CV Jens Kleinjung

Dr. Jens Kleinjung
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Research Interests & Skills

Starting as an experimental protein/peptide chemist, my research activity has encompassed Biophysics of proteins (NMR and optical spectroscopy) and Bioinformatics, where I have worked on a wide range of theoretical aspects of protein sequences and structures. Among those are the parallelisation of multiple sequence alignment, hybrid Molecular Dynamics and Monte Carlo simulations, parametrisation of implicit solvent forces from large-scale simulations, structural alphabets to describe protein structures in terms of canonical fragments and applications to detect allosteric signal transmission in proteins.

In recent years I have focused on the analysis of NGS data, in particular the analysis of single-cell RNA-Seq data. To that end, I have developed an automated pipeline for the complete processing of 'fastq' input data to the final table of transcript counts. My current focus is on modelling the pseudo-temporal gene expression of stem cells along their differentiation to specific cell lineages.

Beside my research activities, I was responsible for the computational ecosystem of the Division of Mathematical Biology at the National Institute for Medical Research (before it was absorbed in the Francis Crick Institute). The core facility of that Division was a Beowulf cluster with a capacity of about 1500 cores and 20TB storage. Additionally, I maintained the shared software, databases and intranet and supported users in software development and cluster usage.

I am an experienced programmer in C, R and Perl and I have used Linux for over a decade in system administration and computational research.

Expertise

- transcriptomics data analysis
- protein sequence and structure analysis
- discrete state models
- molecular simulations
- allostery
- molecular interaction networks
- Linux system administration

Professional Vita

- **since 04.2015** Bioinformatics Officer, The Francis Crick Institute, London, U.K.
- **10.2005-03.2015** Senior Investigator Scientist, Division of Mathematical Biology, National Institute for Medical Research, London, U.K.
- **12.2002-09.2005** Assistant Professor of Bioinformatics, Vrije Universiteit, Amsterdam, The Netherlands
- **01.1998-11.2002** Postdoctoral Research Fellow, National Institute for Medical Research, London, U.K.
- **12.1996-11.1997** Postdoctoral Research Fellow, LCPM-CNRS, Nancy, France
- **04.1996-11.1996** Research assistant, RWTH Aachen University, Germany
- **10.04.1996** Dr. rer. nat. (PhD Chemistry), RWTH Aachen University, Germany
- **01.10.1992-01.04.1996** PhD thesis (Chemistry) 'Insulin-receptor interactions', RWTH Aachen University, Germany
- **01.01.1992-30.06.1992** Diploma thesis (Chemistry) 'Phosphorylated Insulins', RWTH Aachen University, Germany
- **08.1985-12.1991** Studies in chemistry and biology, RWTH Aachen University, Germany

Awards & Grants

- **2010/2012** EMBO long-term fellowship (ALTF 651-2009) to host Dr. J. Baussand
- **2008/2009** European Science Foundation grant of the programme "Frontiers in Functional Genomics" to host Dr. J. Baussand
- **2008-2010** EU project ProtFlexPred (Proposal N° 220256) of the programme "Marie-Curie Intra-European Fellowships for Career development" (Call identifier: PEOPLE-2007-2-1-IEF) to host Dr. A. Pandini
- **2007/2008** European Science Foundation grant of the programme "Frontiers in Functional Genomics" to host Dr. A. Pandini
- **2004** JSPS Invitation Fellowship (6 weeks) for collaborative research at the Global Scientific Information and Computing Center (GSIC), Tokyo with Dr. M. Ota; GRID application of fast protein folding simulations

- **1995-1997** Research grant (2 years) 'Synthesis of Phosphorylated Insulins' from German Research Ministry (DFG)
- **1992-1995** PhD stipend (4 years) of the Land Nordrhine Westphalia for outstanding students

Talks & Lectures

- **11.03.2014** Crick Symposium on Quantitative Biology; 'Signal Transduction in Protein Structures'
- **20.11.2013** BOKU University Wien, Austria; 'Signal Transduction in Protein Structures'
- **15.10.2012** Radboud University Nijmegen, The Netherlands; 'Functional Analysis of Proteins via Structural Alphabets'
- **05-06.2011** Guest professorship at the ETH Zürich, Switzerland; Group of Prof. W.F. van Gunsteren (computer-aided chemistry)
- **05.2010** German Research School for Simulation Sciences, Forschungszentrum Jülich, Germany; Course 'Introduction to Bioinformatics', Group of Prof. P. Carloni, 10 lectures and 3 tutorials
- **05.2009** SISSA International School for Advanced Studies, Trieste, Italy; Course 'Introduction to Bioinformatics', Group of Prof. P. Carloni, 10 lectures and 3 tutorials
- **03.2009** University of Liverpool, Liverpool, U.K.; 'Algorithmic Approaches for Protein Structure Analysis and Design'
- **11.2008** King's College, London, U.K.; 'Alignment Methods for Protein Modelling and Design'
- **09.2008** University of Cagliari, Cagliari, Italy; 'Principles of Biological Sequence Alignment'
- **06.2005** Universitá degli Studi di Milano, Milano, Italy; 'Unified Sequence and Structure Alignment'
- **02.2005** Zentrum für Bioinformatik, Hamburg, Germany; 'Unified Sequence and Structure Alignment'
- **02.2005** CEINGE Institute, Napoli, Italy; 'Flexible Sequence and Structure Alignment Using Constraints'
- **01.2005** Groningen Bioinformatics Centre, Groningen, Netherlands; 'Flexible Sequence and Structure Alignment Using Constraints'
- **08.2004** Quantum Bioinformatics Group, Nara, Japan; 'New Algorithms for Biological Sequence Analysis'

- **08.2004** National Center of Genetics, Mishima, Japan; 'New Algorithms for Biological Sequence Analysis'
- **07.2004** Yokohama City University, Yokohama, Japan; 'Recent Progress in Protein Molecular Dynamics Simulations'
- **11.2003** Biotecnologia 2003, Havana, Cuba; 'Contact-based Sequence Alignment'
- **09.2001** Biophysical Chemistry 2001, Royal Society of Chemistry, London, U.K.; 'Unfolding Simulations Using Leap-dynamics'
- **02.2001** BBSRC Bioinformatics Grantholders' Workshop, Hinxton, U.K.; 'Quest: Iterative Sequence Searching'

Other Professional Activities

- Member of the International Society for Computational Biology
- Academic editor of Scientific Reports
- Academic editor of PLoS ONE
- Reviewer for various research funding organisations

Programs & Servers

- POPS
- POPSCOMP
- more on GitHub

Publications

- on ORCID
- on Google Scholar

1. Lasrado R, Boesmans W, Kleinjung J, Pin C, Bell D, Bhaw L, McCallum S, Zong H, Luo L, Clevers H, Berghe PV and Pachnis V. **Lineage-dependent spatial and functional organization of the mammalian enteric nervous system.** *Science* 356(6339) 722-726 (2017).
2. Gouti M, Delile J, Stamataki D, Wymeersch FJ, Huang Y, Kleinjung J, Wilson V and Briscoe J. **A Gene Regulatory Network Balances Neural and Mesoderm Specification during Vertebrate Trunk Development.** *Developmental Cell* 41(3) 243-261.e7 (2017).
3. Pandini A, Kleinjung J, Rasool S and Khan S. **Coevolved Mutations Reveal Distinct Architectures for Two Core Proteins in the Bacterial Flagellar Motor.** *PloS One* 10 e0142407 (2015).

4. Pandini A, Kleinjung J, Taylor W and Khan S. **The Phylogenetic Signature Underlying ATP Synthase c-ring Dynamics.** *Biophys J* 109 975-987 (2015).

5. Gouti M, Tsakiridis A, Wymeersch FJ, Huang Y, Kleinjung J, Wilson V and Briscoe J. **In Vitro Generation of Neuromesodermal Progenitors Reveals Distinct Roles for Wnt Signalling in the Specification of Spinal Cord and Paraxial Mesoderm Identity.** *PLOS Biology* 12 e1001937 (2014).

6. Kleinjung J and Fraternali F. **Design and Application of Implicit Solvent Models in Biomolecular Simulations.** *Current Opinion in Structural Biology* 25 126-134 (2014).

7. Pernigo S, Fukuzawa A, Pandini A, Holt M, Kleinjung J, Gautel M and Steiner RA. **The Crystal Structure of the Human Titin: Obscurin Complex Reveals a Conserved yet Specific Muscle M-Band Zipper Module.** *J Mol Biol* 427 707-714 (2014).

8. Baussand J and Kleinjung J. **Specific Conformational States of Ras GTPase upon Effector Binding.** *Journal of Chemical Theory and Computation* 9(1) 738-749 (2013).

9. Chakroun N, Fornili A, Prigent S, Kleinjung J, Dreiss CA, Rezaei H and Fraternali F. **Decrypting Prion Protein Conversion into a fi-Rich Conformer by Molecular Dynamics.** *Journal of Chemical Theory and Computation* 9(5) 2455-2465 (2013).

10. Pandini A, Fornili A, Fraternali F and Kleinjung J. **GSATools: analysis of allosteric communication and functional local motions in GROMACS using a Structural Alphabet.** *Bioinformatics* 29 2053-2055 (2013).

11. Kleinjung J and Fraternali F. **Urea-water solvation forces on prion structures.** *Journal of Chemical Theory and Computation* 8 3977-3984 (2012).

12. Kleinjung J, Scott WRP, Allison JR, van Gunsteren WF and Fraternali F. **Implicit Solvation Parameters Derived from Explicit Water Forces in Large-Scale Molecular Dynamics Simulations.** *Journal of Chemical Theory and Computation* 8(7) 2391-2403 (2012).

13. Pandini A, Fornili A, Fraternali F and Kleinjung J. **Detection of allosteric signal transmission by information-theoretic analysis of protein dynamics.** *FASEB Journal* 26 868-881 (2012).

14. Kemena C, Taly JF, Kleinjung J and Notredame C. **STRIKE: Evaluation of Protein Multiple Sequence Alignments using a Single Three Dimensional Structure.** *Bioinformatics* 27 3385-3391 (2011).

15. Fernandes LP, Annibale A, Kleinjung J, Coolen ACC and Fraternali F. **Protein networks reveal detection bias and species consistency when analysed by information- theoretic methods.** *PLoS ONE* 5 e12083 (2010).

16. Pandini A, Fornili A and Kleinjung J. **Structural alphabets derived from attractors in conformational space.** *BMC Bioinformatics* 11 97 (2010).

17. Schmitz S, Schaap IAT, Kleinjung J, Harder S, Grainger M, Calder L, Rosenthal PB, Holder AA and Veigel C. **Malaria parasite actin polymerisation and filament structure.** *J. Biol. Chem.* 285 36577-36585 (2010).

18. Annibale A, Coolen ACC, Fernandes LP, Fraternali F and Kleinjung J. **Tailored graph ensembles as proxies or null models for real networks I: tools for quantifying structure.** *Journal of Physics A: Math. Theor.* 42 485001 (2009).

19. Autore F, Melchiorre S, Kleinjung J, Morgan WD and Fraternali F. **Interaction of Malaria Parasite-Inibitory Antibodies with the Merozite Surface Protein MSP1$_{19}$ by Computational Docking.** *Proteins* 66 513-527 (2007).

20. Pandini A, Bonati L, Fraternali F and Kleinjung J. **MinSet: A general approach to derive maximally representative database subsets by using fragment dictionaries and its application to the SCOP database.** *Bioinformatics* 23 515-516 (2007).

21. Kleinjung J and Fraternali F. **POPSCOMP: An automated interaction analysis of biomolecular complexes.** *Nuc. Acids Res.* 33 W342-W346 (2005).

22. Simossis V, Kleinjung J and Heringa J. **Homology-extended sequence alignment.** *Nuc. Acids Res.* 33 816-824 (2005).

23. Fraternali F and Kleinjung J. **Molecular simulations in structural genomics.** In *Encyclopedia of Genetics, Genomics, Proteomics and Bioinformatics*, volume 4.6, (74). John Wiley & Sons (2004).

24. Shojaee-Moradie F, Chan M P, Telfer M A, Brandenburg D, Sundermann E, Eckey H, Kleinjung J, Sch{"u}ttler A and Jones R H. **Effect of thyroid hormone binding proteins on insulin receptor binding of B1-thyronine-insulin analogues.** *Biochem. J.* 381 51-57 (2004).

25. Kleinjung J, Romein J, Lin K and Heringa J. **Contact-based sequence alignment.** *Nuc. Acids Res.* 32 2464-2473 (2004).

26. Vaccaro L, Cross KJ, Kleinjung J, Straus SK, Thomas DJ, Wharton SA, Skehel JJ and Fraternali F. **Plasticity of Influenza Haemagglutinin Fusion Peptides and their Interaction with Lipid Bilayers.**

Biophys. J. 88 25-36 (2004).

27. Cavallo L, Kleinjung J and Fraternali F. **POPS: a fast algorithm for Solvent Ac- cessible Surface Areas at atomic and residue level.** *Nuc. Acids Res.* 31 3364-3366 (2003).

28. George RA, Kleinjung J and Heringa J. **Predicting protein structural domains from sequence data.** In *Bioinformatics and Genomes - Current Perspectives*, chapter 1, 1-26. Horizon Scientific Press (2003).

29. Kleinjung J, Fraternali F, Martin SR and Bayley PM. **Thermal Unfolding Simulations of Apo-calmodulin using Leap-dynamics.** *Proteins* 50 648-656 (2003).

30. Lin KX, Kleinjung J, Taylor WR and Heringa J. **Testing homolgy with CAO: A contact-based Markov model of protein evolution.** *Comp. Biol. Chem.* 27 93-102 (2003).

31. Simossis V, Kleinjung J and Heringa J. **An overview of Multiple Sequence Alignment.** In **Current Protocols in Bioinformatics*, chapter 3.7, 3.7.1-3.7.25. John Wiley & Sons (2003).

32. Kleinjung J, Douglas N and Heringa J. **Parallelized multiple alignment.** *Bioinformatics* 18 1270-1271 (2002).

33. Kleinjung J, Bayley P and Fraternali F. **Leap-dynamics: efficient sampling of conformational space of proteins and peptides in solution.** *FEBS Letters* 470(3) 257-262 (2000).

34. Kleinjung J and Fabry M. **Photoreactive Insulin Derivatives for the Detection of the Doubly Labeled Insulin Receptor.** *Peptides* 21 401-406 (2000).

35. Kleinjung J, Petit MC, Orlewski P, Mamalaki C A Liolitsas, Tzartos SJ, Tsikaris M V Sakarellos-Daitsiotis, Sakarellos C, Marraud M and Cung MT. **The 3D structure of the Immunogenic Region of the Acetylcholine Receptor: A Combined 2D-NMR, Homology and Molecular Modeling Approach.** *Biopolymers* 53 113-128 (2000).

36. Martin SR, Lu AQ, Xiao J, Kleinjung J, Beckingham K and Bayley PM. **Conformational and metal-binding properties of androcam, a testis-specific, calmodulin-related protein from Drosophila.** *Protein Sci.* 8 2444-2454 (1999).

37. King's College London and Deutsches Wollforschungsinstitut. **Hepatoselective Insulin-Thyroxin Conjugates**, *Patent WO9965941* (1999-12-23).

38. Deutsches Wollforschungsinstitut. **Phosphorylated Insulins**, *Patent DE19535701* (A1) (1997-03-27).