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

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, Department of Chemistry
Faculty of Sciences, Utrecht University
Education Director 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

Contact Address

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3403 AC IJsselstein
the Netherlands

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Mobile : + 31.6.40606226

Major research interests

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

Teaching activities

Teaching directory of the Chemistry bachelor, Utrecht University, Feb-2009 - present

University Senior Teaching Certificate, Utrecht University, Jan. 2003

University Basic Teaching Certificate, Utrecht University, Sept. 2000

Utrecht University College (2000-present): lecturer in the Advanced Chemistry Course: NMR Spectroscopy

Utrecht University (1998-present)
- Lecturer and coordinator of the second year Molecular Modelling and Mathematics course
- Lecturer in the third year Structural Biology course"Computational aspects of NMR structure determination". 1999-present
- Lecturer in the fourth year Structural Biology Methods course "Molecular Dynamics and Simulation". 2001
- Lecturer and co-organizer of the Bijvoet-NSR Research Alliance (BNRA) advanced course for Ph.D. students: "From Data to Structure". 1998-present (every second year)
- Member of the education advisory commission (opleidingadviescommissie) of the Department of Chemistry (until 2009)
- Member of the education commission of the lifescience master of Utrecht University (until 2009)
- Member of the "klankbordoverleg vwo" (high school commission) of the faculty of Chemistry
- Guest lecturer at highschools to promote chemistry in Utrecht
- Tutor for first year chemistry students. 2007-2009
- Responsible for the second year NMR project practical

Memberships

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

Grants & awards

- Bourse de perfectionnement et de recherche from the University of Lausanne, Switzerland (1989)

- Swiss National Science Foundation Fellowship for postdoctoral research work at the Howard Hughes Medical Institute at Yale University, USA, (1994, 1995)

- 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.

- 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.

- 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.

- 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.

- Senior Research Qualification, Utrecht University, August 2004

- 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.

- EC Sixth 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 AIO).

- EC Sixth 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.-).

- 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).

- 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.

- 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 550000.- euros).

- 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 423250.- euros)

Other activities

- Consulting on Molecular Modelling for Nestlé Research Institute, Vers-chez-les-Blanc, CH-1000 Lausanne, Switzerland, 1999-2001

- Member of the advisory panel of the Volkswagen Foundation in Germany in the area of "Conformational Control of Biomolecular Function"

- 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

Ph.D. thesis supervision

- Thesis co-director of Thomas Stockner. “Multidimensional NMR - Protein Structure - Molecular Modelling and Dynamics.” Graz, Austria, April 20, 2001.

- 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 (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. 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. 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. S.J. de Vries. “How proteins get in touch. Interface prediction and docking of protein complexes.” Utrecht, the Netherlands, June, 2009

- Thesis director (promotor) of Drs. M. Krzeminski. “How proteins get in touch. Interface prediction and docking of protein complexes.” Utrecht, the Netherlands, November, 2009

- Thesis director (promotor) of Drs. M. van Dijk. “Modelling protein-DNA interactions. Bend and twist until it fits.” Utrecht, the Netherlands, February, 2010

Invited lectures (1998-present)

- "In computro studies of β-hairpin stability and folding." ISQBP President’s Meeting. Molecular Structure and Dynamics in Biology. September 8-11, 1998, Elba, Italy

- “Hydration Structure and Dynamics of DNA and Collagen by MD Simulation”. Workshop on Modelling Through Numerical Simulations. University of Rome Tor Vergata. January 17,18, 2000, Rome, Italy

- “Hydration Structure and Dynamics of a Collagen Peptide. A Combined NMR and Molecular Dynamics Study”. Molecular Modeling Methods for the Development of NMR in Structural Biology. Centre Européen de Calcul Atomique et Moléculaire (CECAM). October 2-5, 2000, Lyon, France

- “Rational Design of a Subtype-Specific Peptide Vaccine against Neisseria Meningitidis”. 4th User Meeting of the European Large-Scale Facilities for NMR. October 6 and 7, 2000, Noordwijkerhout, the Netherlands

- “The NMR structure of CI2 from secondary chemical shifts and cross-hydrogen bond15N-13C scalar couplings: how far can we get?”. CCPN meeting, Edinburgh, Scotland, April 6-8, 2001

- “Automated assignment and structure calculation with ARIA”. Round Table discussion on automated assignment in NMR. Center for Magnetic Resonance. Florence, Italy, July 6-7, 2001

- “An introduction to molecular dynamics”. EuroLab Course “Advanced Computing in NMR Spectroscopy”. Center for Magnetic Resonance. Florence, September 9-14, 2001

- "Studying protein structure, dynamics and hydration by NMR". Elastin 2002. Acquafredda di Maratea, Italy, July 10-14

- "Computational aspects of NMR structure calculations:. EMBO course "Multidimensional NMR in Structural Biology". Il Ciocco, Castelvecchio Pascoli, Italy, August 11-16,2002

- "New structure-based approach toward designing and selecting peptide-vaccine candidates for Neisseria meningitidis." Conference for the 25th anniversary years of the Chemistry Department. University of Ioannina, Greece, October 22-24, 2002

- "Structure of proteins and of their complexes from sparse (NMR) data". Physical Chemistry Kolloquium. ETHZ, Zurich, Switzerland, November 5, 2002

- "HADDOCK: an approach for protein-protein docking based on biochemical or biophysical data." Keystone Symposium "Frontiers of NMR in molecular biology VIII". Taos, New Mexico, USA, February 4-10, 2003

- "NMR studies of protein-protein interactions". EuroLab Course "Advanced Computing in NMR Spectroscopy". Center for Magnetic Resonance (CERM). Florence, August 31 - September 5, 2003

- "NMR structure determination and validation" Satellite Workshop of the 11th User meeting of the Sincrotrone Trieste on "Validation of Macromolecular Structures and Structure Determination Steps". Trieste, Italy, December 1-3, 2003

- "HADDOCK: high ambiguity driven protein-protein docking." Réunion de l'Intergroupe de Modélisation Moléculaire. Institut Jacques Monod, Jussieu, Paris December 19, 2003

- "NMR-based docking for the study of biomolecular complexes." Gordon Research Conference on Computational Aspects of Biomolecular NMR. Ventura CA, January 18-23, 2004

- "NMR-based high ambiguity driven docking: application to the study of the interaction between two PB1 domains." NMR: a tool for biology VI, Varian NMR meeting. Pasteur Institute, Paris, February 2-4, 2004.

- "NMR-based docking for the study of biomolecular complexes". Chemistry Department Seminar series. Rutgers University, Newark NJ, April 16, 2004.

- "Information-driven docking for the study of biomolecular complexes". CGB-SPINE meeting on "structural proteomics and protein-protein interactions". Amsterdam, June 3-4, 2004

- "Information-driven docking for the study of biomolecular complexes". IIIène journée scientifique de biologie structurale de l'IPBS. "Docking entre macromolécules". Toulouse, France, June 25, 2004

- "Computational aspects of NMR structure calculations". EMBO course "Multidimensional NMR in Structural Biology". Il Ciocco, Castelvecchio Pascoli, Italy, August 15-20,2004

- "Docking approaches for the study of biomolecular complexes" and "HADDOCKing on biomolecular complexes. International BaCaTec Summer School 2004 on "NMR of Biomolecular Complexes". Bayreuth, Germany, October 3-8, 2004

- "Data-driven docking: HADDOCK's adventures in CAPRI". Second CAPRI (criticall assessment of predicted interactions) evaluation meeting. Gaeta, Italy, December 8-10, 2004.

- "Data-driven docking for the study of biomolecular interactions." 11th Bijvoet tutorial symposium on "protein structure in relation to dynamics and interactions". Utrecht, April 7-8, 2005

- "Predicting protein-protein interfaces. Application to data-driven docking." First Benelux Bioinformatics Conference, BBC2005. Gent, April 14-15, 2005

- "Data-driven docking for the study of biomolecular complexes." Protein NMR Summer Course. Copenhagen, Denmark, June 20 – July 1, 2005

- "Data-driven docking for the study of biomolecular complexes." FEBS meeting 2005 "The Protein World". Budapest, Hungary, July 2-7, 2005

- "Data-driven docking for the study of biomolecular complexes." Euromar/EENC 2005. Veldhoven, the Netherlands, July 3-8, 2005

- "HADDOCK's adventures in CAPRI". 15th international BIOMOS symposium on biomolecular molecular dynamics. Burg Arras Alf/Bullay, Germany Aug. 31- Sept. 1, 2005

- "Data-driven modeling of biomolecular interactions". FIGON Platform Pharmacochemie, KNCV/NWO-CV meeting. Lunteren, October 5th, 2005

- "Docking methods for the study of biomolecular complexes" and "HADDOCKing on biomolecular complexes", Second EuCheMS School on Protein Chemistry, Canazei, Italy, January 15-20, 2006

- "Information-driven modeling of biomolecular complexes". Gordon conference on "reversible associations". Ventura, CA, January 17-22, 2006

- "Information-driven modeling of biomolecular complexes". Chemische Kolloquium, TU München May 11, 2006

- "Protein-DNA docking with HADDOCK: it is a matter of flexibility". EU-Coordination Action NMR-Life meeting "Perspective in NMR spectroscopy for studies on protein-protein and protein-DNA complexes, Utrecht, the Netherlands, June 15-16, 2006

- "Direct use of unassigned resonances in NMR structure calculations with PROXY residues". ESF Exploratory Workshop on "Experimental and computational aspects of high-throughput protein NMR", Göteborg, Sweden, June 17-20, 2006

- "Describing partially unfolded states of proteins from sparse NMR data ". 22nd International Conference on Magnetic Resonance in Biological Systems (ICMRBS), Göttingen, Germany, August 20-25, 2006

- "Computational aspects of NMR structure calculations". EMBO course "Multidimensional NMR in Structural Biology". Il Ciocco, Castelvecchio Pascoli, Italy, August 27 – September 1, 2006

- "HADDOCKing on biomolecular complexes". Biochemistry Department Seminar, University of Sao Paulo, Brazil, September 14, 2006

- "Beyond simple protein-protein modeling using HADDOCK". Gordon Conference on "Computational Aspects of Biomolecular NMR". Aussois, France, September 24-29, 2006

- "Information-driven modeling of biomolecular complexes". NCCR structural biology course. ETH Zurich, Switzerland, October 2-6, 2006

- "Protein-DNA docking with HADDOCK: it is a matter of flexibility". CECAM meeting "Recent advances in modeling DNA and RNA: from quantum to coarse grains", Lyon, France, October 16-18, 2006

- "Protein-ligand HADDOCKing: benchmarking on a set of 41 complexes". Coordinated Action NMR-Life workshop on "NMR spectroscopy to study protein-ligand interactions". Frankfurt, Germany, February 26, 2007

- "Information-driven modeling of biomolecular complexes". Ontario Cancer Institute, Toronto, April 22nd, 2007
- "HADDOCKing on biomolecular complexes". FEBS Workshop on Transient Interactions, Sevilla, Spain, May 16-19, 2007
- "Information-driven modeling of biomolecular complexes". FEBS Meeting 2007 "Molecular Machines". Vienna, Austria, June 8-12, 2007
- "Information-driven modeling of biomolecular complexes". 2nd European Conference on Chemistry for Life Sciences, Wroclaw, Poland, September 4-8, 2007
- "Modeling of biomolecular interactions". Bioinformatic Workshop Marie Curie Research Training Network "DNA Enzymes" Warsaw, Poland, October 11-14, 2007
- "Modeling biomolecular complexes". Annual Dutch meeting on Molecular and Cellular Biophysics. Veldhoven, the Netherlands, October 1-2, 2007
- "Information-driven modeling of protein-ligand interactions". Centenary Year Seminar Series 2007, Imperial College, London, UK, October 17, 2007
- "Information-driven modeling of biomolecular complexes". NWO Annual Dutch meeting on Biomolecular Chemistry. Lunteren, the Netherlands, October 29-31, 2007
- "Modeling biomolecular interactions". International Symposium on New NMR in Structural Biology. Frankurt, Germany, November 16-17, 2007
- "Information-driven modeling of biomolecular complexes". SISSA Trieste. Italy, December 20, 2007
- "Information-driven modeling of biomolecular complexes". ENS Lyon. France, February 7, 2008
- "Information-driven modeling of biomolecular complexes". CASP 7.5 meeting. Madrid, Spain, April 21-23, 2008
- "Information-driven modeling of biomolecular complexes". FEBS EU-NMR satellite meeting. Athens, Greece, July 3rd, 2008
- "Computational aspects of NMR structure calculations". EMBO course "Multidimensional NMR in Structural Biology". Il Ciocco, Castelvecchio Pascoli, Italy, August 3-8, 2008
- "Information-driven modeling of biomolecular complexes". Mini NMR symposium, Université de Lyon, Centre Européen de RMN à haut champ. Lyon, France, September 11th, 2008
- "Information-driven modeling of biomolecular complexes". EMBO workshop on "Docking prediction of protein-protein interactions", Barcelona, Spain, October 14-17, 2008
- "Information-driven modeling of biomolecular complexes". EMBO practical course on "solution scattring from biological macromolecules", Hamburg, Germany, October 19-26, 2008
- "eNMR: deploying and unifying the NMR e-infrastructure in systems biology ". 3rd EU-NMR Annual User Meeting, Autrans, France, January 26-29, 2009
- "Information-driven modeling of biomolecular complexes". National Institute for Medical Research (MRC), London, January 13, 2009

- "Information-driven modeling of biomolecular complexes". Keystone meeting on "Frontiers of NMR in Biology", Santa Fe NM, USA, February 15-20, 2009
- "Information-driven modeling of biomolecular complexes". XXIème Conférence du GERM, Fréjus, France, March 8-13, 2009
- "Information-driven modeling of biomolecular complexes". Physical Chemistry Kolloquium. ETHZ, Zurich, Switzerland, May 5, 2009
- "Information-driven modeling of biomolecular complexes". University of Washington, Seattle, May 11, 2009
- "Information-driven modeling of biomolecular complexes". 4th International Symposium on Enabling Technologies for Proteomics, Vancouver, Canada, May 13th, 2009
- "eNMR: deploying and unifying the NMR e-infrastructure in systems biology ". Joint East-NMR / eNMR conference, Florence Italy, June 15-17, 2009
- "eNMR: deploying and unifying the NMR e-infrastructure in systems biology ". Joint East-NMR / eNMR workshop, EBI Hinxton UK, November 4-5, 2009
- "HADDOCK sails the web: features and performance of the HADDOCK web server. Are we ready for large scale docking?". CAPRI meeting, Barcelona Spain, December 9-11, 2009
- "Information-driven modeling of biomolecular complexes". Royal Society Biochemistry meeting on "Experimental approaches to protein-protein interactions, Sheffield, UK, January 11/12, 2010
- "eNMR: deploying and unifying the NMR e-infrastructure in systems biology ". EU-NMR large scale facility meeting, Egmond aan Zee, January 18-21, 2010
- "Information-driven modeling of biomolecular complexes. Perspectives and challenge". Cambridge University biophysical seminar series, UK, January 27, 2010
- "Information-driven modeling of biomolecular complexes". E-WISPOC 2010, Bressanone, Italy, February 1st-5, 2010
- "Information-driven modeling of biomolecular complexes. Perspectives and challenge". FEBS meeting on *Understanding Transient Molecular Interactions in Biology*, Seville, Spain, May 18-21, 2010
- "Information-driven modeling of biomolecular complexes. Perspectives and challenge". University of Science and Technology of China, Hefei, China, May 28, 2010
- eNMR workshop of NMR structure calculation – GRID applications and integrated tools, Vilnius, Lithuania, June 7-11, 2010
- "Information-driven modeling of biomolecular complexes. Perspectives and challenge". Université de Provence / Aix-Marseille I, France, June 18, 2010
- "Information-driven modeling of biomolecular complexes. Perspectives and challenge". INSTRUCT UK meeting, MRC Center, London, UK, July 5, 2010
- "Computational aspects of NMR structure calculations" and "Structure validation". EMBO course "Multidimensional NMR in Structural Biology". Il Ciocco, Castelvecchio Pascoli, Italy, August 1-6, 2010
- "Building macromolecular assemblies by information-driven docking. Challenges and perspectives". 24th International Conference on Magnetic Resonance in Biological Systems (ICMRBS), Cairns, Australia, August 22-27, 2010

- "Building macromolecular assemblies by information-driven docking. Challenges and perspectives". Institute for Molecular Bioscience, University of Queensland, Brisbane, Australia, August 27, 2010

- Workshop on "Information-driven modeling of biomolecular complexes. Challenges and perspectives". Bioinformatic Institute of A-STAR, Singapore, August 31, 2010

Referee

- Agence Nationale française de la Recherche (ANR)
- Applied Bioinformatics
- Biochemistry
- Bioinformatics
- Biophysical Chemistry
- Biophysical Journal
- Biopolymers
- BMC Bioinfomatics
- European Biophysics Journal
- EMBO Journal
- ETH Zurich internal grants
- International Journal of Biological Macromolecules
- International Journal of Quantum Chemistry
- Israel Science Fundation
- Journal of Biomolecular Structure & Dynamics
- Journal of the American Chemical Society
- Journal of Biomolecular NMR
- Journal of Computational Chemistry
- Journal of Computational and Theoretical Chemistry
- Journal of Peptide Research
- Molecular Endocrinology
- Molecular Physics
- Molecular Simulation
- NIH
- Nucleic Acid Research
- NWO-CW Netherlands Organization for Scientific Research
- Proceeding of the National Academy of Sciences
- Proteins: Structure, Function & Bioinformatics
- Swiss National Research fundation
- Welcome Trust Fund, UK

Journal Editorial Board Memberships

Editorial Board and Editorial manager for Proteins: Structure, Function & Bioinformatics

Editorial Board and Editorial manager for the Biophysical Journal

Publication list

International (refereed) journals

1. I. Burghardt, L. Di Bari, A. Bonvin and G. Bodenhausen. (1990). Effect of strong coupling in multiple-quantum-filtered two-dimensional NOE spectroscopy. *J. Magn. Reson.* **86**, 652-656.
2. C. Gonzales, J.A.C. Rullmann, A.M.J.J. Bonvin, R. Boelens and R. Kaptein (1991). Toward an NMR R factor. *J. Magn. Reson.* **91**, 659-664.
3. A.M.J.J. Bonvin, R. Boelens and R. Kaptein (1991). Direct NOE refinement of biomolecular structures using 2D NMR data. *J. Biomol. NMR* **1**, 305-309.
4. A.M.J.J. Bonvin, R. Boelens and R. Kaptein (1991). Direct structure refinement using 3D NOE-NOE spectra of biomolecules. *J. Magn. Reson.* **95**, 626-631.
5. R.M.A. Knegtel, M. Katahira, J.G. Schilthuis, A.M.J.J. Bonvin, R. Boelens, D. Eib, P.T. der Saag and R. Kaptein (1993). The solution structure of the human retinoic acid receptor-b DNA-binding domain. *J. Biomol. NMR* **3**, 1-17.
6. A.M.J.J. Bonvin, J.A.C. Rullmann, R.M.J.N. Lamerichs, R. Boelens and R. Kaptein (1993). Ensemble Iterative Relaxation Matrix Approach: a new NMR refinement protocol applied to the solution structure of crambin. *PROTEINS: Structure, Function & Genetics* **15**, 385-400.
7. A.M.J.J. Bonvin, R. Boelens and R. Kaptein (1994). Direct nuclear Overhauser effect refinement of crambin from 2D NMR data using a slow-cooling simulated annealing. *Biopolymers* **34**, 39-50.
8. A.M.J.J. Bonvin, H. Vis, J.N. Breg, M.J.M. Burgering, R. Boelens and R. Kaptein (1994). NMR solution structure of the Arc repressor using relaxation matrix calculations. *J. Mol. Biol.* **236**, 328-341.
9. A.M.J.J. Bonvin, R. Boelens and R. Kaptein (1994). Time- and ensemble-averaged direct NOE restraints. *J. Biomol. NMR* **4**, 143-149.
10. M.A.A. van Tilborg, A.M.J.J. Bonvin, K. Hard, A.L. Davis, B. Maler, R. Boelens and R. Kaptein (1995). Structure refinement of the glucocorticoid receptor DNA-binding domain from NMR data by relaxation matrix calculations. *J. Mol. Biol.* **247**, 689-700.
11. A.M.J.J. Bonvin and A.T. Brünger (1995). Conformational variability of solution nuclear magnetic resonance structures. *J. Mol. Biol.* **250**, 80-93.
12. M. Slijper, A.M.J.J. Bonvin, R. Boelens and R. Kaptein (1995). Application of structure refinement using 3D NOE-NOE spectroscopy to lac repressor headpiece (1-56). *J. Magn. Reson.* **B107**, 298-301.
13. A.M.J.J. Bonvin and A.T. Brünger (1996). Do NOE distances contain enough information to assess the relative populations of multi-conformer structures? *J. Biomol. NMR* **7**, 72-76.
14. M. Slijper, A.M.J.J. Bonvin, R. Boelens and R. Kaptein (1996). Refined structure of the lac repressor headpiece (1-56) determined by relaxation matrix calculations from 2D and 3D NOE data: change of tertiary structure upon binding to the lac operator. *J. Mol. Biol.* **259**, 761-773.
15. M. Sunnerhagen, V.P. Denisov, K. Venu, A.M.J.J. Bonvin, J. Carey, B. Halle and G. Otting (1998). Water molecules in DNA recognition I: Hydration lifetimes of the trp operator in solution measured by NMR spectroscopy. *J. Mol. Biol.* **282**, 847-858.
16. A.M.J.J. Bonvin, M. Sunnerhagen, G. Otting and W.F. van Gunsteren (1998). Water molecules in DNA recognition II: A molecular dynamics view of the structure and hydration of the trp operator. *J. Mol. Biol.* **282** 859-873.
17. C.A.E.M. Spronk, A.M.J.J. Bonvin, P.K. Radha, G. Melacini, R. Boelens and R. Kaptein (1999). The solution structure of lac repressor headpiece 62 complexed to a symmetrical lac operator sequence determined by NMR and restrained molecular dynamics. *Structure* **7** 6472-6480.
18. A.M.J.J. Bonvin and W.F. van Gunsteren (2000). b-hairpin stability and folding: Molecular dynamics studies of the first b-hairpin of tendamistat. *J. Mol. Biol.* **296**, 255-268.

19. A.M.J.J. Bonvin (2000). Localisation and dynamics of sodium counterions aroud DNA in solution from molecular dynamics simulations. *Eur. Biophys. J.* **29**, 57-60.

20. A.M.J.J. Bonvin, A.E. Mark and W.F. van Gunsteren (2000). The GROMOS96 benchmarks for molecular simulation. *Comput. Phys. Commun.* **128**, 550-557.

21. P.J.A. van Tilborg, M. Czisch, F.A.A. Mulder, G.E. Folkers, A.M.J.J. Bonvin, M. Nair, R. Boelens and R. Kaptein (2000). Changes in dynamical behaviour of the retinoid X receptor DNA-binding domain upon binding to 14 base pair DNA half site. *Biochemistry* **39**. 8747-8757.

22. G. Melacini, A.M.J.J. Bonvin, M. Goodman, R. Boelens and R. Kaptein (2000). Hydration dynamics of the collagen triple-helix by NMR. *J. Mol. Biol.* **300**, 1041-1048.

23. M. van Beest, D. Dooijes, M. van Wetering, S. Kjaerulff, A.M.J.J. Bonvin, O. Nielsen and H. Clevers (2000). Sequence-specific HMG box factors recognize 10-12 base pair minor groove motifs. *J. Biol. Chem.* **275**, 27266-27273

24. A.M.J.J. Bonvin, K. Houben, M. Guenneugues, R. Kaptein and R. Boelens (2001). Rapid protein fold determination using secondary chemical shifts and cross-hydrogen bond ^{15}N-$^{13}C'$ scalar couplings ($^{3hb}J_{NC'}$). *J. Biomol. NMR.* **21**, 221-233.

25. N. D'Amelio, A.M.J.J Bonvin, M. Czisch, P. Barker and R. Kaptein (2002). The C terminus of apocytocrome b562 undergoes fast motions and slow exchange among ordered conformations resembling the folded state. *Biochemistry*, **41**, 5505-5514.

26. S. Singh, G.E. Folkers, A.M.J.J. Bonvin, R. Boelens, R. Wechselberger, A. Niztayev and R. Kaptein (2002). Solution structure and DNA binding properties of the C-terminal domain of UvrC from E-coli. *EMBO J.*, **21**, 6257-6266.

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