcher Engagement and Adoption"

- Consulting for Exscientia, UK, 2022 - present
- Consulting for UBC Pharma, Slough, UK, 2021 - present
- Scientific advisor for Keygene, Wageningen, the Netherlands, 2018 - present
- Project Management Board Member of EOSC-Hub (H2020 project), 2018-2021
- Advisory council member of the Institute of Biomedical Sciences (IBMS), Academia Sinica, Taiwan, Jan. 2017-present
- Scientific advisory board member of PDBe, EBI, Hinxton, Sept. 2016-2022
- Advisory board member of the SURF innovation programme "Reken- en Datainfrastructuren", 2016-2018.
- Project Management Board Member of EGI-Engage (H2020 project), 2015-2017
- Member of the wwPDB task force on integrative models, 2014-present
- External Advisory Board Member of EGI-Inspire (European GRID Initiative), 2010-2015
- Advisory Board Member of CCPN (Collaborative Computing Project in NMR), 2010-present
- Member of the INSTRUCT working group M "Computational Structural Biology", 2008-present
- Board NWO-CW (Dutch Science Chemical Research Council) study section Biomoleculaire Chemie, 2009-2012
- Consulting on Molecular Modelling for Genmab B.V., Utrecht, the Netherlands, 2007-2008
- Member of the advisory panel of the Volkswagen Foundation in Germany in the area of "Conformational Control of Biomolecular Function"
- Consulting on Molecular Modelling for Nestlé Research Institute, Vers-chez-les-Blanc, CH-1000 Lausanne, Switzerland, 1999-2001

Grants & awards

- RVO (Rjksdienst voor Ondernemend Nederland) grant – Demonstratie energie- en klimaatinovatie (DEI+) – *"Experiments on tuning software-systems for greener operation".* Total budget 733'223, UU budget 25'000 euros.
- EC H2020 (HORIZON-EUROHPC-JU-2021-COE-01-02), Centers of Excellences (2022): "*BioExcel3: Centre of Excellence for Computational Biomolecular Research".* Total budget 6'0000'00 euros, UU budget 1'008'000 euros.
- EC Eurostar 3 (2022): "*High-throughput ImmunoTherapy Screening".* Total budget 1'000'000 euros, UU budget 121'000 euros.
- eTEC grant from the Netherlands eScience Center (2021). Title: *"Virtual Research Environment for Integrative Modelling of Biomolecular Complexes*". 500'000 euros.
- EC H2020 e-Infrastructure Programme (H2020-EINFRAEOSC-07) (2020): "*EOSC-ACE".* Total budget 8M euros, UU budget 87'500 euros.
- EU Innovative Medicines Initiative (IMI) (2020). Co-applicant. *"CARE: Corona-accelerated R&D in Europe"*. Total budget 70 million euros (50% of which from EU), UU/Bonvin budget 140'625 euros.
- NWO-ENW high throughput computing grant (2020), for 8 million SBU wall clock hours (4M per year) for the coming two years to support WeNMR and the HADDOCK web portal.
- PPS Technology Area grant from the Netherlands Organization for Scientific Research (NWO-ENW) (2019). Co-applicant. *"Monitoring and Visualizing Protein Societal Behavior in the Cell; an Integrative Approach"*. Total budget 1'100'00 euros, UU/Bonvin budget 269'400 euros.
- PPS programmatoaslag , Topsector Chemie (2019). *"Unravelling the ubiquitin ligase binding landscape"*. 36'450 euros.
- EC H2020 e-Infrastructure Programme (H2020-EINFRAEDU-2018-1, Centers of Excellence) (2018): "*BioExcel2".* Total budget 8'0000'00 euros, UU budget 1'050'000 euros.

- SURFsara programme Machine Learning Enhanced HPC Applications (2018). Title: "3DeepFace: Distinguishing biological interfaces from crystal artifacts in biomolecular complexes using deep learning". 50'000 euros.
- EC H2020 e-Infrastructure Programme (H2020-EINFRA-12-2017) (2018): "*EOSC-Hub".* Total budget 30M euros, UU budget 269'250 euros.
- Accelerating Scientific Discovery (ASDI) grant from the Netherlands eScience Center (2016). Title: *"DeepRank: Scoring 3D protein-protein interaction models using deep learning*". 500'000 euros.
- TOP-PUNT grant from the Netherlands Organization for Scientific Research (NWO-CW) together with Prof. Marc Baldus (2015). Title: *"Caught in the act: a combined magnetic resonance – modelling approach to capture cellular machines at work"*. 2'000'000 euros.
- EC H2020 e-Infrastructure Programme (H2020-EINFRA-5-2015, Centers of Excellence) (2015): "*BioExcel".* Total budget 4'7800'00 euros, UU budget 279'000 euros.
- EC H2020 e-Infrastructure Programme (H2020-EINFRA-9-2015, Virtual Research Environments) (2015): "*West-Life".* Total budget 3'980'000 euros, UU budget 392'250 euros.
- EC H2020 e-Infrastructure Programme (H2020-EINFRA-2014-2) (2015): "*INDIGO-DataCLoud".* Total budget 11'000'00 euros, UU budget 171'000 euros.
- EC H2020 e-Infrastructure Programme (Research & Innovation Actions) (2015): "*EGI-Engage".* Total budget 8'000'00 euros, UU budget 58'000 euros. Leading the MoBrain Competence Center within EGI-Engage.
- Netherlands Organization for Scientific Research (NWO) visitor travel grant for the sabbatical stay of Prof. Jeff Grinstead, University of Puget Sound, USA. Title: "*Defining and Expanding the Limits of HADDOCK for Protein-Ligand Docking".* Grant number 040.11.299. (2011: 12'000.- euros for a six months stay).
- ECHO grant from the Netherlands Organization for Scientific Research (NWO-CW) (2011). Title: *"Zooming into large assemblies: a versatile incorporation of experimental data into biomolecular docking"*. Grant number 711.011.009. (2011-2014: 1 PhD student for 4 years for a total budget of 260'000.- euros).
- Computing grant from NWO / NCF (BG-031-11) entitled "Chemical education in the clouds" for bringing cloud computing into the Utrecht chemistry bachelor curriculum. (2011: 60'000 CPU core hours).
- Utrecht University Focus and Massa grant for one PhD student for a four years period (2010-2014).
- Computing grant from NWO / NCF (BG-002-09) entitled "e-NMR: NMR computational infrastructure" for Grid computing on the national Big Grid infrastructure . (2009: 2'500'000 CPU core hours.)
- EC 7th Framework Programme: Research Infrastructures: *"WeNMR: a worldwide e-Infrastructure for NMR and structural biology"*. Grant number 261572. Coordinator (2010-2013: EU budget 2'150'000.- UU budget including subcontracting 423'250.- euros)
- EC 7th Framework Programme: Research Infrastructures: *"e-NMR: Deploying and unifying the NMR e-Infrastructure in System Biology"*. Grant number 213010. (2007-2010: 4 post-doc years, UU budget including subcontracting 550'000.- euros).
- VICI grant from the Netherlands Organization for Scientific Research (NWO) (2006). Title: *"Predicting, modelling and understanding biomolecular interactions in the post-genomic era."* Grant Nr. 700.65.442. 1'250'000.- euros for five years.
- Participant to various other EU-funded projects and networks:
  - Structural Genomics consortium SPINE and SPINE-II
  - RTD project on structure validation (NMRQual)

- RTD project on NMR methodology for structural genomics (FIND).

- EC 6th Framework Programme FP6-2005-Lifescihealth: Specific Targeted Research Projects (STREP): *"BacAbs: Assessment of Structural Requirements in Complement-Mediated Bactericidal Events: Towards a Global Approach to the Selection of New Vaccine Candidates".* Reg. LSHG-CT-2006-037325. (2007-2009: 1 Post-doc and material credit for a total of Euros 259'620.-).
- EC 6th Framework Programme FP6-2004-Lifescihealth: Specific Targeted Research Projects (STREP): "*Extend NMR: Extending NMR for functional and structural genomics*". Reg. LSHG-CT-2005-018988. (2006-2008: 1 PhD student).
- Scientist in charge of a two year post-doctoral Marie Curie Mobility Action grant (EU 6th framework) to Dr. G. Fuentes (2004). 158'328.- Euros. Title: "*The role of partially unfolded states of proteins in biological signal transduction: Photoactive yellow protein."*
- Senior Research Qualification, Utrecht University, August 2004
- Co-holder of a ALW/FOM Molecule to Cell grant with Prof. R. Kaptein and Prof. R. Boelens (2003). This grant covers two Ph.D. positions for four years and some equipment for a total of Euros 324'600.- Title: "*The role of partially unfolded states of proteins in biological signal transduction: Photoactive yellow protein and Appa."*
- Co-holder of a Netherlands Organization for Scientific Research (NWO) CW-TOP grant with Prof. R. Kaptein and Prof. R. Boelens (2003). This grant covers three Ph.D. positions for four years, equipment and consumable for a total of Euros 500'000.- Title: "*Structural investigation of gene regulation by NMR."*
- Softlink grant from FOM (Stichting voor Fundamenteel Onderzoek der Materie) together with Dr. N. van Nuland and Prof. R. Boelens (2001). This grant covers a three year post-doctoral position and NLG 105'000.- material credit. Title: *"Understanding inactivation of industrial enzymes: a protein folding problem."*
- Jonge Chemici grant from the Netherlands Organization for Scientific Research (NWO) (2001). This grant covers a three year post-doctoral position and NLG 50'000.- for computer equipment. Title: "*Combining protein structure predicition tools with limited NMR data toward fast NMR structure determination."*
- Swiss National Science Foundation Fellowship for postdoctoral research work at the Howard Hughes Medical Institute at Yale University, USA, (1994, 1995)
- Bourse de perfectionnement et de recherche from the University of Lausanne, Switzerland (1989)

Grants & awards from post-docs to join the group

- Dr. Li Xue: VENI grant from the Netherlands Organization for Scientific Research (NWO) (2014). Title: "*Shrinking protein-RNA conformational space with artificial intelligence."*
- Dr. Anna Vangone: EC H2020 Marie Sklodowska-Curie Individual Fellowship (2015). Title: "*A dynamical view of binding affinity."*
- Dr. Irina Moreira: EC H2020 Marie Sklodowska-Curie Individual Fellowship (2015). Title: "*Membrane proteins – development of new computational approaches and its application to G-Protein Coupled Receptors."*
- Dr. Gloria Fuentes: EC FP6 Marie-Curie Intra-European Fellowship (2005). Title: "*Unfolded proteins."*

Ph.D. thesis supervision

- Currently supervising as thesis director two PhD students.
- Thesis director (promotor) of Drs. J. Roel-Touris. *"On the study of biomolecular interactions at different resolutions: Does size matter?"*. Utrecht, the Netherlands, February, 2021
- Thesis director (promotor) of Drs. P. Koukos. *"Integrative Modelling of Biomolecular Complexes: From Small to Large"*. Utrecht, the Netherlands, February, 2020
- Thesis director (promotor) of Drs. C. Geng. *"On Scoring and Binding Affinity Changes in Protein-Protein Interactions"*. Utrecht, the Netherlands, February, 2019
- Thesis director (promotor) of Drs. G.C.P. van Zundert. *"On Explorative and Integrative Modelling of Biomolecular Complexes"*. Utrecht, the Netherlands, November, 2015
- Thesis director (promotor) of Drs. J.P.G.L. Rodrigues. *"Computational Structural Biology of Macromolecular Interactions"*. Utrecht, the Netherlands, December, 2014
- Thesis director (promotor) of Drs. E. Karaca. *"Dissecting biomolecular interactions by integrative modelling"*. Utrecht, the Netherlands, February, 2013
- Thesis director (promotor) of Drs. P.L. Kastritis. *"On the binding affinity of macromolecular complexes. Daring to ask why proteins interact"*. Utrecht, the Netherlands, December, 2012
- Thesis director (promotor) of Drs. M. van Dijk. *"Modelling protein-DNA interactions. Bend and twist until it fits"*. Utrecht, the Netherlands, February, 2010
- Thesis director (promotor) of Drs. M. Krzeminski. *"Intrinsic disorder in biomolecular systems. A modelling challenge"*. Utrecht, the Netherlands, November, 2009
- Thesis co-director (co-promotor) of Drs. S.J. de Vries. *"How proteins get in touch. Interface prediction and docking of protein complexes"*. Utrecht, the Netherlands, June, 2009
- Thesis co-director (co-promotor) of Drs. Aalt D.J. van Dijk. *"Modelling of Biomolecular Complexes by Data-Driven Docking"*. Utrecht, the Netherlands, October 16, 2006
- Thesis co-director (co-promotor) of Drs. Leonardus M.I. Koharudin. *"Protein Structure Determination and Interaction Studies by NMR".* Utrecht, the Netherlands, October 12, 2004
- Thesis co-director (co-promotor) of Drs. Cyril Dominguez. *"NMR-Based Docking of Protein-Protein Complexes. The Human UbcH5B-CNOT4 Ubiquitination complex"*. Utrecht, the Netherlands, June 14, 2004.
- Thesis co-director (co-promotor) of Drs. Danny S.-T. Hsu. *"Biomolecular Recognition Mechanism Studied by NMR Spectroscopy and MD simulations"*. Utrecht, the Netherlands, June 9, 2004.
- Thesis co-director of Thomas Stockner. *"Multidimensional NMR - Protein Structure - Molecular Modelling and Dynamics."* Graz, Austria, April 20, 2001.

Referee

Large variety of journals including PNAS, Nature and Science Journals

Granting agencies

- Agence Nationale française de la Recherche (ANR)
- Austrian Science Fund (FWF)
- BBCRC UK
- Belgian Research Council (FWO)
- DFG (German Research Council)
- European Research Council
- ETH Zurich internal grants

- Italian Cancer Research Association (AIRC)
- Israel Science Foundation
- National Institute of Health, USA
- Netherlands Organization for Scientific Research
- Swiss National Research foundation
- Welcome Trust Fund, UK

Journal Editorial Board Memberships

- Editorial Board and Editorial manager for Proteins: Structure, Function & Bioinformatics (since 2006)
- Editorial Board and Editorial manager for the Biophysical Journal (2008-2014)
- Editorial Board and Editorial manager for Protein Engineering, Design, and Selection (since 2014)
- Advisory Board Member of F1000Research (since 2015)

Conference Organization

- Co-organizer of the EMBO practical course on "Integrative modelling of biomolecular interactions", Izmir, Turkey, September, 2023.
- Co-organizer, together with Drs A. Vargiu, G. Malocci, and R. Apostolov of the BioExcel summerschool on biomolecular simulations. , Sept. 11-15, 2023
- Co-organizer, together with Drs A. Vargiu, G. Malocci, and V. Matser of the BioExcel summerschool on biomolecular simulations. , June 13-14, 2022
- Organizer of the EMBO workshop on "Advances and Challenges in Biomolecular Simulations", Brno, Czech Republic, Online, October 19-21, 2021.
- Co-organizer, together with Drs A. Vargiu, G. Malocci, and V. Matser of the BioExcel summerschool on biomolecular simulations. , Online June 7-11, 2021
- Organizer of the EMBO practical course on "Integrative modelling of biomolecular interactions", Izmir, Turkey, Online, May 31 – June 5, 2021.
- Co-organizer, together with Drs A. Vargiu, G. Malocci, and V. Matser of the BioExcel winterschool on biomolecular simulations. , Online Nov. 20 – Dec. 4, 2020
- Organizer of the Instruct-ERIC/CAPRI Workshop on "Integrated Modelling of Protein-Protein Interactions", EBI Hinxton UK, April 1-2, 2019.
- Co-organizer, together with Drs G. Palermo, V. Tozzini, M. Dal Peraro and R. Amaro of the CECAM meeting on "Multiscale Modelling from Macromolecules to Cell: Opportunities and Challenges of Bimolecular Simulations", Lausanne, Switzerland, Feb. 2019
- Co-organizer, together with Drs A. Vargiu, G. Malocci, and V. Matser of the BioExcel summerschool on biomolecular simulations. , Pula, Sardinia, Italy, Jul. 2018, 2019
- Programme committee member of the International Symposium on Grid and Cloud computing (ISGC), Taipei, Taiwan, March 2014-2021.
- Programme committee member of the 2018 Digital Infrastructure for Research (DI4R) European conference, Lisbon, Portugal, October 2018
- Organizer of the EMBO practical course on "Integrative modelling of biomolecular interactions", Barcelona, Spain, July 2016 and 2018.

- Organizer of the Netherlands Society for Biomolecular Modelling fall meeting, Utrecht, the Netherlands, November 16th, 2016.
- Organizer of the INSTRUCT practical course on "Advanced methods for the integration of diverse structural data with NMR data – 2nd Edition", Utrecht, the Netherlands, April 11-15, 2016.
- Chair of the 2015 Gordon Research Conference on "Computational Aspects of Biomolecular NMR", Il Ciocco, Italy, June 7-12, 2015.
- Vice Chair of the Gordon Research Conference on "Computational Aspects of Biomolecular NMR", Mount Snow Resort, Vermont USA, June 1-8, 2013
- Organizer of the CAPRI 5th evaluation meeting (www.capri2013.nl), Utrecht, April 17-19, 2013
- Co-organizer, together with Drs C. Morris, M. Fynn, J.-M. Carazo and K. Wilson of the CECAM meeting on "Integrated Software for Integrative Structural Biology", Adingdon UK, May 21-23, 2012
- Programme committee member of the 2012 EGI Community Forum, München, Germany, March 26-30, 2012
- Programme committee member of the 2011 EGI Technical Forum, Lyon, France, September 19-23, 2011
- Co-organizer of the WeNMR workshop on "Computational aspects of the joint use of SAXS and NMR", Florence, Italy, May 27th, 2011.
- Co-organizer, together with Prof. D. Beveridge and Dr . P. Carloni, of the CECAM meeting "Recent advances in modeling DNA and RNA: from quantum to coarse grains", Lyon, France, October 16-18, 2006

Invited lectures (2019-present)

- 2019 –

- *"HADDOCK: An integrative modeling platform"*. Biophysical Society satellite workshop: working towards federating structural models and data. Baltimore MD, USA March 1st, 2019.
- *"Integrative modeling of biomolecular complexes"*. 63rd Biophysical Society Meeting. Baltimore MD, USA March 2-6, 2019.
- "*Data-driven HADDOCK strategies in CAPRI rounds 38-45*". 7th CAPRI evaluation meeting, EBI, Hinxton UK, April 3-5, 2019.
- **Keynote:** "*Juggling Research and Services in Bioinformatics*". EMBO practical course: From Research to Service - setting up and running a bioinformatics core facility. Izmir, Turkey, May 8-11, 2019.
- **Keynote:** *"Structural Biology in the Clouds: Past, Present and Future"*. Amsterdam Science Park, the Netherlands, May 6-7, 2019.
- *"Integrative modeling of biomolecular complexes"*. CECAM workshop: "Challenges In Large Scale Biomolecular Simulations 2019: Bridging Theory And Experiments". Cargèse, Corsica, France, May13-17, 2019.
- *"Integrative modeling of biomolecular complexes: from small molecules to membrane systems"*. iNext workshop on Integrated methodologies and approaches for structural biology. Brno, Czech Republic, May 29-31, 2019.
- *"Integrative modeling of biomolecular complexes harvesting evolutionary data".* CECAM workshop on coevolutionary approaches to protein and protein-complexes structure prediction and design. Lausanne, Switzerland, June 17-20, 2019.

- *"Integrative modeling of biomolecular complexes".* EMBO workshop Synergy of experiment and computation in quantitative systems biology. Nove Hrady, Czech Republic, June 23-28, 2019.
- *"Integrative modeling of biomolecular complexes"*. BioExcel Summerschool on biomolecular simulations. Pula, Italy, July 1-5, 2019.
- *"Integrative modelling of biomolecular interactions".* Pasteur/EMBO course on integrative structural biology, Paris, France, July 9-11, 2019. https://www.pasteur.fr/en/integrative-structural-biology
- **Keynote:** *"Structural Biology in the Clouds: Past, Present and Future"*. 48th Asia Pacific Advanced Network conference, Putrajaya, Malaysia, July 22-66, 2019.
- "*Exploring protein docking with HADDOCK*", Structural Bioinformatics course. EMBL-EBI, Hinxton UK, September 17-18, 2019.
- "*Structural Biology in the Clouds: Past, Present and Future* ", CompBioMed 2019 conference. London UK, September 25-27, 2019.
- *"Integrative modeling of biomolecular complexes"*. CECAM BImMS 2019 school. Lugano, Switzerland, October 7, 2019.
- *"Integrative modeling of biomolecular complexes"*. Aviesan symposium on Deciphering the Functional Mechanisms of Biological Macromolecules. Paris, France, October 8, 2019
- EMBO Global Exchange Lecture Course *"Structural and biophysical methods for biological macromolecules in solution"*, Santiago, Chile, October 14-20, 2019
- *"Integrative modeling of biomolecular complexes"*. From Protein Complexes to Cell-Cell Communication. Esztergom, Hungary, October 27-29, 2019.
- EMBO practical course on *"Practical Integrative Structural Biology*", Hamburg, Germany, November 3-8, 2019
- *"Integrative modeling of biomolecular complexes"*. GIDRM meeting on Computation methods and NMR spectroscopy: A powerful synergy for chemistry, materials science and biology. Pisa, Italy, December 10th , 2019.
- *"HADDOCK workshop on Integrative modeling of biomolecular complexes"*. Coimbra University, Portugal, December 18-19 , 2019.

- 2020–

- *"Integrative modeling of biomolecular complexes"*. Applied Bioinformatics in Life Sciences, Leuven, Belgium, February 13-14, 2020.
- *"WeNMR - Structural biology in the cloud - 10 years of experience of using EGI services".* EGI Webinar, April 27, 2020
- *"WeNMR - Structural biology in the cloud - 10 years of experience of using EGI services".* EOSC-week conference , May 19th, 2020
- Interview and live demo of HADDOCK in the closing plenary of the EOSC-week conference, May 20th, 2020
- *"Comment résoudre des puzzles tridimensionnels contribue à attaquer le virus.".* Webinar Franco-Sciences, May 26, 2020
- *"Integrative modeling of biomolecular complexes"*. Online BioExcel Summerschool on biomolecular simulations. July 22-26, 2020.
- **Keynote:** "*Juggling Research and Services in Bioinformatics*". Online EMBO practical course: From Research to Service - setting up and running a bioinformatics core facility. Sept. 29th, 2020.
- *"Integrative modeling of biomolecular complexes"*. CCPBioSim online training week. Oct. 2-9, 2020.

- *"Integrative modeling of biomolecular complexes"*. North Jersey ACS NMR Topical Group - 2020 Virtual NMR Symposium. Oct. 20, 2020.
- "*Exploring protein docking with HADDOCK*", Structural Bioinformatics course. EMBL-EBI, Hinxton UK, Nov. 26, 2020.
- *"Integrative modeling of biomolecular complexes"*. Online BioExcel Winterschool on biomolecular simulations. Nov. 30 – Dec. 4 , 2020.
- *"Integrative modeling of biomolecular complexes"*. Online Thermofischer Winterschool on integrative structural biology. China, Dec. 2 – Dec. 4 , 2020.
- *"Drug repurposing against SARS-Cov2 using HADDOCK"*. Interdisciplinary consortia for the study of pandemics, CIC biomaGUNE Spain, Dec. 15, 2020.

- 2021–

- *"Juggling research, education and services in structural bioinformatics"*. WiSS 2021 – Online First Women in Science Symposium, International Institute of Molecular and Cell Biology, Warsaw, Poland, March 4-5, 2021.
- *"Integrative modeling of biomolecular complexes"*. Online HADDOCK workshop at the International Symposium on Grid and Cloud computing. Taipei, March 22nd, 2021.
- *"Unravelling the social life of proteins by integrative modelling"*. CROP-IB 2021 Breakthroughs in technology development, vegetable trait and crop improvement - https://www.cropib.com . April 12-13, 2021.
- *"Integrative modeling of biomolecular complexes"*. Online webinar series for the 50 years of the Molecular Biophysics and 100 year birth anniversary of Prof. G.N. Ramachandran at IIT Bangalore, April 13nd, 2021.
- *"Solving 3D puzzles by integrative modelling using PDB structures".* ASBMB special symposium celebrating the 50th anniversary of the Protein Data Bank, May 4-5, 2021
- *"Integrative modeling of biomolecular complexes"*. EMBO practical course on Integrative modelling of biomolecular complexes. Online, May 30 – June 5, 2021
- *"Integrative modeling of biomolecular complexes"*. Online BioExcel Summerschool on biomolecular simulations. June 7-11, 2021.
- *"Integrative modeling of biomolecular complexes"*. Webinar for the PhD school at SISSA, Italy. June 16th, 2021
- *""Integrative modelling of biomolecular complexes with HADDOCK"*. SBGrid webinar, June 19th, 2021.
- *"Deep-learning approaches to Learn Interaction Patterns from Protein-Protein Interfaces"*. Deep Learning on Supercomputers Workshop co-located with ISC'21, July 2nd, 2021
- *"Integrative modelling of biomolecular complexes - toward interactome modelling".* HPC EU-ASEAN virtual Summer School. July 5-9, 2021
- *"Integrative modelling of biomolecular complexes".* PRACE autumn School on fundamentals of biomolecular simulations and virtual drug development. Sept. 20-24, 2021
- **Keynote:** "*Juggling Research, Teaching and Services in Bioinformatics*". EMBO practical course: From Research to Service - setting up and running a bioinformatics core facility. Online, Oct. 4-8, 2021.
- "*Exploring protein docking with HADDOCK*", Structural Bioinformatics online course. EMBL-EBI, Hinxton UK, Oct. 14, 2021.
- *"WeNMR under EGI: A 10+ years happy symbiosis"*. EGI conference 2021, online, Oct. 19-21, 2021.

- *"WeNMR project: boosting structural biology research with DIRAC services"*. EGI conference 2021, online, Oct. 19-21, 2021.
- **Keynote:** *"Integrative modelling of biomolecular complexes".* 5th international Symposium on Bioinformatics. Dec. 15-17, 2021

- 2022–

- **Keynote:** *"Solving 3D puzzles of biomolecular interactions by integrative modelling".* SoScience-IEEE online conference, Turkey, Feb. 26, 2022
- *"Integrative modeling of biomolecular complexes"*. Online BioExcel Winterschool on biomolecular simulations. Mar. 25 – Apr. 1st, 2022.
- *"European Research Projects as EOSC Service Providers – The HADDOCK/WeNMR use case"*. EOSC future providers days, Apr. 26-28, 2022.
- *"Combining different sources of experimental data in modeling".* FEBS workshop: Lost in Integration - Probing Biomolecules with Electrons, Photons, Neutrons and Magnetic Spins. Spetses, Greece. May 9-14, 2022
- *"Integrative Modelling of Biomolecular complexes."* HADDOCK workshop. Budapest, Hungary. May 23-25, 2022
- *"Integrative Modelling of Biomolecular complexes."* KAUST conference on Modern trends in targeted structure-based drug design and discovery. Saudi Arabia. June 6-9, 2022
- *"Integrative modeling of biomolecular complexes"*. BioExcel Summerschool on biomolecular simulations. Pula, Italy, June 13-17, 2022.
- Impact of AlphaFold on teaching and training in life sciences. EBI webinar, June 22, 2022. DOI: 10.6019/TOL.AlphaFoldTeaching-w.2022.00001.1
- *"Dissecting biomolecular interactions: scoring and binding affinity challenges"*. EMBL-EBI Industry workshop on "AI/ML for Biologics and Protein Evolutionary Modelling". EBI Hinxton, UK, June 28-*29, 2022*
- *"Integrative Modelling of Biomolecular complexes."* EMBO practical course on integrative structural biology,. Paris, France. July 4-9, 2022
- *"Solving 3D puzzles of biomolecular interactions by integrative modelling"*. Protein Society meeting. San Fransisco, USA, July 6-10, 2022.
- *"Solving 3D puzzles of biomolecular interactions by integrative modelling"*. Online Instruct-ERIC practical course on "Instruct-ing Structural Biologists Towards Integration". Florence, Italy, July 18-21, 2022.
- *"Solving 3D puzzles of biomolecular interactions by integrative modelling"*. EMBO workshop "When predictions meet experiments: The future of structure determination". Palermo, Italy, Sept. 5-8, 2022.
- **Keynote:** *"Solving 3D puzzles of biomolecular interactions by integrative modelling"*. RNAct final conference "Tailoring RNA-binding proteins and RNA targeting". Valencia, Spain, Sept. 14-15, 2022.
- "*Exploring protein docking with HADDOCK*", Structural Bioinformatics online course. EMBL-EBI, Hinxton UK, Oct. 20, 2022.
- EMBO practical course on *"Practical Integrative Structural Biology*", Hamburg, Germany, November 6-13, 2022
- *"Integrative modelling of biomolecular complexes".* EU-ASEAN HPC School. Bangkok, Thailand, Dec. 5-10, 2022

- 2023–

- *"Integrative modelling of biomolecular complexes".* Bioinformatics and Computational Biology, CNS advanced course, Coimbra, Portugal, Jan. 2-13, 2023
- *"Integrative modelling with HADDOCK".* Workshop at the International Symposium on Grid and Cloud computing, Taipei, Taiwan, March 20, 2023
- *"A Virtual Research Environment for Integrative Modelling of Biomolecular Complexes with the New Modular Version of HADDOCK"*. International Symposium on Grid and Cloud computing, Taipei, Taiwan, March 21-24, 2023
- ***Keynote*** *"Solving 3D puzzles of biomolecular complexes by integrative modelling"*. ICGEB Course "NMR for combatting diseases: from cancer to SARS-CoV-2". Florence, Italy, March 27-31, 2023
- *"Solving 3D puzzles of biomolecular complexes with HADDOCK".* Structural Proteomics symposium, Utrecht, April 25-26, 2023
- ***Keynote*** *"Solving 3D puzzles of biomolecular complexes with HADDOCK".* BioSB conference, Egmond aan Zee, the Netherlands, May 8-10, 2023
- *"Toward accurate antibody-antigen complex structure prediction from sequence using AI and integrative modelling."* MPI meeting, Lawrence KS, USA, May 25-27, 2023
- *Panelist on "From Millions to Billions: 20 Years of Excellence in Scientific Computing in Europe"* at the EGI2023 conference, Poznan, Poland, June 20-22, 2023
- *"Towards accurate antibody-antigen complex prediction from sequence using AI and integrative modelling".* Roche symposium, Penzberg, Germany, July 11th, 2023
- *"Integrative modeling of biomolecular complexes"*. EMBO practical course on Integrative modelling of biomolecular complexes. Izmir, Turley, Sept. 17-20, 2023
- "*Solving 3D puzzles of biomolecular interactions by integrative modelling*", Structural Bioinformatics course. EMBL-EBI, Hinxton UK, Oct. 4th, 2023.
- BioExcel Workshop on *"Integrative modeling of biomolecular complexes"*. University of Bratislava, Slovakia, October 19, 2023
- HADDOCK Workshop on *"Integrative modeling of biomolecular complexes"*. Copenhagen University, PhD school. Copenhagen, Denmark, October 24-25, 2023
- ***Keynote*** *"Toward accurate antibody-antigen complex structure prediction from sequence using AI and integrative modelling."* ISBU symposium, Copenhagen University, Denmark, October 27, 2023
- *"The molecules of life and structural biology approaches to study them."* ENZA zaden, Enkhuizen, the Netherlands, November 3, 2023
- *"Sailing biomolecular interactions for 20 years!"***,** HADDOCK 20 years symposium, Huizen, Netherlands, November 8-9, 2023
- *"Toward accurate antibody-antigen complex structure prediction from sequence using AI and integrative modelling."* EMBL Grenoble, November 14, 2023
- ***Keynote*** *"Solving 3D puzzles of biomolecular complexes by integrative modelling".* Reedijk symposium, Leiden University, the Netherlands, November 17, 2023
- *"Solving 3D puzzles of biomolecular complexes by integrative modelling".* EMBO workshop on "Computational models of life", San Feliu, Spain, November 27-30, 2023
- *"Toward accurate antibody-antigen complex structure prediction from sequence using AI and integrative modelling."* EMBO conference on computational structural biology, EMBL Heidelberg, Germany, December 6-8, 2023
- *"Integrative modeling of biomolecular complexes"*. EU-ASEAN HPC School, Bogor, West Java, Indonesia, December 11-15, 2023

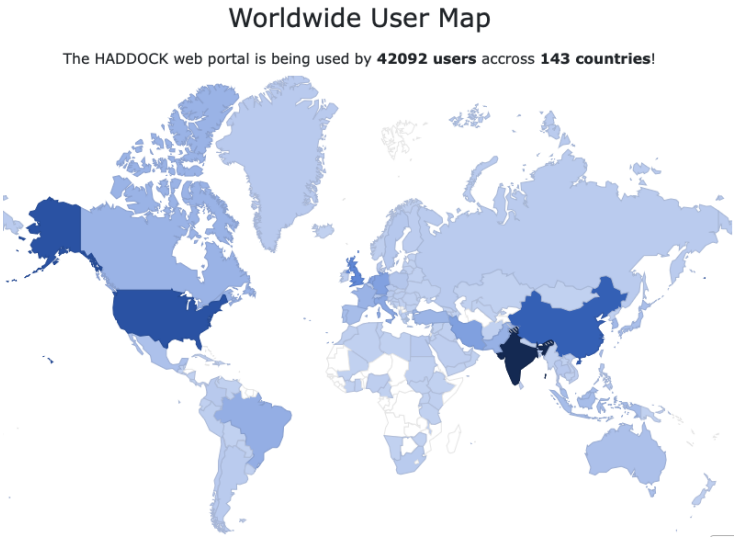
Software

Software developed in my group are made freely available to the community through:

- open repositories via our lab GitHub organization: https://github.com/haddocking
- web services available from https://wenmr.science.uu.nl

We are promoting open science, data and software.

The major software developed by the group in HADDOCK, our integrative modelling platform for the modelling of biomolecular complexes. It is made available from through a user-friendly web portal (https://wenmr.science.uu.nl/haddock2.4) which counts to date >42'000 registered users distributed over 143 countries. The software is also used in educational programmes in various universities worldwide and by major pharma and biotech companies.



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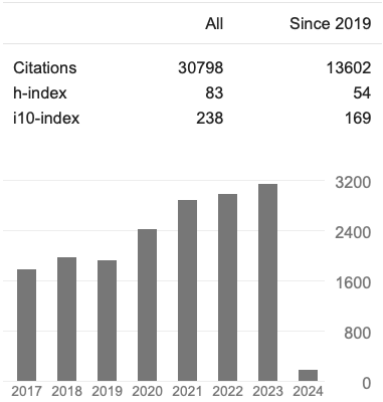
Publication list

Output statistics from Google Scholar January 17th, 2024



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- Google Scholar Citations: (h-index: 83)
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- Scopus Author ID: 7003870500 (h-index: 72)

Preprints

1. M. Giulini, C. Schneider, D. Cutting, N. Desai, C. Deane and **A.M.J.J. Bonvin**. Towards the accurate modelling of antibody-antigen complexes from sequence using machine learning and information-driven docking. ***BioRxiV***. 10.1101/2023.11.17.567543 (2023).

International (refereed) journals

2. M. Giulini, R.V. Honorato, J.L. Rivera, **A.M.J.J. Bonvin**. ARCTIC-3D: Automatic Retrieval and ClusTering of Interfaces in Complexes from 3D structural information. ***Comm. Biol.*** 7:49, p. 1-9 (2024).
3. X. Xu, **A.M.J.J. Bonvin**. DeepRank-GNN-esm: A Graph Neural Network for Scoring Protein-Protein Models using Protein Language Model. ***Bioinfo. Adv.*** vbad191, _Advanced Online Publication (2024).
4. F. van der Krift, D.W. Zijlmans, R. Shukla, A. Javed, P.I. Koukos, L.L.E. Schwarz, E.P.M. Timmermans-Sprang, P.E.M. Maas, D. Gahtory, M. van den Nieuwboer, J.A. Mol, G.J. Strous, A.M.J.J. Bonvin, M. van der Stelt, E.J.A. Veldhuizen, M.s Weingarth, M. Vermeulen, J. Klumperman, M.M. Maurice. A novel antifolate suppresses growth of FPGS-deficient cells and overcomes methotrexate resistance. ***Life Science Alliance***, 6, e202302058 (2023).
5. M. Lensink, G. Brysbaert, N. Raouraoua, P. Bates, M. Giulini, R. Vargas Honorato, C. van Noort, J. Teixeira, **A.M.J.J. Bonvin**, R. Kong, H. Shi, X. Lu, S. Chang, J. Liu, Z. Guo, X. Chen, A. Morehead, R. Roy, T. Wu, N. Giri, F. Quadir, C. Chen, J. Cheng, C. Del Carpio, E. Ichiishi, L. Rodriguez-Lumbreras, J. Fernández-Recio, A. Harmalkar, L. Chu, S.Canner, R. Smanta, J. Gray, H. Li, P. Lin, J.a He, H. Tao, S. Huang, J. Roel, B. Jimenez-Garcia, C. Christoffer, A. Jain J, Y. Kagaya, H. Kannan, T. Nakamura, G. Terashi, J. Verburgt, Y. Zhang, Z. Zhang, H. Fujuta, M. Sekijima, D. Kihara, O. Khan, S. Kotelnikov, U. Ghani, D. Padhorny, D. Beglov, S. Vajda, D. Kozakov, S. Negi S, T. Ricciardelli, D. Barradas-Bautista, Z. Cao, M. Chawla, L. Cavallo, R. Oliva, R. Yin, M. Cheung, J. Guest, J. Lee, B. Pierce, B. Shor, T. Cohen, M. Halfon, D. Schneidman-Duhovny, S. Zhu, R. Yin, Y. Sun, Y. Shen, M. Maszota-Zieleniak, K. Bojarski K, E. Lubecka, M. Marcisz, A. Danielsson, L. Dziadek, M. Gaardlos, A. Giełdoń, J. Liwo, S. Samsonov, R. Slusarz, K. Zieba, A. Sieradzan, C. Czaplewski , S. Kobayashi, Y. Miyakawa, Y. Kiyota, M. Takeda-Shitaka, K. Olechnovič, L. Valančauskas, J. Dapkūnas, C. Venclovas, B. Wallner, L. Yang, C. Hou, X. He, S. Guo, S. Jiang, X. Ma, R. Duan, L. Qiu, X. Xu, X. Zou, S. Velankar, S. Wodak. Impact of AlphaFold on Structure Prediction of Protein Complexes: The CASP15-CAPRI Experiment ***Proteins: Struc. Funct. & Bioinformatics*** *12*, 1658-1683 (2023).
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9. Y. Jung, C. Geng, **A.M.J.J. Bonvin**, L.C. Xue, V.G. Honavar. MetaScore: A novel machine-learning based approach to improve traditional scoring functions for scoring protein-protein docking conformations. ***Biomolecules,*** 13, 121 (1-20) (2023).

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12. A. Basciu, L. Callea, S. Motta, **A.M.J.J. Bonvin**, L. Bonati and A.V. Vargiu. No dance, no partner! A tale of receptor flexibility in docking and virtual screening. **Annual Reports in Medicinal Chemistry** 59, 43-97 (2022)

13. R. Shukla, F. Lavore, So. Maity, M.G.N. Derks, C.R. Jones4, B.J.A. Vermeulen, A. Melcrová, M.A. Morris, L.M. Becker, X. Wang, R. Kumar, J. Medeiros-Silva, R.A.M. van Beekveld, **A.M.J.J. Bonvin**, J. Lorent, M. Lelli, J. Nowick, H.D. MacGillavry, A.J. Peoples, A.L. Spoering, L.L. Ling, D.E. Hughes, W.H. Roos, E. Breukink, K. Lewis and M. Weingarth. Teixobactin kills bacteria by a two-pronged attack on the cell envelope. ***Nature*** 608, 390-396 (2022)

14. C.J. Buchanan, B. Gaunt, P.J. Harrison, Y. Yang, J. Liu, A. Khan, A.M. Giltrap, A. Le Bas, P.N. Ward, K. Gupta, M. Dumoux, T.K. Tan, L. Schimaski, S. Daga, N. Picchiotti, M. Baldassarri, E. Benetti, C. Fallerini, F. Fava, A. Giliberti, P.I. Koukos, M.J. Davy, A. Lakshminarayanan, X. Xue, G. Papadakis, L.P. Deimel, V. Casablancas-Antràs, T.D.W. Claridge, **A.M.J.J. Bonvin**, Q.J. Sattentau, S. Furini, M. Gori, J.Huo, R.J. Owens, C. Schaffitzel, I. Berger, A. Renieri, GEN-COVID Multicenter Study, J.H. Naismith, A. Baldwin, B.G. Davis. Pathogen-sugar interactions revealed by universal saturation transfer analysis. ***Science*** doi:10.1126/science.abm3125 (2022).

15. V. Charitou, S.C. van Keulen and **A.M.J.J. Bonvin**. A Cyclisation and Docking Protocol for Cyclic Peptide-Protein Modelling using HADDOCK2.4. ***J. Chem. Theory Comput.*** 18, 4027-4040 (2022).

16. N. Rosário-Ferreir, **A.M.J.J. Bonvin** and Irina S. Moreira. Using machine-learning-driven approaches to boost hot-spot's knowledge. ***WIREs Comp. Mol. Sci.***, 12, e1602 (2022).

17. B. Garofalo, **A.M.J.J. Bonvin**, A. Bosin, F.P. Di Giorgio, R. Ombrato and A.V. Vargiu. Molecular Insights Into Binding and Activation of the Human KCNQ2 Channel by Retigabine. ***Frontiers Mol. Biosci.*** *9*, 839249 (2022).

18. T Neijenhuis, S.C. van Keulen and **A.M.J.J. Bonvin**. Interface Refinement of Low-to-Medium Resolution Cryo-EM Complexes using HADDOCK2.4. ***Structure*** *30*, 476-484 (2022).

19. N.Renaud, C. Geng, S. Georgievska, F. Ambrosetti, L. Ridder, D.F Marzella, **A.M.J.J. Bonvin*** and L.C. Xue*. DeepRank: A deep learning framework for data mining 3D protein-protein interfaces. ***Nature Comm.*** *12*, 7068 (2021).

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