DR. SEBASTIAN WILL — CURRICULUM VITAE, 08/2019

Researcher
TBI—Theoretical Biochemistry Group
Institute for Theoretical Chemistry
University of Vienna

email: *sebastian.will@univie.ac.at*
`www.tbi.univie.ac.at/~will`
phone: *+43 1 4277 52749*

SUMMARY

70+ peer-reviewed publications in international journals and conference proceedings (among them various well-cited first author publications); H-index 27 (according to Google scholar). Developer of the widely-used software package LocARNA (the original publication alone was cited 441 times). Class lecturer at University of Vienna; formerly, University of Leipzig, University of Freiburg, and MIT.

MAIN RESEARCH INTERESTS

Algorithmic bioinformatics of RNA and protein structure; Structure prediction, comparative analysis, design, interaction, and folding kinetics of RNAs; Genome-wide de-novo prediction of non-coding RNAs; Downstream analysis of high-throughput NGS data; Declarative methods in bioinformatics

SELECTED PUBLICATIONS

S. Hammer, W. Wang, S. Will*, and Y. Ponty* Fixed-parameter tractable sampling for RNA design with multiple target structures. *BMC Bioinformatics*, 20 no. 1 pp. 209, 2019.

H. Jabbari, I. Wark, C. Montemagno, and S. Will* Knotty: efficient and accurate prediction of complex RNA pseudoknot structures. *Bioinformatics*, 34 no. 22 pp. 3849–3856, 2018.

S. Will, Ch. Otto, M. Miladi, M. Möhl, and R. Backofen* SPARSE: quadratic time simultaneous alignment and folding of RNAs w/o sequence-based heuristics. *Bioinformatics*, 31 no. 15 pp. 2489–96, 2015.

S. Will, M. Yu, and B. 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. 900–14, 2012.

S. Will, K. Reiche, I. Hofacker, P. Stadler, and R. Backofen*. Inferring non-coding RNA families and classes by means of genome-scale structure-based clustering. *PLOS Comp Biol*, 3(4):e65, 2007.

GRANTS AND HONORS

German Research Foundation postdoctoral research fellowship: grant WI 3628/1-1

Doctorate *"summa cum laude"*

Doctoral fellowship of the graduate program "Logic in Computer Science" at LMU, Munich

CONTRIBUTIONS TO THE SCIENTIFIC COMMUNITY

2019	Guest editor of IJMS (MDPI) special issue "RNA Structure Prediction"
since 2014	PC member of WABI'15, BIOINFORMATICS'17–19, RECOMB'18, '19, & '20
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; 2007 special issue of Constraints
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

Teaching Experience (summary)

2017–2019	Classes at University of Vienna ("Structure and Dynamics of Biomacromolecules", "Algorithmic Bioinformatics", "Algorithms and Program Development for Biological Chemistry (APBC)"); all classes taught several times
2012–2016	Classes at University of Leipzig, including undergrad class "Algorithms and Data Structures" ($\sim$ 300 students) and graduate classes on advanced methods in bioinformatics, 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"; as TA, with Bonnie Berger: Seminar 18.418 "Topics in Computational Biology"
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	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	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

Degrees

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

Selected Software

2018	Infrared / RNARedprint. FPT generic Boltzmann sampling and RNA sampling with multiple target structures *(C++, Python, Boost.Python)*
2018	Knotty. Space-efficient prediction of CCJ pseudoknots *(C++)*
2016–2019	GitCATS Git-based multilingual continuous integration testing system (written for teaching a programming class (APBC), where—using Github—students submit and revise their programs, which the system tests automatically) *(Python)*
2015	SparseMFEFold. Space-efficient RNA structure prediction *(C++)*
since 2012	SPARSE. Very efficient structure-based alignment of RNAs; distributed as part of the LocARNA package *(C++)*
2011–2013	REAPR. A pipeline for fast structure-based realignment for de-novo prediction of structural non-coding RNAs in whole eukaryotic genomes *(C++, Python)*
since 2010	CARNA. Constraint-based Alignment of RNAs with structures of unrestricted complexity — a competitive tool for alignment of pseudoknots and multi-stable RNAs *(C++, Gecode)*
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. *(C++, Perl)*
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. *(C++, Perl)*
2006	CTE-Alignment. Constrained alignment by Cluster-Tree-Elimination — declarative integration of complex constraints preserving efficiency *(C++)*
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. *(Mozart/Oz)*

Selected Talks and Visits

2019	Talk WABI'19 (algorithmic bioinf. conference), Niagara Falls NY
2019	Keynote Talk at meeting of the former DFG Priority Program SPP 1258, Freiburg
2019	Invited Talk and visit at École Polytechnique, Palaiseau
2018	Talk at RECOMB (major algorithmic bioinformatics conference), Paris
2018	Talk at the Vienna RNA meeting, Vienna
2018	Talk at the Benasque RNA meeting (E. Rivas, E. Westhof), Benasque
2017	Invited Talk at Ribonets workshop, Düsseldorf
2015	Two Talks at the Benasque RNA meeting (E. Rivas, E. Westhof), Benasque
2014/15	Talks at WABI'15, Atlanta and WABI'14, Wrocław
2012/13	Talk at RECOMB'12 in Vancouver and two Talks at RECOMB'13, Beijing
2010	Invited Talk Prof. Jérôme Waldispühl, McGill, Montreal
2010	Invited Talk Prof. Cenk Sahinalp, SFU, Vancouver
2009	Talk at the Benasque RNA meeting, Benasque
2008	Invited Talks Prof. Bonnie Berger, MIT, Cambridge MA

SELECTED SCIENTIFIC CONTRIBUTIONS

Structure-Based Comparative Analysis of RNAs

Motivation Structural non-coding RNAs (ncRNAs) play an essential 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 — 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. 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, I developed sparsified algorithms to predict RNA-RNA-interaction and RNA pseudoknots , which significantly improves performance and space consumption. Furthermore, I developed fixed parameter-tractable and polynomial algorithms for the alignment of RNA pseudoknots .

Structure Prediction in 3D Protein Models and Symmetry Breaking in Constraint Search

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.
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 I 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.
Motivated by the work on structure prediction, I 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.

TEACHING ACTIVITIES (DETAILED)

2019 Invited lectures at Winter School "Algorithms in Structural Bioinformatics": two lectures and two hands-on lab classes "Comparative methods for structure analysis" (Marseille, `https://algosb2019.sciencesconf.org`)

2017–19 University of Vienna; class "Algorithmic Bioinformatics" for Bioinformatics MSc students (with Arndt von Haeseler and Heiko Schmidt), 3× 1/3 of 56h

2017–19 University of Vienna; lab class "Algorithms and Program Development for Biological Chemistry" for Chemistry MSc and PhD students, 3 × 56h

2017&18 University of Vienna; class "Structure and Dynamics of Biological Macromolecules", 2×56h

2015/16 University of Leipzig; Organization of recitation classes to "Algorithms and Data Structures (I+II)" (∼ 400 students; 12 parallel recitation classes); 56h

2013 University of Leipzig; class "Algorithms and Data Structures" (∼ 300 students) for first-semester Computer Science and Mathematics BSc students (with Peter Stadler); 1/2 of 112h

2012–16 University of Leipzig; classes for Bioinformatics MSc students (with Peter Stadler)

- 2016 "Theoretical biology", 1/2 of 28h
- 2014/15 "Graph theory", 1/2 of 28h
- 2013 "Recent methods in RNA Structure Prediction", 1/2 of 28h
- 2014/15 & 12/13 "Advanced methods in bioinformatics", 2 × 1/2 of 28h

2011 MIT Math Department; class 18.417: "Introduction to Computational Molecular Biology — Foundations of Structural Bioinformatics"; 24h

2010 MIT CSAIL; Seminar 18.418 "Topics in Comp. Biology" with Bonnie Berger; 26h

2006–12 University of Freiburg; classes for Bioinformatics and CS MSc students:

- 2009/10 & 08/09 "RNA Bioinformatics", 26h
- 2009 & 08 "Protein Folding and Energy Landscapes", 2 × 26h
- 2007/08 "Bioinformatics II", 26h
- 2007 "Bioinformatics I", 26h
- 2006/07 "Constraint Programming", 26h

2006 Invited lecture at Summer School BCI (Biology, Computation, and Information) on "Optimal Constrained-Based Protein Structure Prediction"

2002–05 University of Jena; classes for Bioinformatics MSc students

- 2006 class "Simplified Protein Models", 26h
- 2005/06 seminar "Constraint-Satisfaction-Problems in Bioinformatics", 2× 26h
- 2005 lab class "Data Mining & Sequence Analysis", 3× 52h