Dr. Sebastian Will

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Summary

Over 60 peer-reviewed publications in international journals and conference proceedings (among them various well-cited first author publications); class lecturer at University of Vienna; formerly, at Universities of Leipzig, Freiburg University, and Massachusetts Institute of Technology

Main Research Interests

Algorithmic bioinformatics of RNA and protein structure; Structure prediction, design, interaction, folding dynamics, and comparative analysis of structural RNAs; Genome-wide de-novo prediction of non-coding RNAs; Declarative methods in bioinformatics

Selected Publications

S. Will, Ch. Otto, M. Miladi, M. Möhl, and R. Backofen. SPARSE: quadratic time simultaneous alignment and folding of RNAs without sequence-based heuristics. *Bioinformatics*, **31** no. 15 pp. 2489–2496, 2015.

S. Will, Michael Yu, and Bonnie Berger. Structure-based whole genome realignment reveals many novel non-coding RNAs. *Genome Res*, **23** no. 6 pp. 1018-27, 2013.

S. Will, T. Joshi, I. L. Hofacker, P. F. Stadler, and R. Backofen. LocARNA-P: Accurate boundary prediction and improved detection of structural RNAs. *RNA*, 18 no. 5 pp. 900-914, 2012.

Raheleh Salari, Mathias Möhl, S. Will, S. Cenk Sahinalp, and Rolf Backofen. Time and space efficient RNA-RNA interaction prediction via sparse folding. In Bonnie Berger, editor, Proc. of RECOMB 2010, volume 6044 of LNCS, pages 473-490. Springer-Verlag, 2010.

Grants and Honors

- German Research Foundation postdoctoral research fellowship: **grant WI 3628/1-1**
- PhD "summa cum laude" (with highest honors)
- Doctoral fellowship of the graduate program "Logic in Computer Science" at LMU, Munich

Contributions to the Scientific Community

since 2006	**Reviewer** for scientific journals, e.g. *Bioinformatics, NAR, Algorithms*, and international conferences, e.g. *RECOMB, ISMB, WABI*
since 2011	**Associate editor** of AMB thematic series
since 2006	**Co-chair** of Workshops on Constraints in Bioinformatics (WCB) collocated with international constraint and logic programming conferences CP and ICLP
since 2004	**Supervision** of students for Bachelor's, Master's/Diploma, and PhD Theses
since 2000	**Development, maintenance, and deployment** of free scientific software (prominently, the *LocARNA package*); in 2015–16 as member of the German Initiative for Bioinformatics Infrastructure (de.NBI)

Teaching Experience

2017	**Classes** at University of Vienna ("Algorithmic Bioinformatics", "Algorithms and Program Development for Biological Chemistry")
2012-16	**Classes** at University of Leipzig, including undergrad class "Algorithm and Data Structures" ($\sim$ 300 students) and graduate classes on advanced methods in bioinformatics and RNA analysis, graph theory, and theoretical biology.
2011	**Class** 18.417 as instructor of the MIT Math Dept.: "Introduction to Computational Molecular Biology — Foundations of Structural Bioinformatics"; Seminar 18.418 "Topics in Computational Biology" (TA, with Bonnie Berger)
2006 – 2012	**Classes** at Department of Computer Science, University Freiburg, Germany, covering "RNA Bioinformatics", "Protein Folding and Energy Landscapes", "Bioinformatics I+II", "Constraint Programming", "Structure Prediction in Simplified Protein Models" (**all classes in English**)
2006	**Invited Class** at Summer School BCI (Biology, Computation, and Information) on "Optimal Constrained-Based Protein Structure Prediction"
2002 – 2005	**Classes** at Department of Computer Science, University Jena, Germany covering class "Simplified Protein Models", seminar "Constraint-Satisfaction-Problems in Bioinformatics", lab class "Data Mining & Sequence Analysis"

Positions and Fellowships

since 2016	**Researcher** (Universitätsassistent, post-doc) at University of Vienna with Prof. Ivo Hofacker
2012-2016	**Postdoctoral Researcher** at University of Leipzig with Prof. Peter Stadler
2005-2012	**Akademischer Rat** at the Albert-Ludwigs-University in Freiburg with Prof. Rolf Backofen
2011	**Instructor** at Math Department, Massachusetts Institute of Technology (MIT)
2011	**Postdoctoral Associate** at Computer Science and Artificial Intelligence Lab (CSAIL), MIT, with Prof. Bonnie Berger
2010	**Postdoctoral Fellow**; Scholarship granted by the German Research Foundation, CSAIL, MIT, with Prof. Bonnie Berger
2002 – 2005	**Postdoctoral Researcher** at University Jena, Bioinformatics Group
2000 – 2002	**Doctoral Fellow**; granted by PhD program "Logic in Computer Science"; LMU Munich; Advisers: Prof. Peter Clote, Rolf Backofen

Education

2005	**Dr. rer. nat. in Computer Science** — *Summa Cum Laude* Friedrich-Schiller-University Jena, Germany
2000	**Diplom($\approx$ M.Sc.) in Computer Science** — *best in class* Ludwig-Maximilians-University Munich, Germany

CV Appendix

Selected Software

2015	**SparseMFEFold**. Space-efficient RNA structure prediction.
since 2012	**SPARSE**. Very efficient structure-based alignment of RNAs; distributed as part of the LocARNA package.
2011-2013	**REAPR**. A pipeline for fast structure-based realignment for de-novo prediction of structural non-coding RNAs in whole eukaryotic genomes.
since 2010	**CARNA**. Constraint-based Alignment of RNAs with structures of unrestricted complexity — a competitive tool for alignment of pseudoknots and multi-stable RNAs.
since 2009	**LocARNA-P**. Reliabilities of RNAs sequence-structure alignment — LocARNA-P computes reliabilities and match probabilities of sequence-structure alignments and enables advanced comparative RNA analysis.
since 2005	**LocARNA**. Multiple alignment of RNAs — LocARNA is one of the most accurate and fastest tools for pairwise and multiple alignment of RNA. LocARNA is enjoying widespread, active use in RNA research, is constantly extended, and inspires further algorithmic development.
2006	**CTE-Alignment**. Constrained alignment by Cluster-Tree-Elimination — declarative integration of complex constraints preserving efficiency.
2000 – 2005	**PSP**. Constrained-based Protein Structure Prediction — first exact prediction in face-centered cubic and cubic models. PSP has set the foundations for the CPSP package.

Selected Talks and Visits

2015	Two **Talks** at the Benasque RNA meeting (E. Rivas, E. Westhof), Benasque
2015	**Talk** at WABI (algorithmic bioinformatics conference), Atlanta
2014	**Talk** at WABI, Wrocław
2013	Two **Talks** at RECOMB (major bionformatics conference), Beijing
2012	**Talk** at RECOMB, Vancouver
2010	**Invited Talk** Prof. Jérôme Waldispühl, McGill, Montreal
2010	**Invited Talk** Prof. Cenk Sahinalp, SFU, Vancouver
2010	**Invited Talk** Prof. Rolf Backofen, ALU, Freiburg
2009	**Talk** at the Benasque RNA meeting, Benasque
2008	**Invited Talks** Prof. Bonnie Berger, MIT, Cambridge MA

Main Scientific Contributions

Efficient and Accurate Multiple Alignment of Structural RNA for Comparative Analysis and Its Applications

Motivation	Structural non-coding RNA (ncRNA) is playing a very important role in cells. Analysis of RNA requires fast and space efficient structure-based alignment methods. However, the gold-standard for this purpose has prohibitive complexity. Fast methods enable new biological applications.

Results The LocARNA software package — very time and space-efficient algorithms for multiple alignment of RNA by simultaneous alignment and folding.
The tool LocARNA has been used for large scale clustering of structural RNAs. SPARSE improves ensemble-based sparsification over LocARNA, resulting in even more efficient alignment and folding. LocARNA-P extends the approach for computing reliabilities of sequence-structure RNA alignment, which allowed me to predict accurate boundaries of ncRNAs in computational predictions and improve the predictive power of de-novo ncRNA prediction. I have applied the tool in the modENCODE project and revealed many novel ncRNA candidates in *Drosophila melanogaster* based on a further algorithmic extension of LocARNA.

Prediction of RNA-RNA-Interaction, Pseudoknot Prediction and Alignment

Motivation Folding and alignment of RNA molecules is indispensable for current biological research. However, for considering pseudoknots in the study of RNA-RNA-interaction, efficiency is still limiting.

Results Applying a sparsification technique, we developed sparsified algorithms to predict RNA-RNA-interaction and RNA pseudoknots, which significantly improves performance and space consumption. Furthermore, we developed fixed parameter-tractable and polynomial algorithms for alignment of RNA pseudoknots. Thereby, we improved the theoretical complexity as well as practical applicability of pseudoknot alignment algorithms.

Predicting Globally Optimal Structures in Three-Dimensional Protein Models

Motivation Protein models are valuable tools for the study of protein folding and evolution, as well as for benchmarking heuristic optimization. Many of these applications require optimal structure prediction, however effective approaches for unrestricted models didn't exist.

Results We developed a fast approach for optimal prediction of structures in cubic and face-centred-cubic HP and HPNX protein models. The implementation CPSP is freely available and is used in protein studies.

Symmetry Breaking in Constraint-Search

Motivation Symmetry breaking is often essential for the efficient solving of constraint models, but most specialized methods interfere with the search heuristic and complicate constraint modeling.

Results We devised a general symmetry breaking scheme that works by introducing constraints during the search. The scheme has been used in a number of constraint models, among them our own models for protein structure prediction. The idea contributed significantly to the advancement of the field.