

REMO ROHS, Ph.D.

Professor and Founding Chair of Quantitative and Computational Biology
Professor of Chemistry, Physics and Astronomy, and Computer Science
University of Southern California, Los Angeles, CA, United States

Rohs Lab: <https://www.rohslab.org>; Email: rohs@usc.edu

QCB Department: <https://www.qcb-dornsife.usc.edu>

Research of the Rohs Lab established the field of DNA shape analysis in protein-DNA binding and transcription factor binding specificity. To achieve this, the Rohs Lab successfully integrated the fields of structural biology and genomics. Many tools and papers in both areas of research now use the approaches pioneered by the Rohs Lab. The Rohs Lab has expanded their work on deciphering molecular mechanisms and interactions based on the three-dimensional shapes of molecules to proteins, RNA, and drug design. The Rohs Lab currently develops machine learning and artificial intelligence (AI) methods and other computational and experimental approaches to reveal molecular mechanisms of binding. Dr. Rohs is an Alfred P. Sloan Research Scholar, and he was elected as a Fellow of the American Association for the Advancement of Science (AAAS).

EDUCATION, ACADEMIC DEGREES, AND TRAINING

01/2006-08/2010	Postdoctoral Training in Computational Biology and Bioinformatics, Columbia University, New York, NY, USA
12/2009	Professional Achievement Certificate in Business (Accounting, Finance, Management, Marketing), Columbia University, New York, NY, USA
03/2003-12/2005	Postdoctoral Training in Computational Structural Biology, Weizmann Institute of Science, Rehovot, Israel
01/2003	Ph.D. in Biochemistry, Department of Biology, Chemistry and Pharmacy, Freie Universität Berlin, Germany
09/1997	M.Sc. in Physics, Faculty of Natural Sciences, Humboldt Universität Berlin, Germany

POSITIONS AND APPOINTMENTS

01/2021-present	Full Professor (with Tenure) and Founding Chair of the newly established Department of Quantitative and Computational Biology (18 core and 23 joint faculty, 60 Ph.D., 20 M.Sc., and more than 120 undergraduate students) University of Southern California, Los Angeles, CA, USA
08/2016-12/2020	Full Professor (with Tenure), Quantitative and Computational Biology Section, Department of Biological Sciences, University of Southern California, Los Angeles, CA, USA
01/2016-08/2016	Associate Professor (with Tenure), Molecular and Computational Biology Section, Department of Biological Sciences, University of Southern California, Los Angeles, CA, USA
2013-present	Courtesy appointment, Department of Computer Science, Viterbi School of Engineering, University of Southern California, Los Angeles, CA, USA
2012-present	Courtesy appointment, Department of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA
2011-present	Member, Norris Comprehensive Cancer Center, Keck School of Medicine, University of Southern California, Los Angeles, CA, USA
2011-present	Courtesy appointment, Department of Chemistry, University of Southern California, Los Angeles, CA, USA
08/2010-01/2016	Tenure-track appointment, Molecular and Computational Biology Section, Department of Biological Sciences, University of Southern California, Los Angeles, CA, USA
2009-2010	Associate Research Scientist (Advisor: Barry Honig), Howard Hughes Medical Institute, Center for Computational Biology and Bioinformatics,

	Department of Biochemistry and Molecular Biophysics, Columbia University, New York, NY, USA
2006-2008	Research Associate (Advisor: Barry Honig), Howard Hughes Medical Institute, Center for Computational Biology and Bioinformatics, Department of Biochemistry and Molecular Biophysics, Columbia University, New York, NY, USA
2003-2005	Postdoctoral Fellow (Advisor: Zippora Shakked), Department of Structural Biology, Weizmann Institute of Science, Rehovot, Israel

HONORS AND AWARDS

Personal Awards and Fellowships

2024	Elected Fellow, Asia-Pacific Artificial Intelligence Association (AAIA), Hongkong
2022	Elected Fellow, American Association for the Advancement of Science (AAAS), Biological Sciences Section
2016	USC Mentoring Award in the category Faculty Mentoring Graduate Students, University of Southern California, Los Angeles, CA, USA
2016	American Chemical Society OpenEye Outstanding Junior Faculty Award in Computational Chemistry presented at the ACS Spring 2016 National Meeting, San Diego, CA
2013	Alfred P. Sloan Research Fellowship, Alfred P. Sloan Foundation, New York, NY
2012	Certificate of Appreciation from LCUSD Governing Board for dedication to students of La Cañada High School and supporting the field of science
2011	Selected by GenomeWeb as Annual Young Investigator
2010	Keynote Address, 2 nd India-Japan Symposium on Bioinformatics, Indian Institute of Technology, New Delhi, India
2005	Postdoctoral Fellowship, Kimmelman Center for Biomolecular Structure and Assembly, Weizmann Institute of Science, Rehovot, Israel
2003	Minerva Fellowship, Max Planck Society for the Advancement of Science, Munich, Germany
1998	Humboldt Prize for M.Sc. Thesis, Humboldt Universität, Berlin, Germany

Paper Awards

2024	Weller <i>et al.</i> J. Chem. Inf. Model. paper on drug design is featured on the journal cover
2024	Mitra <i>et al.</i> Nucleic Acids Res. paper on RNA structure is featured on the journal cover
2017	Yang <i>et al.</i> Mol. Syst. Biol. paper received a RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2016/17
2016	Dror <i>et al.</i> Genome Res. paper received a RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2015/16
2016	Zhou <i>et al.</i> PNAS paper was selected for a Highlight presentation at the RECOMB 2016 conference
2015	Zhou <i>et al.</i> PNAS paper received a RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2014/15
2015	Abe <i>et al.</i> Cell paper received a RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2014/15

2014	Yang <i>et al.</i> Nucleic Acids Res. paper received a RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2013/14
2014	Slattery <i>et al.</i> Trends Biochem. Sci. review paper was featured on the journal cover
2014	Yang <i>et al.</i> Nucleic Acids Res. paper was selected as NAR Breakthrough Article, a designation received by < 1% of articles published in NAR
2014	Yang <i>et al.</i> Nucleic Acids Res. paper was featured on the journal cover
2014	Barozzi <i>et al.</i> Mol. Cell paper received a RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2013/14
2013	Gordân <i>et al.</i> Cell Rep. paper received a RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2012/13
2013	Lazarovici <i>et al.</i> PNAS paper received a RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2012/13
2012	Slattery <i>et al.</i> Cell paper received the RECOMB/ISCB Top-10 Paper Award for being one of the ten most influential publications in the fields of regulatory and systems genomics in 2011

PROFESSIONAL ACTIVITIES

Member of Editorial and Professional Boards

2023-present	Member, Board of Directors, Center for Applied Mathematical Sciences (CAMS), University of Southern California
2014-2017	Member, Editorial Board, Proteopedia, Israel Structural Proteomics Center, Weizmann Institute of Science, Rehovot, Israel
2012-2014	Member, Academic Advisory Board, zSpace Inc., Sunnyvale, CA
2011-2016	Faculty Member, Faculty of 1000 in Biology (Structural Biology, Section Structure: Transcription and Translation), London, UK
2011	Guest Editor, PLOS Computational Biology, Public Library of Science
2010-present	Associate Editor, BMC Bioinformatics, BioMed Central, London, UK
2010-present	Member, Editorial Board, Journal of Biomolecular Structure & Dynamics, Taylor & Francis, Albany, NY

Meeting Organizer, Session Chair, Program and Poster Awards Committee Member

2022	Co-organizer of RECOMB Satellite Meeting for Dr. Michael Waterman's birthday and establishment of QCB as new USC department celebration
2022	Co-organizer of ACS Meeting Symposium for Dr. Barry Honig's birthday celebration, American Chemical Society National Meeting Spring 2022
2017	Program Committee Member, 25 th Annual International Conference on Intelligent Systems in Molecular Biology (ISMB)/16 th European Conference on Computational Biology (ECCB), Prague, Czech Republic
2015	Co-organizer of Workshop "Rules of protein-DNA recognition: computational and experimental advances", funded by Banff International Research Station for Mathematical Innovation and Discovery, Banff, Canada, and held at Casa Matemática Oaxaca, Mexico
2015	Invited session chair, Keystone Symposia on DNA Methylation and Epigenomics, Keystone, CO, USA
2014	Invited session chair, Symposium "Modeling the effects of water and solvation in biological systems: Developments and applications" at 248 th National Meeting, American Chemical Society, San Francisco, CA, USA

2013	Program Committee Member, 21 st Annual International Conference on Intelligent Systems in Molecular Biology (ISMB)/12 th European Conference on Computational Biology (ECCB), Berlin, Germany
2013	Invited session chair, 18 th Conversation on Biomolecular Structure & Dynamics, Albany, NY, USA
2011	Co-organizer of Professor Barry Honig's Birthday Symposium, Columbia University, New York, NY, USA
2009	Co-organizer of symposium "Computer Simulation of Biological Macromolecules", Berlin, Germany
2005	Co-organizer of symposium "New Horizons in Computational Biology", Weizmann Institute of Science, Rehovot, Israel
2000	Chair of organization committee, "Berlin Humboldt School on Structural Biology", Berlin, Germany

Member of Review Panels, Reviewer of Grants and Manuscripts

2024	Member, Review panel, NIH Director's Transformative Research Award, National Institutes of Health, Bethesda, MD, USA
2023	Grant reviewer, European Research Council, ERC grant proposals, Brussels, Belgium
2022	Member, External review panel, Department of Mathematics, University Committee of Academic Review (UCAR), University of Southern California
2022	Grant reviewer, Minerva Weizmann Foundation and Max Planck Society, Munich, Germany
2015	Grant reviewer, Human Frontiers Science Program (HFSP), Strasbourg, France
2015	Grant reviewer, Canada First Research Excellence Fund, NSERC/SSHRC/CIHR granting agencies, Ottawa, Canada
2015	Grant reviewer, Division of Molecular and Cellular Bioscience, National Science Foundation, Arlington, VA, USA
2014	Ad hoc member, NIH study section "Genome, Computational Biology and Technology (GCAT)", National Institutes of Health, Bethesda, USA
2014	Ad hoc reviewer, NSF CAREER awards, National Science Foundation, Arlington, VA, USA
2014-2016	Grant reviewer, Biotechnology and Biological Sciences Research Council (BBRC), London, UK
2014	Grant reviewer, Medical Research Council (MRC), London, UK
2014	Grant reviewer, Los Alamos National Laboratory, Los Alamos, NM, USA
2013-2016	Member, Standing Committee of External Evaluators, Italian Institute of Technology (IIT), Genova, Italy
2012-2015	Member, HHMI Fellowship Review Panel, Howard Hughes Medical Institute, Chevy Chase, USA (reviewed >100 proposals in 4 years)
2012-2017	Grant reviewer, Israel Science Foundation (ISF), Jerusalem, Israel
2011	Reviewer, Banff International Research Station (BIRS), Banff, Canada
2010	Grant reviewer, Wellcome Trust, London, UK
2004-present	Manuscript reviewer for (among others) Nature (multiple), Cell (multiple), Nat. Struct. Mol. Biol. (multiple), Nat. Methods (multiple), Nat. Commun. (multiple), Proc. Natl. Acad. Sci. USA (multiple), Genome Res. (multiple), Dev. Cell, Cell Syst. (multiple), Cell Rep. (multiple), Gene, Epigenetics & Chromatin (multiple), PLOS Comput. Biol. (multiple), Nucleic Acids Res. (multiple), J. Mol. Biol. (multiple), Bioinformatics (multiple), Protein Sci., PLOS ONE (multiple), BMC Bioinformatics (multiple), FEBS Letters, J. Struct. Biol., Biophys. J. (multiple), Biochemistry (multiple), Biopolymers, Photochem. Photobiol., J. Chem. Theor. Comput., J. Biomol. Struct. Dyn. (multiple), Curr. Opin. Struct. Biol. (multiple), and others

UNIVERSITY SERVICE

2021-present	Founding Department Chair of the newly established Department of Quantitative and Computational Biology (18 core and 23 joint faculty members, 60 Ph.D., 20 M.Sc., more than 100 undergraduate major and 20 undergraduate minor students), University of Southern California
2018-2020	Section Head (Department Chair equivalent position), newly established Quantitative and Computational Biology section (14 core and 15 joint faculty members, 60 Ph.D., 10 M.Sc., and 60 undergraduate students), University of Southern California
2019-2020	Chair, Tenure-track Faculty Search Committee, Computational Structural, Synthetic, or Systems Biology, University of Southern California
2016-2020	Member, Executive Committee of Department of Biological Sciences, University of Southern California
2016-2019	Vice Chair of Department of Biological Sciences, University of Southern California
2016-2018	Head of Computational Biology and Bioinformatics group (prior to establishment of Quantitative and Computational Biology section; 10 faculty members), University of Southern California
2018-2022	Ad hoc member, Dornsife Committee for Appointments, Promotions, and Tenure (DCAPT) for multiple tenure evaluation meetings, Dornsife College for Letters, Arts and Sciences, University of Southern California
2017-2018	Member, RTPC Faculty Search Committee (hiring 3 new teaching faculty), Department of Biological Sciences, University of Southern California
2017-present	Program Director, Quantitative Biology (B.Sc.) and Quantitative and Computational Biology (M.Sc.), University of Southern California
2016-present	Chair, Executive Committee, then Curriculum Committee for Quantitative Biology Undergraduate Major and Quantitative and Computational Biology Master's Program, University of Southern California
2016-2019	Co-chair, Curriculum Committee, Department of Biological Sciences, University of Southern California
2016-2017	Member, Science and Engineering Subcommittee of University Committee on Curriculum, University of Southern California
2016-2017	Member, Faculty Search Committee, Multi-scale modeling and data-intensive computing for biology, University of Southern California
2016	Member, Data Science Advisory Board, Michelson Center for Convergent Biosciences, University of Southern California
2015	Member, Dean's advisory committee for department chair selection, Department of Biological Sciences, University of Southern California
2015	Member, Dean's self-study steering/"uber" committee, Department of Biological Sciences, University of Southern California
2015	Member, Self-study subcommittee "undergraduate programs", Department of Biological Sciences, University of Southern California
2015-2018	Member, Advisory Board, Women in Science and Engineering (WiSE) Program, University of Southern California
2015-2018	Member, Executive Committee for NIH training grant at Chemistry/Biology Interface, University of Southern California
2015-2016	Chair, High-performance Computing Committee, Computational Biology and Bioinformatics section, University of Southern California
2015-2018	Member, Building Committee, Ray R. Irani Hall, Molecular and Computational Biology section University of Southern California
2014-2018	Chair, Space Committee, Computational Biology and Bioinformatics section, University of Southern California
2014-2018	Member, Retreat Committee, Molecular and Computational Biology section, University of Southern California

2011-2016	Member, Screening Committee, Ph.D. Program in Computational Biology and Bioinformatics, University of Southern California
2011-2013	Organizer, Seminar Series in Computational Biology and Bioinformatics, University of Southern California
2010-2016	Member, Admissions Committee, Ph.D. Program in Computational Biology and Bioinformatics, University of Southern California

TEACHING AND MENTORING

Course and Curriculum Development

2021-2022	Redesigned undergraduate, Master's, and Ph.D. programs of the Department of Quantitative and Computational Biology; established new courses; introduced and received university approval for new curriculum
2018-2019	Developed new Master's program (M.Sc. and Progressive Master's) in Quantitative and Computational Biology
2018-2019	Developed new Honors program for B.Sc. in Quantitative Biology (QBIO), including Honors Seminar and Thesis courses, QBIO 493 and QBIO 494
2016-2017	Developed new Major (B.Sc.) in Quantitative Biology (QBIO), including a new course QBIO 105 "Introduction in Quantitative Biology"
2016	Developed new content for and restructured undergraduate course BISC 321 "Science, Technology, and Society"
2014	Co-developed course proposal for new general education course (with F. Sun and M. Waterman)
2012-2016	Co-developed new undergraduate level course BISC/QBIO 481 "Structural Bioinformatics from Atoms to Cells" (with F. Alber)
2011-2014	Initiated and taught "Bioinformatics Institute" at La Cañada High School, La Cañada Flintridge, CA

Placements of Trainees, Honors and Awards Received by Graduate Students in Rohs Lab

Tianyin Zhou (*graduated in 09/2014, was hired by Google as Software Engineer, promoted to Senior Software Engineer, Staff Software Engineer, and Senior Staff Software Engineer*):

2014	Ph.D. Achievement Award in recognition of outstanding academic research, Graduate School, University of Southern California (Rohs as advisor received a Graduate School Mentoring Award)
2014	Harrison M. Kurtz Award given to the most outstanding Ph.D. student in the Biological Sciences, University of Southern California

Iris Dror (*joint with Technion, Israel; graduated in 09/2015; joined UCLA as Postdoctoral Associate in 11/2015*):

2014	Women in Science Fellowship, Israeli Ministry of Science
2013	Paper of the Month Award (with Dror as first and Rohs as last author), Department of Biology, Technion – Israel Institute of Technology
2012	Irwin and Joan Jacobs Fellowship, Graduate School, Technion – Israel Institute of Technology

Lin Yang (*graduated in 06/2016 and was hired by Google as Software Engineer*):

2016	Ph.D. Achievement Award in recognition of outstanding academic research, Graduate School, University of Southern California (Rohs as advisor received a Graduate School Mentoring Award)
2015	Dan David Prize Scholarship in the "Future" category Bioinformatics, Dan David Foundation and Tel Aviv University, Tel Aviv, Israel
2015	Harrison M. Kurtz Award given to the most outstanding Ph.D. student in the Biological Sciences, University of Southern California

Ana Carolina Dantas Machado (graduated in 08/2016; joined the University of California San Diego in 01/2019 as Postdoctoral Associate and was promoted to Assistant Project Scientist):

- 2016 Harrison M. Kurtz Award given to the most outstanding Ph.D. student in the Biological Sciences, University of Southern California
- 2015 William E. Trusten Award given to the most outstanding Ph.D. student in the Biological Sciences, University of Southern California
- 2014 WiSE Merit Fellowship given to Ph.D. students who demonstrate exceptional work in their field, Women in Science and Engineering Program, University of Southern California

Tsu-Pei Chiu (graduated in 06/2018; was Postdoctoral Associate and Lecturer at USC and promoted in 2024 to Assistant Professor (Teaching) of Quantitative and Computational Biology):

- 2018-2020 USC-Taiwan Postdoctoral Fellowship
- 2017-2018 Manning Endowed Fellowship of the USC Graduate School
- 2016-2017 Research Enhancement Fellowship of the USC Graduate School
- 2016 William E. Trusten Award given to the most outstanding Ph.D. student in the Biological Sciences, University of Southern California

Beibei Xin (graduated in 06/2018; joined China Agricultural University in Beijing as Faculty Member in 10/2019 where she is currently an Associate Professor):

- 2018 William E. Trusten Award given to the most outstanding Ph.D. student in the Biological Sciences, University of Southern California
- 2018 WiSE Merit Fellowship given to Ph.D. students who demonstrate exceptional work in their field, Women in Science and Engineering Program, University of Southern California
- 2017-2018 Research Enhancement Fellowship of the USC Graduate School

Satyanarayan Rao (graduated in 06/2018; joined the University of Colorado at Denver as Postdoctoral Associate in 11/2018; now tenure-track Assistant Professor at the Indian Institute of Technology Roorkee as of 08/2023)

Richard Li (graduated in 05/2019; joined Wuxi NextCode Genomics in Boston as Senior Computational Associate)

Jared Sagendorf (graduated in 06/2020; joined the University of California San Francisco as Academic Coordinator in 04/2023 after a period as Postdoctoral Associate and Lecturer at USC):

Jinsen Li (graduated in 9/2021; currently Postdoctoral Associate and Instructor at USC)
2019-2020 Research Enhancement Fellowship of the USC Graduate School

Brendon Cooper (graduated in 7/2022; joined Beckman Coulter as Development Scientist in 04/2023 after a short period as Postdoctoral Associate at USC)

2021-2022 Inaugural Michael S. Waterman Awardee in Computational Biology

Raktim Mitra (graduated in 10/2024; joined 2024 Nobel Laureate Dr. David Baker's laboratory at the University of Washington, Seattle, as Postdoctoral Associate)

- 2023-2024 Michael S. Waterman Awardee in Computational Biology and Bioinformatics, University of Southern California
- 2024-2025 Phi Kappa Phi Student Achievement Award, University of Southern California

Yibei Jiang

2023-2024 Inaugural Awardee for Excellence in Teaching in Computational Biology

TALKS AND SEMINARS**Invited talks at international conferences (08/2010-present; since joining USC)**

1. **Visualizing Biological Data (VIZBI) Conference 2024**, Los Angeles, CA, USA, March 13-15, 2024. Molecular visualization methods quantify and reveal mechanisms of interaction.
2. **APS Meeting Symposium** “Harnessing the Power of Machine Learning in Studying Biomolecular Dynamics”, **American Physical Society Meeting**, Minneapolis, MN, March 3-8, 2024. Deep learning methods reveal mechanisms of protein-nucleic acid binding.
3. **Multiscale Genome Organization Symposium** at the **Biophysical Society Annual Meeting**, Philadelphia, PA, USA, February 10-14, 2024. Biophysical mechanisms of protein-DNA binding revealed through deep learning approaches.
4. **Keynote Speaker, RECOMB-ISCB Conference on Regulatory Genomics & Systems Genomics 2023**, Los Angeles, CA, USA, November 28-30, 2023. Deep learning approaches for studies of protein-nucleic acid binding.
5. **Conference on Rules of Protein-DNA Recognition 2023**, Cancun, Mexico, October 9-13, 2023. Deep learning approaches for studies of protein-nucleic acid binding.
6. **Conference on Modeling Protein Interactions 2023**, Lawrence, KS, USA, May 25-27, 2023. Deep learning approaches for studies of protein-nucleic acid binding.
7. Joint CECAM-CSF Conference **on Multiscale simulations of DNA from electrons to nucleosomes: 22 years of the Ascona B-DNA Consortium**, Ascona, Switzerland, April 16-21, 2023. Deep learning to predict DNA structure and probe protein-DNA binding.
8. **Workshop on Protein-DNA Interactions: from Biophysics to Cell Biology**, Weizmann Institute of Science, Rehovot, Israel, October 18-20, 2022. Deep learning methods reveal mechanisms of protein-DNA binding.
9. Symposium in the Honor of Dr. Tom Tullius' 70th Birthday, **Bioinformatics Program, Boston University**, Boston, MA, USA, September 30, 2022. Deep learning methods reveal mechanisms of protein-DNA binding.
10. **11th Annual Southern California Systems Biology Symposium**, UCLA, Los Angeles, CA, USA, April 2, 2022. Deep learning methods reveal of protein-DNA binding.
11. Symposium in the Honor of Dr. Barry Honig's 80th Birthday, **American Chemical Society Spring 2022 Meeting**, San Diego, CA, USA, March 20-24, 2022. Deep learning methods reveal of protein-DNA binding.
12. **1st International Conference on Mathematical Multiscale Modeling in Biology**, Guanacaste, Costa Rica, October 21-25, 2019. Multiscale modeling of protein-DNA binding specificity.
13. **2nd Molecular Biosystems Conference on Eukaryotic Gene Regulation & Functional Genomics**, Puerto Varas, Chile, September 30 – October 4, 2019. Proteins can't read: DNA is much more than its sequence.
14. **Howard Hughes Medical Institute Think Tank** discussing new future research directions for their **Janelia Farm Research Campus**, Ashburn, VA, September 23-25, 2019. Tackling challenges in biology from a computational biologist's perspective.
15. Mann-tastic 30 years of Excellence and Beyond, **Mortimer B. Zuckerman Mind Brain Behavior Institute, Columbia University**, New York, NY, USA, June 14, 2019. Mann-tastic journey introducing DNA shape to genomics.
16. **Keynote Evening Talk, Retreat of the Graduate School of Quantitative Biosciences Munich**, Ludwig Maximilians University, Technical University Munich, Max Planck Institute of Biochemistry, and Helmholtz Center Munich, Tutzing, Germany, June 12-14, 2019. Integrating genomics and structural biology reveals mechanisms of gene regulation.
17. **Colloque 60 ans du Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique**, Paris, France, April 9-11, 2019. How DNA shape advanced our understanding of gene regulation.
18. **4th International Conference on Mathematical and Computational Medicine**, Cancun, Mexico, December 3-7, 2018. How DNA shape advanced our understanding of gene regulation.

19. **Keynote and Opening Talk. Regulatory and Systems Genomics COSI Track, 26th International Conference on Intelligent Systems for Molecular Biology (ISMB)**, Chicago, IL, USA, July 6-10, 2018. A tale of DNA shape analysis: a user manual and next steps.
20. **3rd Workshop on Rules of Protein-DNA Recognition: Computational & Experimental Advances, Casa Matemática Oaxaca and Banff International Research Station for Mathematical Innovation and Discovery**, Oaxaca, Mexico, June 4-8, 2018. A tale of DNA shape analysis: a user manual and next steps.
21. **4th International Conference on Protein and RNA Structure Prediction**, Montego Bay, Jamaica, December 4-8, 2017. Mechanisms of transcription factor-DNA binding are protein family specific.
22. **1st Molecular Biosystems Conference on Eukaryotic Gene Regulation & Functional Genomics**, Puerto Varas, Chile, September 23-26, 2017. Integrating genomics and structural biology reveals mechanisms of gene regulation.
23. **Symposium on Molecular Recognition: Revealing the Effects Associated with Receptor-Ligand Binding, 254th National Meeting, American Chemical Society**, Washington, DC, USA, August 20-24, 2017. Structural analysis and quantitative modeling of protein-DNA interactions.
24. **Symposium on Modeling Water & Solvation in Biochemistry: Developments & Applications, 252nd National Meeting, American Chemical Society**, Philadelphia, PA, USA, August 21-25, 2016. Integration of electrostatics and solvation into statistical machine learning approaches for the quantitative modeling of protein-DNA binding.
25. **Workshop on Measuring and Modeling Quantitative Sequence-Function Relationships**, Banbury Center, **Cold Spring Harbor Laboratory**, NY, USA, July 5-8, 2016. Quantitative modeling of TF-DNA binding: Beyond DNA shape towards biophysical features.
26. **Workshop on Healthy Aging, Japan Science and Technology Agency and Leibniz Association**, Tokyo, Japan, June 20-22, 2016. Transcriptional regulation in the aging genome.
27. **Workshop on Regulatory Genomics and Epigenomics, Simons Institute for the Theory of Computing, University of California at Berkeley**, Berkeley, CA, USA, March 7-10, 2016. Quantitative modeling of transcription factor binding specificities using DNA shape.
28. **2nd Workshop on Rules of Protein-DNA Recognition: Computational & Experimental Advances, Casa Matemática Oaxaca and Banff International Research Station for Mathematical Innovation and Discovery**, Oaxaca, Mexico, June 21-25, 2015. Quantitative modeling of transcription factor binding specificities using DNA shape.
29. **19th Conversation on Biomolecular Structure & Dynamics**, Albany, NY, USA, June 9-13, 2015. Quantitative modeling of transcription factor binding specificities using DNA shape.
30. **Symposium on Modeling the Effects of Water and Solvation in Biological Systems: Developments and Applications, 248th National Meeting, American Chemical Society**, San Francisco, CA, USA, August 10-14, 2014. High-throughput prediction of minor groove electrostatic potential in studies of protein-DNA recognition.
31. **Zing Conference on Protein Folding**, organized by Zing Conferences, Cambridge, UK; held in Punta Cana, Dominican Republic, July 16-19, 2014. Protein family-specific DNA readout mechanisms derived from genomic data using machine learning.
32. **1st Workshop on Rules of Protein-DNA Recognition: Computational & Experimental Advances, Banff International Research Station for Mathematical Innovation and Discovery**, Banff, Alberta, Canada, June 16-21, 2013. Genome analysis based on the integration of DNA sequence and shape.
33. **DNA @ 60, The 60th Anniversary of the Discovery of the DNA Double Helix**, Technion – Israel Institute of Technology, Haifa, Israel, May 26-29, 2013. The structure of the double helix in the genomic era.
34. **International Conference on Biomolecular Forms and Functions, A Celebration of 50 Years of the Ramachandran Map**, Indian Institute of Science, Bangalore, India, January 8-11, 2013. DNA shape in the genomic era.
35. **243rd National Meeting, American Chemical Society, Symposium in honor of Professor Andrew McCammon**, San Diego, CA, USA, March 25-28, 2012. Nuance in the double helix: The role of shape in sequence-specific protein-DNA recognition.

36. **Keystone Symposium, Nucleic Acid Therapeutics: From Base Pairs to Bedsides**, Santa Fe, NM, USA, January 10-15, 2012. High-throughput prediction of DNA shape on a genome-wide scale.
37. **Symposium in honor of Professor Barry Honig, Columbia University**, New York, NY, USA, December 15-16, 2011. Genome-wide analysis of DNA shape.
38. **17th Conversation on Biomolecular Structure & Dynamics**, Albany, NY, USA, June 14-18, 2011. High-throughput prediction of DNA shape on a genomic scale.
39. **Conference on Modeling Electrostatics in Molecular Biology**, Clemson, SC, USA, April 4-6, 2011. DelPhi in the genomic era: Mapping electrostatic potential as a function of DNA sequence.
40. **6th Congress of the Federation of the Israel Societies for Experimental Biology**, Eilat, Israel, February 7-11, 2011. Origins of specificity in protein-DNA recognition.
41. **1st Annual Southern California Systems Biology Conference**, Irvine, CA, USA, January 29-30, 2011. Origins of protein-DNA specificity revealed through an integrative approach of structural and systems biology.
42. **4th India-Japan Symposium on Cell Engineering and Bioinformatics, Indian Institute of Technology**, New Delhi, India, December 13-14, 2010. The role of DNA shape in protein-DNA recognition.
43. **2nd India-Japan Symposium on Bioinformatics, Indian Institute of Technology**, New Delhi, India, December 10-11, 2010. The role of DNA shape in protein-DNA recognition.

Contributed talks at international conferences (08/2010-present; since joining USC)

44. **Highlight Talk RECOMB 2016 Conference**, Santa Monica, CA, USA, April 17-21, 2016. Quantitative modeling of transcription factor binding specificities using DNA shape.
45. **Cold Spring Harbor Meeting on Systems Biology: Global Regulation of Gene Expression**, Cold Spring Harbor Laboratory, NY, USA, March 15-19, 2016. Deciphering layers of transcription factor-DNA binding on a protein family-specific basis.
46. **Epigenomics 2016 Meeting**, Rio Mar, Puerto Rico, USA, January 31-February 5, 2016. Deciphering layers of transcription factor-DNA binding on a protein family-specific basis.
47. **Keystone Symposia on DNA Methylation and Epigenomics**, Keystone, CO, USA, March 29-April 2, 2015. Modeling of the effect of DNA methylation on DNA shape and protein-DNA binding.
48. **Cold Spring Harbor Meeting on Systems Biology: Global Regulation of Gene Regulation**, held in Rio Mar, Puerto Rico, USA, January 28-February 1, 2015. Quantitative modeling of transcription factor binding specificities using DNA shape.
49. **4th Zing Nucleic Acids Conference**, organized by Zing Conferences, Cambridge, UK; held in Cancun, Mexico, December 5-9, 2014. Structural insights into protein-DNA recognition derived from sequencing data using machine learning.
50. **7th Annual RECOMB/ISCB Conference on Regulatory and Systems Genomics**, San Diego, CA, USA, November 9-14, 2014. Quantitative modeling of transcription factor binding specificities using DNA shape.
51. **Regulatory Genomics Special Interest Group, 22nd Annual International Conference on Intelligent Systems for Molecular Biology (ISMB)**, Boston, MA, USA, July 12, 2014. Quantitative modeling of transcription factor binding specificities using DNA shape.
52. **5th Annual RECOMB Conference on Regulatory and Systems Genomics**, San Francisco, CA, USA, November 12-15, 2012. Genome analysis based on the integration of DNA sequence and shape.
53. **Regulatory Genomics Special Interest Group, 20th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB)**, Long Beach, CA, USA, July 14, 2012. Genome analysis based on the integration of DNA sequence and shape.
54. **3Dsig, Structural Bioinformatics and Computational Biophysics Satellite Meeting, ISMB**, Long Beach, CA, USA, July 13-14, 2012. Genome-wide analysis of DNA shape.

Invited departmental seminars (08/2010-present; since joining USC)

55. **Max Planck Institute for Molecular Genetics**, Berlin, Germany, October 27, 2022. Deep learning methods reveal mechanisms of protein-DNA binding.
56. **Distinguished Speaker Series, Edmond J. Safra Center for Bioinformatics, Tel Aviv University**, Tel Aviv, Israel, October 24, 2022. Computational biology reveals mechanisms of protein-DNA binding.
57. Joint Seminar, **Institute of Mathematics and School of Life Sciences, Swiss Federal Institute of Technology (EPFL)**, Lausanne, Switzerland, April 26, 2022. Statistical machine learning methods reveal of protein-DNA binding.
58. **Department of Chemical and Structural Biology, Weizmann Institute of Science**, Rehovot, Israel, June 14, 2022. Deep learning methods reveal mechanisms of protein-DNA binding.
59. **Fulgent Genetics**, Temple City, CA, May 26, 2021. The interface of next-generation sequencing and machine learning.
60. **European Molecular Biology Laboratory (EMBL)**, Heidelberg, Germany, February 5-6, 2020. Quantitative modeling of protein-DNA binding specificity.
61. **Computational Biology Department, Carnegie Mellon University**, Pittsburgh, PA, USA, January 21-22, 2020. Quantitative modeling of protein-DNA binding specificity.
62. **Berlin Institute of Medical Systems Biology, Max Delbrück Center for Molecular Medicine**, Berlin, Germany, June 11, 2019. Integrating genomics and structural biology reveals mechanisms of gene regulation.
63. Faculty of Biological Sciences, **Pontificia Universidad Católica de Chile**, Santiago, Chile, September 28, 2017. Integrating genomics and structural biology reveals mechanisms of gene regulation.
64. Department of Bioinformatics and Genomics, **University of North Carolina, Charlotte**, NC, USA, April 28, 2017. Integrating genomics and structural biology reveals mechanisms of gene regulation.
65. Department of Chemistry, **University of Utah, Salt Lake City**, UT, USA, April 13, 2017. Integrating genomics and structural biology reveals mechanisms of gene regulation.
66. Chemical and Structural Biology Division, College of Biological Sciences, **University of Minnesota Twin Cities, Minneapolis**, MN, USA, March 22, 2017. Integrating genomics and structural biology reveals mechanisms of gene regulation.
67. Program in Quantitative and Computational Biology, **Lewis Sigler Institute for Integrative Genomics, Princeton University**, Princeton, NJ, USA, March 9, 2017. Integrating genomics and structural biology reveals mechanisms of gene regulation.
68. **Keynote Seminar**, Biozentrum, Faculty of Biology, **Ludwig Maximilians University, Munich**, Germany, December 16, 2016. Revealing mechanisms of gene regulation by integrating genomics and structural biology.
69. Institute Colloquium, **Leibniz Institute on Aging - Fritz Lipmann Institute**, Jena, Germany, July 21, 2016. Deconvolving the mechanisms of transcriptional regulation.
70. Institute of Systems Genetics, **New York University School of Medicine**, New York, NY, USA, June 9, 2016. Revealing mechanisms of gene regulation by integrating genomics and structural biology.
71. Scientific **Symposium “Computational Biology of Aging”, Leibniz Institute on Aging - Fritz Lipmann Institute**, Jena, Germany, March 23, 2016. Deconvolving the mechanisms of transcriptional regulation.
72. Bioinformatics and Computational Biology Research Center, **Cedars-Sinai Medical Center**, Los Angeles, CA, USA, January 19, 2016. Quantitative modeling of transcription factor binding specificities using DNA shape.
73. Special Guest Lecture, Azrieli Institute for Systems Biology, **Weizmann Institute of Science**, Rehovot, Israel, May 20, 2015. Quantitative modeling of transcription factor binding specificities using DNA shape.
74. Lecture in Bioinformatics, **Tel Aviv University**, Ramat Aviv, Israel, May 19, 2015. Quantitative modeling of transcription factor binding specificities using DNA shape.
75. Systems Biology Seminar, Program in Bioinformatics, **Boston University**, Boston, MA, USA, April 9, 2015. Quantitative modeling of TF binding specificities using DNA shape.

76. Bioinformatics and Computational Biology Program, **Iowa State University**, Ames, IA, USA, March 25, 2015. Quantitative modeling of transcription factor binding specificities using DNA shape.
77. Dept. of Biochemistry, **New York University School of Medicine**, New York, NY, USA, March 5, 2015. Quantitative modeling of transcription factor binding specificities using DNA shape.
78. Joint Program in Computational Biology, Dept. of Computational and Systems Biology, University of Pittsburgh and Carnegie Mellon University, Pittsburgh, PA, USA, February, 27, 2015. Quantitative modeling of transcription factor binding specificities using DNA shape.
79. Dept. of Computational Molecular Biology **Max Planck Institute for Molecular Genetics**, Berlin, Germany, February 9, 2015. The role of DNA shape in transcription factor-DNA recognition and nucleosome formation.
80. Duke Center for Genomic and Computational Biology, **Duke University**, Durham, NC, USA, November 17, 2014. Quantitative modeling of transcription factor binding specificities using DNA shape.
81. Dept. of Systems Biology, **Columbia University Medical Center**, New York, NY, USA, June 9, 2014. Quantitative modeling of TF binding specificities using DNA shape.
82. Dept. of Systems Biology, **Harvard Medical School**, Boston, USA, May 22, 2014. Quantitative modeling of transcription factor binding specificities using DNA shape.
83. Center for Computational Molecular Biology, **Brown University**, Providence, RI, USA, May 20, 2014. Quantitative modeling of TF binding specificities using DNA shape.
84. Dept. of Biochemistry, **University of Wisconsin – Madison**, WI, USA, May 5, 2014. Quantitative modeling of transcription factor binding specificities using DNA shape.
85. **Fred Hutchinson Cancer Research Institute**, Seattle, WA, USA, April 24, 2014. Quantitative modeling of transcription factor binding specificities using DNA shape.
86. Dept. of Genome Sciences, **University of Washington**, Seattle, WA, USA, April 23, 2014. Quantitative modeling of transcription factor binding specificities using DNA shape.
87. Center for Nonlinear Studies, **Los Alamos National Laboratory**, Los Alamos, NM, USA, April 7, 2014. Quantitative modeling of TF binding specificities using DNA shape.
88. Dept. of Genetics, **Washington University**, St. Louis, MO, USA, March 20, 2014. Quantitative modeling of transcription factor binding specificities using DNA shape.
89. Bioinformatics Program, **University of California, Los Angeles (UCLA)**, CA, USA, January 23, 2012. High-throughput prediction of DNA shape on a genome-wide scale.
90. Cell, Molecular, and Developmental Biology Program, **University of California, Riverside**, CA, USA, November 16, 2011. DNA shape is a source of protein-DNA specificity.
91. Center for Theoretical Biological Physics, **University of California, San Diego (UCSD)**, CA, USA, October 7, 2011. DNA shape is a source of protein-DNA specificity.
92. Department of Biochemistry and Molecular Biology, **Tel Aviv University**, Tel Aviv, Israel, February 20, 2011. The role of DNA shape in protein-DNA recognition.
93. Faculty of Biology, **Technion – Israel Institute of Technology**, Haifa, Israel, February 16, 2011. The role of DNA shape in protein-DNA recognition.
94. Dept. of Structural Biology, **Weizmann Institute of Science**, Rehovot, Israel, February 15, 2011. The role of DNA shape in protein-DNA recognition.
95. Dept. of Microbiology and Molecular Genetics, **Hebrew University of Jerusalem**, Jerusalem, Israel, February 14, 2011. The role of DNA shape in protein-DNA recognition.
96. **Sanford-Burnham Medical Research Institute**, San Diego, CA, USA, January 10, 2011. Shape readout mediates specificity in protein-nucleic acid interactions.
97. Dept. of Computational Molecular Biology **Max Planck Institute for Molecular Genetics**, Berlin, Germany, December 7, 2010. The role of DNA shape in transcription factor-DNA recognition and nucleosome formation.
98. **Accelrys, Inc.**, San Diego, CA, USA, November 14, 2010. The role of DNA shape in protein-DNA recognition.

Invited USC seminars (08/2010-present; since joining USC)

99. **Department of Biomedical Engineering**, Viterbi School of Engineering, University of Southern California, Los Angeles, CA, November 1, 2024. Engineering+: AI-driven discovery in biology.
100. **Division of Oncology, Department of Medicine**, Keck School of Medicine, University of Southern California, Los Angeles, CA, October 22, 2024. Answering biological and biomedical questions by integrating structural biology and genomics.
101. **Workshop on Predictive Intelligence for Pandemic Prevention**, Viterbi School of Engineering, University of Southern California, Los Angeles, CA, April 6-7, 2023. AI methods for the study of structural molecular mechanisms.
102. **Genetic and Epigenetic Regulation Program Retreat, Norris Comprehensive Cancer Center**, Keck School of Medicine, University of Southern California, Los Angeles, CA, May 23, 2019. Quantitative modeling of transcriptional regulation.
103. **Workshop “Mathematical Oncology: Modeling Clinical Data for Maximum Patient Benefit”**, University of Southern California, Los Angeles, CA, May 24, 2017. Computational opportunities in biological datasets.
104. **Keck School of Medicine**, University of Southern California, Los Angeles, CA, November 21, 2016. Integrating genomics and structural biology reveals mechanisms of gene regulation.
105. **Bridge@USC Science Faculty Luncheon**, University of Southern California, Los Angeles, CA, November 16, 2016. Transcriptional regulation in the aging genome.
106. **Bridge@USC and Michelson Center for Convergent Biosciences Retreat**, Catalina Island, CA, February 5-7, 2016. Building a bridge between structural biology and Genomics.
107. **The Bridge Institute**, University of Southern California, Los Angeles, CA, February 25, 2015. Building a bridge between structural biology and genomics.
108. **Department of Biological Sciences Intersection Seminar**, University of Southern California, Los Angeles, CA, September 18, 2014. Genome-wide studies of DNA structure, function and evolution.
109. **Symposium “30 Years of Computational Biology at USC”**, University of Southern California, Los Angeles, CA, March 29 - April 1, 2012. Genome-wide analysis of DNA shape.
110. **Department of Physics and Astronomy**, University of Southern California, Los Angeles, CA, February 24, 2012. Physical principles are the basis for molecular mechanisms in biology.
111. **Department of Chemistry**, University of Southern California, Los Angeles, CA, October 6, 2011. DNA shape is a source for protein-DNA specificity.
112. **Bioinformatics Workshop, USC Keck School of Medicine**, University of Southern California, Los Angeles, CA, August 31, 2011. Adding dimensions to linear sequence information.

PUBLICATIONS**Peer-reviewed journal articles (08/2010-present, since joining USC)**

1. **R. Mitra[#], A.S. Cohen[#], J.M. Sagendorf**, H.M. Berman, and **R. Rohs^{*}**. DNAProDB: an updated database for the automated and interactive analysis of protein-DNA complexes. **Nucleic Acids Res.** 53, D396-D402 (2025).
2. **R. Mitra, J. Li, J.M. Sagendorf, Y. Jiang, A.S. Cohen, T.P. Chiu, C.J. Glasscock, and R. Rohs^{*}**. Geometric deep learning for interpretable prediction of protein-DNA binding specificity. **Nat. Methods** 21, 1674-1683 (2024).
3. **J. A. Weller and R. Rohs^{*}**. Structure-based drug design with a deep hierarchical generative model. **J. Chem. Inf. Model.** 64, 6450-6463 (2024).
4. **J.M. Sagendorf, R. Mitra, J. Huang, X.S. Chen, and R. Rohs^{*}**. Structure-based prediction of protein-nucleic acid binding using graph neural networks. **Biophys. Rev.** 16, 297-314 (2024).
5. V.A. Bonnell, Y. Zhang, A.S. Brown, J. Horton, G.A. Josling, **T.P. Chiu, R. Rohs, S. Mahony, R. Gordân, M. Llinás^{*}**. DNA sequence and chromatin differentiate sequence-specific

- transcription factor binding in the human malaria parasite *Plasmodium falciparum*. **Nucleic Acids Res.** 52, 10161-10179 (2024).
6. J. Li and R. Rohs*. Deep DNASHape webserver: prediction and real-time visualization of DNA shape considering extended *k*-mers. **Nucleic Acids Res.** 52, W7-W12 (2024).
 7. R. Mitra[#], A.S. Cohen[#], and R. Rohs*. RNAScape: geometric mapping and customizable visualization of RNA structure. **Nucleic Acids Res.** 52, W354-W361 (2024).
 8. J. Li, T.P. Chiu, and R. Rohs*. Predicting DNA structure using a deep learning method. **Nat. Commun.** 15, 1243 (2024).
 9. Y. Jiang, T.P. Chiu, R. Mitra, and R. Rohs*. Probing the role of the protonation state of a minor groove-linker histidine in Exd-Hox–DNA binding. **Biophys. J.** 123, 248-259 (2024).
 10. Y. Li, B.H. Cooper, Y. Liu, D. Wu, X. Zhang, R. Rohs, and P.Z. Qin*. CRISPR-Cas9 activities with truncated 16-nucleotide RNA guides are tuned by target duplex stability beyond RNA/DNA hybrid. **Biochemistry** 62, 2541-2548 (2023).
 11. B.H. Cooper, A.C. Dantas Machado, Y. Gan, O.M. Aparicio, and R. Rohs*. DNA binding specificity of all four *Saccharomyces cerevisiae* forkhead transcription factors. **Nucleic Acids Res.** 51, 5621-5633 (2023).
 12. T.P. Chiu, S. Rao, and R. Rohs*. Physicochemical models of protein–DNA binding with standard and modified base pairs. **Proc. Natl. Acad. Sci. USA.** 120, e2205796120 (2023).
 13. B.H. Cooper, T.P. Chiu, and R. Rohs*. Top-Down-Crawl: a method for the ultra-rapid and motif-free alignment of sequences with associated binding metrics. **Bioinformatics** 38, 5121-5123 (2022).
 14. T.P. Chiu, J. Li, Y. Jiang, and R. Rohs*. It is in the flanks: conformational flexibility of transcription factor binding sites. **Biophys. J.** 121, 3765-3767 (2022).
 15. E. Oberbeckmann, N. Krietenstein, V. Niebauer, Y. Wang, K. Schall, M. Moldt, T. Straub, R. Rohs, K.-P. Hopfner*, P. Korber*, S. Eustermann*. Genome information processing by the INO80 chromatin remodeler positions nucleosomes. **Nat. Commun.** 12, 3231 (2021).
 16. C.S.K. Lee, M. F. Cheung, J. Li, Y. Zhao, W.H. Lam, V. Ho, R. Rohs, Y. Zhai*, D. Leung*, and B.-K. Tye*. Humanizing the yeast origin recognition complex. **Nat. Commun.** 12, 33 (2021).
 17. Y. Le Poul, Y. Xin, L. Ling, B. Mühling, R. Jaenichen, D. Hörl, D. Bunk, H. Harz, H. Leonhardt, Y. Wang, E. Osipova, M. Museridze, D. Dharmadhikari, E. Murphy, R. Rohs, S. Preibisch, B. Prud'homme*, and N. Gompel*. Regulatory encoding of quantitative variation in spatial activity of a *Drosophila* enhancer. **Sci. Adv.** 6, eabe2955 (2020).
 18. S. Lara-Gonzalez, A.C. Dantas Machado, S. Rao, A.A. Napoli, J. Birktoft, R. Di Felice, R. Rohs*, and C.L. Lawson*. The RNA polymerase α subunit recognizes the DNA shape of the upstream promoter element. **Biochemistry** 59, 4523-4532 (2020).
 19. A.C. Dantas Machado, B.H. Cooper, X. Lei, R. Di Felice, L. Chen, and R. Rohs*. Landscape of DNA binding signatures of myocyte enhancer factor-2B reveals a unique interplay of base and shape readout. **Nucleic Acids Res.** 48, 8529-8544 (2020).
 20. X. Lei*, J. Zhao, J.M. Sagendorf, N. Rajashekar, J. Xu, A.C. Dantas Machado, C. Sen, R. Rohs, P. Feng, and L. Chen*. Crystal structures of ternary complexes of MEF2 and NKX2-5 bound to DNA reveal a disease related protein-protein interaction interface. **J. Mol. Biol.** 432, 5499-5508 (2020).
 21. X. Wu, B. Cao, P. Aquino, T.P. Chiu, C. Chen, S. Jiang, Z. Deng, S. Chen, R. Rohs, L. Wang*, J.E. Galagan*, and P.C. Dedon*. Epigenetic competition reveals density-dependent regulation and target site plasticity of phosphorothioate epigenetics in bacteria. **Proc. Natl. Acad. Sci. USA** 117, 14322-14330 (2020).
 22. J.F. Kribelbauer, X.J. Lu, R. Rohs, R.S. Mann, and H.J. Bussemaker*. Toward a mechanistic understanding of DNA methylation readout by transcription factors. **J. Mol. Biol.** 432, 1801-1815 (2020).
 23. T.P. Chiu, B. Xin, N. Markarian, Y. Wang, and R. Rohs*. TFBSshape: an expanded motif database for DNA shape features of transcription factor binding sites. **Nucleic Acids Res.** 48 (D1), D246-D255 (2020).
 24. J.M. Sagendorf, N. Markarian, H.M. Berman, and R. Rohs*. DNAproDB: an expanded database and web-based tool for structural analysis of DNA-protein complexes. **Nucleic Acids Res.** 48 (D1), D277-D287 (2020).

25. C. Chu[#], Z. Li^{#,*}, **B. Xin[#]**, F. Peng, C. Liu, **R. Rohs**, Q. Luo, and J. Zhou^{*}. Deep graph embedding for ranking optimization in E-commerce. **Proc. ACM Int. Conf. Inf. Knowl. Manag.** 2007-2015 (2018).
26. **X. Wang[#]**, **T. Zhou^{#,*}**, Z. Wunderlich, M.T. Maurano, A.H. DePace, S.V. Nuzhdin, and **R. Rohs^{*}**. Analysis of genetic variation indicates DNA shape involvement in purifying selection. **Mol. Biol. Evol.** 35, 1958-1967 (2018).
27. **B. Xin** and **R. Rohs^{*}**. Relationship between histone modifications and transcription factor binding is protein family specific. **Genome Res.** 28, 321-333 (2018).
28. **S. Rao**, **T.P. Chiu**, J.F. Kribelbauer, R.S. Mann, H.J. Bussemaker^{*}, and **R. Rohs^{*}**. Systematic prediction of DNA shape changes due to CpG methylation explains epigenetic effects on protein-DNA binding. **Epigenetics Chromatin** 11, 6 (2018).
29. **R.Y. Li**, **R. Di Felice**, **R. Rohs^{*}**, and D.A. Lidar^{*}. Quantum annealing versus classical machine learning applied to a simplified computational biology problem. **npj Quantum Information** 4, 11 (2018).
30. R.N. Azad, D. Zafiropoulos, D. Ober, Y. Jiang, **T.P. Chiu**, **J.M. Sagendorf**, **R. Rohs^{*}**, and T.D. Tullius^{*}. Experimental maps of DNA structure at nucleotide resolution distinguish intrinsic from protein-induced DNA deformations. **Nucleic Acids Res.** 46, 2636-2647 (2018).
31. **J. Li**, **J.M. Sagendorf**, **T.P. Chiu**, M. Pasi, A. Pérez, and **R. Rohs^{*}**. Expanding the repertoire of DNA shape features for genome-scale studies of transcription factor binding. **Nucleic Acids Res.** 45, 12877-12887 (2017).
32. **T.P. Chiu**, **S. Rao**, R.S. Mann, B. Honig, and **R. Rohs^{*}**. Genome-wide prediction of minor-groove electrostatic potential enables biophysical modeling of protein-DNA binding. **Nucleic Acids Res.** 45, 12565-12576 (2017).
33. W. Ma, **L. Yang**, **R. Rohs^{*}**, and W.S. Noble^{*}. DNA sequence+shape kernel enables alignment-free modeling of transcription factor binding. **Bioinformatics** 33, 3003-3010 (2017).
34. J. Li, **A.C. Dantas Machado**, M. Guo, **J.M. Sagendorf**, Z. Zhou, L. Jiang, X. Chen, D. Wu, L. Qu, Z. Chen, L. Chen^{*}, **R. Rohs^{*}**, and Y. Chen^{*}. Structure of the forkhead domain of FOXA2 bound to a complete DNA consensus site. **Biochemistry** 56, 3745-3753 (2017).
35. **J.M. Sagendorf**, H.M. Berman^{*}, and **R. Rohs^{*}**. DNAProDB: an interactive tool for structural analysis of DNA-protein complexes. **Nucleic Acids Res.** 45, W89-W97 (2017).
36. N.S. Tangprasertchai, **R. Di Felice**, X. Zhang, I.M. Slaymaker, C. Vazquez Reyes, W. Jiang, **R. Rohs^{*}**, and P.Z. Qin^{*}. CRISPR-Cas9 mediated DNA unwinding detected using site-directed spin labeling. **ACS Chem. Biol.** 12, 1489-1493 (2017).
37. S. Kasinathan, G.E. Zentner, **B. Xin**, **R. Rohs**, and S. Henikoff^{*}. Correspondence: Reply to 'DNA shape is insufficient to explain binding'. **Nat. Commun.** 8, 15644 (2017).
38. **L. Yang[#]**, Y. Orenstein[#], A. Jolma, Y. Yin, J. Taipale, R. Shamir^{*}, and **R. Rohs^{*}**. Transcription factor family-specific DNA shape readout revealed by quantitative specificity models. **Mol. Syst. Biol.** 13, 910 (2017).
39. S. Schwörer, F. Becker, C. Feller, A.H. Baig, U. Köber, H. Henze, J.M. Kraus, **B. Xin**, A. Lechel, D.B. Lipka, C.S. Varghese, M. Schmidt, **R. Rohs**, R. Aebersold, K.L. Medina, H. A. Kestler, F. Neri, J. von Maltzahn^{*}, S. Tümpel^{*}, and K.L. Rudolph^{*}. Epigenetic stress responses induce muscle stem-cell ageing by Hoxa9 developmental signals. **Nature** 540, 428-432 (2016).
40. S. Schöne, M. Jurk, M.B. Helabad, **I. Dror**, I. Lebars, B. Kieffer, P. Imhof, **R. Rohs**, M. Vingron, M. Thomas-Chollier^{*}, and S.H. Meijsing^{*}. Sequences flanking the core-binding site modulate glucocorticoid receptor structure and activity. **Nat. Commun.** 7, 12621 (2016).
41. A. Mathelier, **B. Xin**, **T.P. Chiu**, **L. Yang**, **R. Rohs^{*}**, and W.W. Wasserman^{*}. DNA shape features improve transcription factor binding site predictions *in vivo*. **Cell Syst.** 3, 278-286 (2016).
42. G. Kuzu[#], E.G. Kaye[#], J. Chery, T. Siggers, **L. Yang**, J. Dobson, S. Boor, J. Bliss, W. Liu, G. Jogl, **R. Rohs**, N.D. Singh, M.L. Bulyk, M.Y. Tolstorukov^{*}, and E. Larschan^{*}. Expansion of GA dinucleotide repeats increases the density of CLAMP binding sites on the X-chromosome to promote *Drosophila* dosage compensation. **PLOS Genet.** 12, e1006120 (2016).
43. **I. Dror**, **R. Rohs**, and Y. Mandel-Gutfreund^{*}. How motif environment affects transcription factor search dynamics: finding a needle in a haystack. **BioEssays** 38, 605-612 (2016).
44. **T.P. Chiu[#]**, F. Comoglio[#], **T. Zhou**, **L. Yang**, R. Paro, and **R. Rohs^{*}**. DNASHapeR: an R/Bioconductor package for DNA shape prediction and feature encoding. **Bioinformatics** 32,

- 1211-1213 (2016).
45. G.E. Zentner, S. Kasinathan, **B. Xin, R. Rohs**, and S. Henikoff*. ChEC-seq kinetics discriminates transcription factor binding sites by DNA sequence and shape. **Nat. Commun.** 6, 8733 (2015).
 46. **I. Dror**, T. Golan, C. Levy, **R. Rohs***, and Y. Mandel-Gutfreund*. A widespread role of the motif environment in transcription factor binding across diverse protein families. **Genome Res.** 25, 1268-1280 (2015).
 47. Z. Deng, Q. Wang, Z. Liu, M. Zhang, **A.C. Dantas Machado, T.P. Chiu**, C. Feng, Q. Zhang, L. Yu, L. Qi, J. Zheng, X. Wang, X.M. Huo, X. Qi, X. Li, W. Wu, **R. Rohs***, Y. Li*, and Z. Chen*. Mechanistic insights into metal ion activation and operator recognition by the ferric uptake regulator. **Nat. Commun.** 6, 7642 (2015).
 48. F. Comoglio, T. Schlumpf, V. Schmid, **R. Rohs**, C. Beisel, and R. Paro*. High-resolution profiling of *Drosophila* replication start sites reveals a DNA shape and chromatin signature of metazoan origins. **Cell Rep.** 11, 821-834 (2015).
 49. N. Abe, **I. Dror, L. Yang**, M. Slattery, **T. Zhou**, H.J. Bussemaker, **R. Rohs***, and R.S. Mann*. Deconvolving the recognition of DNA sequence from shape. **Cell** 161, 307-318 (2015).
 50. M. Levo, E. Zalckvar, E. Sharon, **A.C. Dantas Machado**, Y. Kalma, M. Lotan-Pompan, A. Weinberger, Z. Yakhini, **R. Rohs**, E. Segal*. Unraveling determinants of transcription factor binding outside the core-binding site. **Genome Res.** 25, 1018-1029 (2015).
 51. **T. Zhou**[#], N. Shen[#], **L. Yang**, N. Abe, J. Horton, R.S. Mann, H.J. Bussemaker, R. Gordân*, and **R. Rohs***. Quantitative modeling of transcription factor binding specificities using DNA shape. **Proc. Natl. Acad. Sci. USA** 112, 4654-4659 (2015).
 52. T. Hadžić, D. Park, K.C. Abruzzi, **L. Yang**, J.S. Trigg, **R. Rohs**, M. Rosbash, and P.H. Taghert*. Genome-wide features of neuroendocrine regulation in *Drosophila* by the basis helix-loop-helix transcription factor dimmed. **Nucleic Acids Res.** 43, 2199-2215 (2015).
 53. **T.P. Chiu**[#], **L. Yang**[#], **T. Zhou**, B.J. Main, S.C.J. Parker, S.V. Nuzhdin, T.D. Tullius, and **R. Rohs***. GBshape: a genome browser database for DNA shape annotations. **Nucleic Acids Res.** 43, D103-D109 (2015).
 54. **A.C. Dantas Machado**[#], **T. Zhou**[#], **S. Rao**[#], **P. Goel**[#], C. Rastogi[#], A. Lazarovici, H.J. Bussemaker*, and **R. Rohs***. Evolving insights on how cytosine methylation affects protein-DNA binding. **Brief. Funct. Genomics** 14, 61-73 (2015).
 55. M. Slattery*, **T. Zhou**[#], **L. Yang**[#], **A.C. Dantas Machado**[#], R. Gordân*, and **R. Rohs***. Absence of a simple code: how transcription factors read the genome. **Trends Biochem. Sci.** 39, 381-399 (2014).
 56. I. Barozzi, M. Simonatto, S. Bonifacio, **L. Yang**, **R. Rohs**, S. Ghisletti, and G. Natoli*. Coregulation of transcription factor binding and nucleosome occupancy through DNA features of mammalian enhancers. **Mol. Cell** 54, 844-857 (2014).
 57. X. Zhang, **A.C. Dantas Machado**, Y. Ding, Y. Chen, **Y. Lu**, K. Tham, L. Chen, **R. Rohs***, and P.Z. Qin*. Conformations of p53 response elements in solution deduced using site-directed spin labeling and Monte Carlo sampling. **Nucleic Acids Res.** 42, 2789-2797 (2014).
 58. **L. Yang**, **T. Zhou**, **I. Dror**, A. Mathelier, W.W. Wasserman, R. Gordân, and **R. Rohs***. TFBSshape: a motif database for DNA shape features of transcription factor binding sites. **Nucleic Acids Res.** 42, D148-D155 (2014).
 59. **I. Dror**, **T. Zhou**, Y. Mandel-Gutfreund*, and **R. Rohs***. Covariation between homeodomain transcription factors and the shape of their DNA binding sites. **Nucleic Acids Res.** 42, 430-441 (2014).
 60. A. Eldar, H. Rozenberg, Y. Diskin-Posner, **R. Rohs**, and Z. Shakked*. Structural studies of p53 inactivation by DNA-contact mutations and its rescue by suppressor mutations via alternative protein-DNA interactions. **Nucleic Acids Res.** 41, 8748-8759 (2013).
 61. Y. Chen*, X. Zhang, **A.C. Dantas Machado**, Y. Ding, Z. Chen, P.Z. Qin, **R. Rohs**, and L. Chen*. Structure of p53 binding to the BAX response element reveals DNA unwinding and compression to accommodate base-pair insertion. **Nucleic Acids Res.** 41, 8368-8376 (2013).
 62. **T. Zhou**, **L. Yang**, **Y. Lu**, **I. Dror**, **A.C. Dantas Machado**, **T. Ghane**, **R. Di Felice**, and **R. Rohs***. DNASHape: a method for the high-throughput prediction of DNA structural features on a genome-wide scale. **Nucleic Acids Res.** 41, W56-W62 (2013).

63. S.P. Hancock, D. Cascio, **T. Ghane, R. Rohs, R. Di Felice**, and R.C. Johnson*. Control of DNA minor groove widths and Fis protein binding by the purine 2-amino group. **Nucleic Acids Res.** 41, 6750-6760 (2013).
64. A. Lazarovici, **T. Zhou**[#], A. Shafer[#], **A.C. Dantas Machado**[#], T.R. Riley, R. Sandstrom, P.J. Sabo, **Y. Lu, R. Rohs**^{*}, J.A. Stamatoyannopoulos^{*}, and H.J. Bussemaker^{*}. Probing DNA shape and methylation state on a genomic scale with DNase I. **Proc. Natl. Acad. Sci. USA** 110, 6376-6381 (2013).
65. R. Gordân, N. Shen[#], **I. Dror**[#], **T. Zhou**[#], J. Horton, **R. Rohs**^{*}, and M.L. Bulyk^{*}. Genomic regions flanking E-box binding sites influence DNA binding specificity of bHLH transcription factors through DNA shape. **Cell Rep.** 3, 1093-1104 (2013).
66. Y.P. Chang, M. Xu, **A.C. Dantas Machado**, X.J. Yu, **R. Rohs**^{*}, and X.S. Chen^{*}. Origin DNA recognition by the SV40 large tumor antigen: Insights into the mechanism of initiator assembly. **Cell Rep.** 3, 1117-1127 (2013).
67. Y. Chen, D.L. Bates, R. Dey, P.H. Chen, **A.C. Dantas Machado**, I.A. Laird-Offringa, **R. Rohs**, and L. Chen^{*}. DNA binding by GATA transcription factor suggests mechanisms of DNA looping and long-range gene regulation. **Cell Rep.** 2, 1197-1206 (2012).
68. M. Slattery, T. Riley, P. Liu, N. Abe, P. Gomez-Alcala, **I. Dror, T. Zhou, R. Rohs**^{*}, B. Honig^{*}, H.J. Bussemaker^{*}, and R.S. Mann^{*}. Cofactor binding evokes latent differences in DNA binding specificity between Hox proteins. **Cell** 147, 1270-1282 (2011).
69. E.P. Bishop[#], **R. Rohs**[#], S.C.J. Parker[#], S.M. West, P. Liu, R.S. Mann, B. Honig, and T.D. Tullius^{*}. A map of minor groove shape and electrostatic potential from hydroxyl radical cleavage patterns of DNA. **ACS Chem. Biol.** 6, 1314-1320 (2011).

Peer-reviewed journal articles (until 08/2010; before joining USC)

70. **R. Rohs**[#], X. Jin[#], S.M. West, R. Joshi, B. Honig^{*}, and R.S. Mann^{*}. Origins of specificity in protein-DNA recognition. **Ann. Rev. Biochem.** 79, 233-269 (2010).
71. M. Kitayner[#], H. Rozenberg[#], **R. Rohs**[#], O. Suad, D. Rabinovich, B. Honig^{*}, and Z. Shakked^{*}. Diversity in DNA recognition by p53 revealed by crystal structures with Hoogsteen base pairs. **Nat. Struct. Mol. Biol.** 17, 423-429 (2010).
72. S.M. West, **R. Rohs**, R.S. Mann^{*}, and B. Honig^{*}. Electrostatic interactions between arginines and the minor groove in the nucleosome. **J. Biomol. Struct. Dyn.** 27, 861-866 (2010).
73. **R. Rohs**[#], S.M. West[#], A. Sosinsky, P. Liu, R.S. Mann^{*}, and B. Honig^{*}. The role of DNA shape in protein-DNA recognition. **Nature** 461, 1248-1253 (2009).
74. **R. Rohs**, S.M. West, P. Liu, and B. Honig^{*}. Nuance in the double helix and its role in protein-DNA recognition. **Curr. Op. Struct. Biol.** 19, 171-177 (2009).
75. R. Joshi, J. M. Passner[#], **R. Rohs**[#], R. Jain[#], A. Sosinsky[#], M. A. Crickmore, V. Jacob, A. K. Aggarwal^{*}, B. Honig^{*}, and R. S. Mann^{*}. Functional specificity of a Hox protein mediated by the recognition of minor groove structure. **Cell** 131, 530-43 (2007).
76. H. Sklenar^{*}, D. Wüstner, and **R. Rohs**. Using internal and collective variables in Monte Carlo simulations of nucleic acid structures: chain breakage/closure algorithm and associated Jacobians. **J. Comput. Chem.** 27, 309-315 (2006).
77. **R. Rohs**^{*}, I. Bloch, H. Sklenar, and Z. Shakked. Molecular flexibility in ab initio drug docking to DNA: binding-site and binding-mode transitions in all-atom Monte Carlo simulations. **Nucleic Acids Res.** 33, 7048-7057 (2005).
78. **R. Rohs**^{*}, H. Sklenar, Z. Shakked. Structural and energetic origins of sequence-specific DNA bending: Monte Carlo simulations of papillomavirus E2 protein-DNA binding sites. **Structure** 13, 1499-1509 (2005).
79. **R. Rohs**^{*} and H. Sklenar. Methylene blue binding to DNA with alternating AT base sequence: minor groove binding is favored over intercalation. **J. Biomol. Struct. Dyn.** 21, 699-711 (2004).
80. **R. Rohs** and H. Sklenar^{*}. Methylene blue binding to DNA with alternating GC base sequence: continuum treatment of salt effects. **Indian J. Biochem. Biophys.** 38, 1-6 (2001).
81. **R. Rohs**, H. Sklenar^{*}, R. Lavery, and B. Röder. Methylene blue binding to DNA with alternating GC base sequence: a modeling study. **J. Am. Chem. Soc.** 122, 2860-2866 (2000).
82. **R. Rohs**, C. Etchebest, and R. Lavery^{*}. Unraveling proteins: a molecular mechanics study. **Biophys. J.** 76, 2760-2768 (1999).

Invited News & Views articles (08/2010-present; since joining USC)

83. **R. Rohs***, **A.C. Dantas Machado**, and **L. Yang**. Exposing the secrets of sex determination. **Nat. Struct. Mol. Biol.** 22, 437-438 (2015).
84. B. Honig* and **R. Rohs***. Biophysics: Flipping Watson and Crick. **Nature** 470, 472-473 (2011).

Peer-reviewed book chapters (08/2010-present; since joining USC)

85. N.S. Tangprasertchai, X. Zhang, Y. Ding, K. Tham, **R. Rohs**, I.S. Haworth, and P.Z. Qin*. Integrated spin-labeling/computational-modeling approaches for mapping global structures of nucleic acids. **Methods Enzymol.** 564, 427-453 (2015).
86. R. Harris#, T. Mackoy#, **A.C. Dantas Machado#**, D. Xu, **R. Rohs***, and M.O. Fenley*. Opposites attract: Shape and electrostatic complementarity in protein-DNA complexes. Chapter 3, vol. 2 in T. Schlick, editor. **Innovations in Biomolecular Modeling and Simulation.** 53-80 (2012). Biomolecular Sciences series, Royal Society of Chemistry, RCS Publishing, London, UK.

Educational peer-reviewed publication (08/2010-present; since joining USC)

87. **A.C. Dantas Machado**, **S.B. Saleebyan#**, **B.T. Holmes#**, **M. Karelina#**, **J. Tam#**, **S.Y. Kim#**, **K.H. Kim#**, **I. Dror**, E. Hodis, E. Martz, P.A. Compeau, and **R. Rohs***. Proteopedia: 3D visualization and annotation of transcription factor-DNA readout modes. **Biochem. Mol. Biol. Educ.** 40, 400-401 (2012).

GRANTS AND RESEARCH SUPPORT**Current research support**

Role: PI

Project/Proposal Title: AI-driven discovery of novel BMAL1 modulators for the treatment of Circadian dysregulation and cancer

Source of Support: Office of Research and Innovation SBIR/STTR Planning Award Program

Total Amount Awarded: \$350,000

Total Award Period Covered: 12/04/2024– 01/31/2026

Role: PI

Project/Proposal Title: Quantitative modeling of transcription factor-DNA binding

Source of Support: NIH/NIGMS (R35 MIRA)

Total Amount Awarded: \$2,657,022

Total Award Period Covered: 07/09/2019 – 06/30/2025

Previous Research Support (since joining USC)

Role: Co-PI (with Gompel and Preibisch)

Project/Proposal Title: Quantitative dissection of molecular determinants of enhancer function

Source of Support: HFSP

Total Amount Awarded: \$900,000 (\$325,000 for Rohs)

Total Award Period Covered: 10/01/2018-09/30/2022

Role: co-I (PI Bussemaker)

Project/Proposal Title: Inferring gene regulatory circuitry from functional genomics data

Source of Support: NIH/NHGRI (R01)

Total Amount Awarded: \$444,972 (for Rohs)

Total Award Period Covered: 07/01/2017 – 06/30/2022

Role: PI

Project/Proposal Title: Genome analysis based on the integration of DNA sequence and shape

Source of Support: NIH/NIGMS (R01)
Total Amount Awarded: \$1,255,884
Total Award Period Covered: 02/01/2014 – 01/31/2020

Role: co-I (PI XJ Chen)
Project/Proposal Title: Structural Basis of APOBEC Functions and Interactions with HIV-Vif
Source of Support: NIH/NIGMS (R01)
Total Amount Awarded: \$75,000
Total Award Period Covered: 09/15/2016 – 06/30/2019

Role: PI
Project/Proposal Title: Alfred P. Sloan Research Fellowship
Source of Support: Alfred P. Sloan Foundation
Total Amount Awarded: \$50,000
Total Award Period Covered: 09/15/2013 – 09/14/2017

Role: PI (multi-PI)
Project/Proposal Title: Multi-scale modeling of genetic variation in a developmental network
Source of Support: NIH/NIGMS (U01)
Total Amount Awarded: \$1,978,533
Total Award Period Covered: 09/30/2013 – 06/30/2017

Role: co-I (PI Bussemaker)
Project/Proposal Title: Inferring gene regulatory circuitry from functional genomics data
Source of Support: NIH/NHGRI (R01)
Total Amount Awarded: \$358,836 (for Rohs)
Total Award Period Covered: 07/15/2013 – 06/30/2017

Role: PI
Project/Proposal Title: Collaborative Research: Experimental and computational studies of DNA binding by human paralogous transcription factors
Source of Support: NSF/MCB
Total Amount Awarded: \$102,637
Total Award Period Covered: 09/15/2014 – 08/31/2017

Role: PI (multi-PI with Fraser and Roberts)
Project/Proposal Title: Bridging gene regulation from molecules to organisms
Source of Support: Bridge@USC Institute
Total Amount Awarded: \$33,333 (for Rohs)
Total Award Period Covered: 07/01/2016 – 06/30/2017

Role: PI
Project/Proposal Title: Deciphering molecular mechanisms of p53-DNA recognition
Source of Support: American Cancer Society
Total Amount Awarded: \$30,000
Total Award Period Covered: 07/01/2012 – 06/30/2013