CARLOS SIMMERLING, PH.D.

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PROFESSIONAL EXPERIENCE

2018-present	Marsha Laufer Endowed Professor of Physical and Quantitative Biology
2015-present	Affiliated Faculty Member, SBU Institute for Advanced Computational Science
2010-present	Associate Director, Laufer Center for Physical and Quantitative Biology
2008-present	Professor, Department of Chemistry, Stony Brook University (SBU)
2006-present	Member, Graduate Program in Bioengineering, SBU
2005-present	Affiliated Faculty Member, Dept. of Applied Mathematics and Statistics, SBU
2005-present	Member, Brookhaven National Laboratory, Computational Science Center
2004-2008	Associate Professor, Department of Chemistry, SBU
2004-present	Member, Institute for Chemical Biology and Drug Discovery, SBU
2001-present	Member, Graduate Program in Pharmacological Sciences, SBU
2001-present	Member, Graduate Program in Biochemistry and Structural Biology, SBU
2000-present	Member, Graduate Program in Molecular and Cellular Biology, SBU
1998-2004	Assistant Professor, Department of Chemistry, SBU
1998-present	Member, Center for Structural Biology, SBU

EDUCATION

1994-1998	Postdoctoral Researcher, University of California, San Francisco, Dept. of Pharmaceutical Chemistry (with Peter Kollman)
1994	Ph.D., University of Illinois at Chicago, Dept. of Chemistry (with Ron Elber)
1991	B.A., University of Illinois at Chicago, Dept. of Chemistry

HONORS AND AWARDS

2021	Gordon Bell Special Prize for COVID-19
2021	SUNY Chancellor's Award for Excellence in Scholarship and Creative Activities
2016	Fellow, American Chemical Society
2007	"Humanitarian Impact Innovation Prize", Itanium Solutions Alliance (a coalition of Microsoft, Intel, HP, Oracle and other technology industry leaders)
2004/05/07/08/09	Outstanding Mentor, Siemens Foundation
2003	"Excellence in the Pursuit of Knowledge", SUNY Chancellor's Award
2001	Cottrell Scholar, Research Corporation for Science Advancement
2000	"Young Investigator in Women's Cancers", Academic Medicine Development Corp

POSITIONS HELD

2019-present	Academic Advisory Board member, Open Force Field Initiative
2019-present	MOLSSI Associate, The Molecular Sciences Software Institute
2014-present	Chair, Investigator Conflict of Interest Committee, SBU (member since 2006)
2011-present	Editorial board member, Reports in Theoretical Chemistry
2010-2014	NSF Scientific Advisory Board for Teragrid Supercomputing
2007-2012	Director of Computational Biology, Institute for Chemical Biology and Drug Discovery, SBU
2007-2014	Advisory Board Member, New York Center for Computational Science
2007-2012	Councilor, American Chemical Society, Division of Computers in Chemistry (COMP)

2006-present	Executive Committee Member, American Chemical Society, Division of Computers in Chemistry (COMP)
2005-2011	Section Editor, American Chemical Society "Annual Report in Computational Chemistry"

RESEARCH SUMMARY

Professor Simmerling's research interests focus on the dynamic aspects of biomolecular function, and how conformational changes affect important processes such as protein folding, molecular recognition and enzymatic function. Specific applications of interest are the role of dynamics in drug resistance, recognition/repair of DNA damage, and the nature of the unfolded/disordered state of peptides and proteins. Most of his recent publications on biological systems have been co-authored with experimental collaborators, with a significant focus on integration of computation and experiment.

The biomolecular simulation field remains immature and thus improvement of methods and models is also a focus of the Simmerling lab. Prof. Simmerling has a long history of development and application of a variety of simulation methods, and is currently one of six members of the leadership team for the widely used Amber molecular simulation program (installed at over 12,000 sites, with over 10,000 site licenses; http://www.ambermd.org).

The accuracy of molecular simulations is crucially dependent on the physics model (the "force field") used to describe energies. Simmerling has been an international leader in protein force field development for over a decade. The Simmerling lab's ff99SB Amber force field set a new standard for protein model accuracy, with an impact extending well beyond Amber; it is available in every modern MD package and has been cited independently of Amber over 5,000 times. The force field served as a foundation for other groups' subsequent adaptation and adjustment, which have collectively received thousands of additional citations. Simmerling's follow up models ff12SB and ff14SB further improved accuracy, and have received over 2,000 citations, and the newest model, ff19SB, was recently released. The Simmerling lab also develops the primary implicit water models for Amber, with 5 articles each having >100 citations independent of Amber.

ENCOURAGING DIVERSITY AND EARLY ENGAGEMENT OF STEM STUDENTS IN RESEARCH

Prof. Simmerling is deeply committed to encouraging diversity in STEM, with **8 female of 25 total PhDs, and 3 female of 6 total postdocs.** Four of 6 current PhD candidates in the lab are URM and/or female. Two URM graduate students have obtained NIH F31 NRSA fellowships. Undergraduates represent a significant part of Simmerling's research group (**61** total; 58% female, 23% URM); 9 of 10 current lab undergrads are URM and/or female. Most go on to MD or PhD programs; our two 2021 graduates (both female/URM) went to PhD programs at Yale and U Chicago. Two undergraduate mentees received "Minority Access to Research Careers" (MARC) fellowships, one a 2014 HHMI EXROP award, and one captained the team that won the Student Cluster Challenge at the 2009 Supercomputing Conference. Simmerling also recruits and mentors local high school students (**47 total**; 38% female, 9% minority), including 8 Intel Science Talent Search (STS) and 9 Siemens Competition semi-finalists, 4 Intel STS national finalists, winner of the Best in Category Award (Biochemistry/Biology) at the 2010 International Science & Engineering Fair, a 2008 Davidson Fellow Laureate ($50,000), and winner of the 2009 national first-prize award in the Siemens Competition ($100,000). In the past 5 years, 6 high school and undergraduate students were co-authors on 6 peer-reviewed publications, and 4 more are co-authors on manuscripts under review. Simmerling has received the Siemens Foundation "Outstanding Mentor" award 5 times, and his efforts were described in the 2012 Newsday article "The Mentor Experiment", and the 2013 New York Times article "A Laboratory Grows Young Scientists".

POSTDOCTORAL FELLOWS MENTORED AND CURRENT POSITIONS (6 TOTAL)

Name	Program	Topic	Date
Hornak, Viktor	Chemistry	New Methods for Biomolecular Simulations	1999-2000

	Investigator III, Novartis Institutes for Biomedical Research		
Song, Kun	Chemistry	Recognition of DNA Damage	2007-2008
	Computational Chemist, AstraZeneca		
Fu, Lin	Pharmacology	Recognition of DNA Damage	2009-2011
	Wenzhou Medical University		
Pias, Sally	Chemistry	Simulation Methods for Drug Resistance	2009-2011
	Associate Professor, New Mexico Tech Department of Chemistry		
Carvalho, Alexandra	Chemistry	DNA Scanning by Repair Enzymes	2010-2013
	Assistant Investigator, University of Coimbra, CNC-Center for Neuroscience and Cell Biology		
Miguez, Angela	Chemistry	Proofreading Mechanism of DNA Polymerase	2015-2017
	Assistant Professor, SUNY Oneonta		

GRADUATE STUDENTS MENTORED AND CURRENT POSITIONS (29 TOTAL)

Name	**Program**	**Topic**	**Degree/Date**
Cui, Guanglei	Chemistry	New methods for biomolecular simulations	PhD, 2003
	Computational Chemist, GlaxoSmithKline Pharmaceuticals		
Cheng, Xiaolin	Chemistry	Simulations of modified DNA	PhD, 2004
	Associate Professor, College of Pharmacy, The Ohio State University		
Strockbine, Bentley	Pharmacology	Simulating folding of small proteins	PhD, 2006
	Forensic Psychiatrist		
Geney, Raphael	Chemistry	Structure-based drug design of paclitaxel	PhD, 2005
	Patent Associate, Galapagos		
Okur, Asim	Chemistry	New methods for biomolecular simulations	PhD, 2006
	Scientific Information Officer, National Institute of Mental Health (NIMH)		
Song, Kun	Chemistry	Enzyme ecognition of DNA damage	PhD, 2007
	Computational Chemist, AstraZeneca		
Roe, Daniel	Chemistry	Improved solvation models for simulations	PhD, 2007
	Staff Scientist, National Institutes of Health		
Rafi, Salma	Chemistry	Structure and inhibition of enoyl reductase	PhD, 2008
	Principal Scientist at Schrödinger		
Wickstrom, Lauren	Chemistry	Comparison of simulation and NMR data	PhD, 2009
	Associate Professor, Borough of Manhattan Community College		
Ding, Fangyu	Biochemistry	Simulations of HIV-1 protease mutants	PhD, 2010
	unknown		
Campbell, Arthur	Chemistry	Structure and dynamics of crosslinked DNA	PhD, 2011
	Group Leader, Senior Computational Chemist I at Broad Institute		
Bergonzo, Christina	Chemistry	Enzyme recognition of DNA damage	PhD, 2012
	Research Chemist, National Institutes of Standards & Technologies (NIST)		
Shang, Yi	Chemistry	Dynamics of drug resistant HIV-1 protease	PhD, 2013
	Postdoc, Icahn School of Medicine at Mt. Sinai		
Carr, Amber	Chemistry	Self-guided MD simulation methods	PhD, 2013
	Lecturing Fellow, Duke University		
Martinez, Carmenza	Chemistry	Improving protein force fields	PhD, 2013
	unknown		
Lai, Cheng-Tsung	Biochemistry	Rational design of slow-binding inhibitors	PhD, 2014
	Postdoctoral Fellow, Northwestern University		
Li, Haoquan	Chemistry	Enzyme recognition of DNA damage	PhD, 2014
	Software Development Engineer II at Amazon Drive		
Nguyen, Hai	Chemistry	Improved implicit solvent for biopolymers	PhD, 2015
	Senior Scientist II, Schrödinger		
Maier, James	Biochemistry	Improved protein side chain force field	PhD, 2015

	Data Scientist, Viasat Inc.		
Hauser, Kevin	Chemistry	Recognition of DNA by transcription factors	PhD, 2016
	Senior Scientist, Vir Biotechnology Inc		
Huang, He	Chemistry	New methods for nonpolar solvation	PhD, 2018
	Postdoctoral Scholar at Tufts University		
Zou, Junjie	Chemistry	Application of alchemical free energy methods	PhD, 2019
	Senior Scientist, Xtalpi Inc.		
Tian, Chuan	Chemistry	Improved protein backbone force field	PhD, 2019
	Research Scientist, Eli Lilly		
Kasavajhala, Koushik	Chemistry	Using structure reservoirs to speed sampling	PhD, 2020
	Principal Scientist at Schrödinger		
Belfon, Kellon	Chemistry	Conformational studies of retroviral proteases	PhD, 2021
	Project Modeling Investigator, Roivant Sciences		
Lam, Kenneth	Mol Cell Bio	Improved methods for simulations of RNA	PhD, 2020
Raguette, Lauren	Chemistry	Simulations of phosphorylated proteins	PhD, 2022 (*est*)
Fallon, Zachary	Chemistry	Proofreading mechanism of DNA polymerase	PhD, 2022 (*est*)
Wang, Yuzhang	Chemistry	More accurate protein implicit solvent models	PhD, 2024 (*est*)
Darya Stepanenko	Applied Mathematics	Modeling the SARS-CoV-2 Spike	PhD, 2025 (est)

UNDERGRADUATE STUDENTS MENTORED IN RESEARCH (60 TOTAL)

Padma Kandadai (1999), Thomas Canseco (1999-2000), Ruth Li (1999), William Olivo (1999), Hitomi Oda (1999), My Tu (2001-2002), Brock Adams (2002), Mfon Akpan (2001), Kinning Poon (2002), Patrice Leahy (2003), Kerri Goldgraben (2003), Jing Moy (2003), Noel Carascal (2003 -2004), Isaac Pflaum (2004), Eric Absgarten (2006-2007), Lester Leong (2006-2007), Marie Majkut (2007), Richard Yao (2007-2008), Dan Talmasov (2007-2008), Aaron Pellman-Isaacs (2008-2009), Dan Martingano (2008-2011), Catherine Kelso (2008), Michael Sperandeo (2008), Henry Lederer (2008), James Maier (2008-2009), Yinglin Gao (2008-2009), Nora Asamoah (2008-2010), Paraskevas Xenophontos (2009-2010), Esther Shin (2009-2010), Jon McGinn (2009), Ben Sherman (2010), Lukas Klees (2010), Neville Bethel (2009-2013), Sherry Bermeo (2012-2015), James Alrassi (2014), Victoria Perrone (2014-2017), Emily Liu (2014-2015), Bernard Essuman (2014, 2019-presen), Dillon Higginson (2015), Gabriela Witek (2015-2017), Rebecca Chang (2017), Grace Manalo (2017), Jorge Pincay (2017-2020), Kelley Chiu (2018-present), Jackelyne Garcia Cruz (2018-2019), Christian Arty (2018), Jose Guerra (2019-2021), Abbigayle Cuomo (2019-2021), Juliana Pham (2019-2021), Stephanie Helbock (2020-present), Isabel Yang (2020-2021), Stephanie Budhan (2020-present), Sarah Varghese (2020-present), Sarah Jacobson (2020-2021), Michelle Twan (2020-2021), Samer Mahmoud (2021-present), Sarah Gunasekera (2021-present), Isra Ahmed (2021-present), Sharena Brown (2021-present), Kezia Kelley (2021)

HIGH SCHOOL STUDENTS MENTORED IN RESEARCH (46 TOTAL)

Michael Lee (1999), Kristen Regan (2000), Asad Sheth (2000), Dan Noe (2000-2001), Max Bernstein (2001), Jason Barell (2002), Kevin Wang (2003, 2004), Zack Goldberg (2003), Jillian Cypser (2003), David Rosenman (2004), Catherine Kelso (2004-2007), Julian Hershowitz (2004,2005), Oleksandr Dagayev (2005-2006), Rachel Orifici (2005), Alex Iyer (2005), Stephanie Clemente (2006), Karthik Kasaraneni (2006), Tom Petracca (2006), Zuha Qazi (2006), Jaime Campos (2007), Christine Shrock (2007-2009), Viraj Shah (2007), Ruoyi Jiang (2008-2009), Brian Miranda (2008-2010), Evan Tilley (2009), Prashant Kota (2009-2010), Kevin Zhao (2009), Dianna Hu (2009-2010), Hannah Kenagy (2010-2011), Anvit Kalra-Lall (2011), Carlos Pena-Lobel (2011), Daniel Wang (2011-2012), John Gee (2012), Anna Whitney (2011), Mayuri Sridhar (2012), Elissa (Yiqing) He (2014), Brandon Gong (2015), Ben Schiffer (2015), Ziheng (Tony) Wang (2015), Rinni Bhansali (2015), Anna Lou (2016-2017), Annie Chang (2016-2017), Merrick Cai (2017-2018), Shobhita Sundaram (2017-2018), Keene Lu (2018), Kyra Ramonetti (2019-present)

AWARDS AND FELLOWSHIPS RECEIVED BY MENTORED GRADUATE STUDENTS

Kellon Belfon: 2018 NIH/NIGMS NRSA F31 Fellowship, 2017 ACM SIGHPC/Intel Computational & Data Science Fellowship, 2017 AGEP Travel Award, 2014-2019, the Dr. W. Burghardt Turner Fellowship, 2014-2016 IMSD-MERGE Graduate Fellowship

Lauren Raguette: 2018 Chemistry Award for First-Year Graduate Student Teaching Assistant

Zachary Fallon: 2017 Graduate Assistance in Areas of National Need Fellowship

Chuan Tian: 2019 IACS Travel Scholarship, 2018 Sigma Xi Travel Award, Image Challenge Winner at the 2016 7th Annual Center for Functional Nanomaterials (CFN) retreat

James Maier: 2013 Sigma Xi Travel Award

Kevin Hauser: 2014 AGEP-T FRAME Conference Travel Award, 2014 American Chemical Society NVIDIA GPU Research Award, 2012-2016 NIH/NIGMS NRSA F31 Fellowship, Invited participant for the 2013 Lindau Meeting of Nobel Laureates, 2011-2012 NIH CBTP T32 Fellowship, 2009-2011 NSF LSAMP-BD Fellowship, 2011 NSF GRFP Honorable Mention, 2011 NSF AGEP Travel Award

Cheng-Tsung (Eric) Lai: Fall 2014 American Chemical Society CCG Graduate Research Excellence Award, 2013 New York Structural Biology Discussion Group 8th Winter Meeting Poster Award, 2011 Institute for Chemical Biology & Drug Discovery Best Poster Award

Hai Nguyen: 2012 Sigma Xi Award

Miranda Yi Shang: Fall 2011 American Chemical Society CCG Graduate Research Excellence Award

Christina Bergonzo: Spring 2011 American Chemical Society CCG Graduate Research Excellence Award

Amber Carr: 2013 Chemistry Award for Outstanding Service, 2011-2012, 2012-2103 IBM Research Fellowship, 2010 American Chemical Society Peter Kollman Graduate Award in Supercomputing

Ding Fangyu: Fall 2009 American Chemical Society CCG Graduate Research Excellence Award, Sigma Xi Excellence in Research Award

Lauren Wickstrom: 2007 Sigma Xi Excellence in Research award, Fall 2007 American Chemical Society CCG Research Excellence Award

Salma Rafi: Spring 2007 American Chemical Society CCG Graduate Research Excellence Award

Kun Song: 2007 Merck Achievement Award by the Chemical Toxicology Division of the American Chemical Society, 2005 American Chemical Society CCG Graduate Research Excellence Award

Raphaël Geney: Fall 2004 American Chemical Society CCG Graduate Research Excellence Award

Melinda Layten: 2004 Kevin King and John Miller Scholarship

Asim Okur: Spring 2004 American Chemical Society CCG Graduate Research Excellence Award

Xiaolin Cheng: Spring 2004 American Chemical Society CCG Graduate Research Excellence Award

Guanglei Cui: 2003 ACS American Chemical Society CCG Graduate Research Excellence Award

Ben Strockbine: 2003 American Chemical Society CCG Graduate Research Excellence Award

TEACHING EXPERIENCE

General Chemistry (1200+ students per semester), General Chemistry Lab, Honors General Chemistry Lab, Physical Chemistry, Physical Chemistry for Life Sciences, Theoretical Chemistry, Computational Structural Biology, Advanced Structural Biology, Principles of Pharmacology, Modern

Drug Discovery, Introductory Synthetic and Spectroscopic Laboratory Techniques, Tools of Chemistry

CURRENT SUPPORT

NIH R01GM107104 (Simmerling, PI) 08/01/2013 - 6/30/2022
New solvent models, sampling methods and maintenance of Amber software
The goal of this program is to support the continued development, maintenance, testing and evaluation of existing software.

NIH RM1 GM135136 (Dill, PI; Simmerling- co-PI) 04/1/2020 – 03/31/2025
Solvation modeling for next-gen biomolecule simulations
To understand biological processes in health and disease, and to develop drugs and other therapies, we need computational models for proteins and how they interact with each other in the wet environments inside and around our cells. Here we develop models based on physical principles and geometrical descriptions of the interactions that determine how proteins behave.

NSF CTMC-1665159 (Simmerling, PI, Wu co-investigator) 07/01/2017 - 06/30/2021
Chemical Theory, Models and Computational Methods
Improving the Accuracy of the Amber Force Field for Biomolecular Simulation
This project is centered on developing more accurate physics models (force fields) that will facilitate a much broader and more reliable application of simulation tools to biophysics problems.

R43 GM134756 (Tsai, Simmerling, Shen MPI) 07/01/2019 - 06 /30/2021
A Cloud-Based Web Application To Accelerate Targeted Covalent Drug Discovery
This project seeks to develop a cloud-based on-demand web application that offers rapid and accurate predictions of covalently targetable hotspots in proteins and more broadly the protonation states of any titratable sites in macromolecules to accelerate drug discovery.

NIH R01 GM102864 (Tonge PI; Simmerling co-investigator) 09/15/2012 - 03/31/2022
Mechanism of Slow Onset Enzyme Inhibition and Drug Target Residence Time
The goal is to determine the mechanism by which some enzyme inhibitors exhibit slow-onset kinetics. Further studies include the rational design of inhibitors with longer residence times.

Research Corporation for Scientific Advancement (Simmerling, PI) 06/15/2020 – 06/14/2021
Pan-Covid-19 MultiValent Binders (MVBs) to Block Virus Entry
This project aims to determine the mechanism of membrane fusion induced by coronavirus spike proteins, and work with experimental collaborators to identify inhibitors.

Research Corporation for Scientific Advancement (Simmerling, PI) 06/15/2020 – 06/14/2021
Modulating Ribosomal Frameshifts to Interfere with Viral Protein Translation
This project aims to model the structure and interactions of the coronavirus RNA pseudoknot, and develop ligands to interfere with the pseudoknot role in transcript of viral RNA

Software license fees,"*Amber*" Period: ongoing
Principal Investigators: David Case, Tom Cheatham, Ken Merz, Adrian Roitberg, Carlos Simmerling
This project involves the development and distribution of the Amber suite of programs for molecular simulation. The core developers listed above equally share the proceeds from license fees to support algorithm and code development in their labs.

COMPLETED SUPPORT

AMDeC Foundation 07/1/2000 - 06/30/2003
Computer Simulations: A New Tool in the Detection and Treatment of Cancer

NIH R01 GM061678 (Simmerling, PI) 06/01/2000 - 03/31/2011

Computational Studies of Model Systems for Protein Unfolded States

Research Corporation for Science Advancement (Simmerling, PI) 07/01/2000 - 06/30/2002
Using Large Clusters of Personal Computers to Improve Simulations in the Condensed Phase

NIH S10 RR017855 (Smith, PI; Simmerling, Co-investigator) 03/01/2004 - 02/28/2007
Computational Facility for Structural Biology

Academy of Applied Science (Simmerling, PI) 06/01/2005 - 05/30/2006
Research Engineering and Apprenticeship Program

Academy of Applied Science (Simmerling, PI) 06/01/2006 - 05/30/2007
Research Engineering and Apprenticeship Program
NIH R37 CA017395 (Grollman, PI, Simmerling, co-Investigator) 04/01/2007 - 03/31/2012
Molecular Pharmacology of Oxidative DNA Damage: Structure and Energetics

Academy of Applied Science (Simmerling, PI) 06/01/2007 - 05/30/2008
Research Engineering and Apprenticeship Program

SBU/BNL SEED grant (Simmerling, PI) 06/01/2007 - 05/30/2008
Simulations of Biomolecular Systems on Massively Parallel Supercomputers

NIH R01 GM079383 (Duan, PI; Simmerling MPI) 07/01/2007 - 06/30/2011
AMBER force field consortium: a coherent biomolecular simulation platform

NSF/Computing Research Association CIF-A-231 (Simmerling, PI) 09/15/2009 - 10/14/2011
Computing Innovation Fellow

Academy of Applied Science (Simmerling, PI) 06/01/2011 - 05/30/2012
Research Engineering and Apprenticeship Program

NIH R01 GM098102 (Hall, PI; Simmerling, Cheatham MPI) 09/30/2011 - 08/31/2016
RNA-ligand interactions: simulation and experiment

AstraZeneca Pharmaceuticals LP 2000281000 (Simmerling, PI) 11/07/2011 - 06/05/2012
Developing Computational Chemistry Tools for Modeling Time Dependent Inhibition

NSF 1137097 (Dongarra, PI; Simmerling co-PI) 04/15/2012 - 03/31/2014
Beacon: A Strategic Path to Scientific Discovery Enabled by the Intel MIC Architecture

Academy of Applied Science (Simmerling, PI) 06/01/2012 - 05/30/2013
Research Engineering and Apprenticeship Program

NIH/NCI R01 CA165911(Schärer, PI; Simmerling, co-investigator) 07/01/2012 - 04/30/2017
Synthesis, structure and repair of DNA interstrand crosslinks

NIH F31 GM101946 NIH Fellowship (Kevin Hauser) 08/01/2012 - 07/31/2016
NRSA: Modeling the mechanism of MTERF1-DNA binding and recognition

NIH F31 GM123767 NIH Fellowship (Kellon Belfon) 03/10/2018 - 03/11/2020
NRSA: Characterization of a Potential Allosteric Target in the Dimer Interface of Retroviral Proteases

IBM PhD Fellowship Award 08/01/2012 - 07/31/2014
Fellowship for Amber Carr

Academy of Applied Science 06/01/2013 - 05/30/2014
Research Engineering and Apprenticeship Program

SUPERCOMPUTER TIME SUPPORT

National Cancer Institute, Advanced Biomedical Computing Center 04/01/2000 – 03/31/2001
Refinement of Cancer-Related Biomolecular Structures

NSF NRAC MCA02N028 10/01/2002 – 09/30/2003
Improving Biomolecular Simulations: Energy Functions and Conformational Sampling

NSF NRAC MCA02N028 04/01/2004 - 03/31/2005
Computer Simulations of Biomolecular Structure and Dynamics

NSF NRAC MCA02N028 04/01/2005 - 03/31/2006
Computer Simulations of Biomolecular Structure and Dynamics

NSF LRAC MCA02N028 04/01/2006 - 03/31/2007
Computer Simulations of Biomolecular Structure and Dynamics

NSF LRAC MCA02N028 04/01/2007 - 03/31/2008
Computer Simulations of Biomolecular Structure and Dynamics

NSF TRAC MCA02N028 04/01/2009 - 03/31/2010
Computer Simulations of Biomolecular Structure and Dynamics

NSF XSEDE MCA02N028 04/01/2010 - 03/31/2011
Computer Simulations of Biomolecular Structure and Dynamics

NSF OCI-1036208 (PI: Cheatham; co-PIs Simmerling, York, Walker, Roitberg) 12/01/10 - 4/30/14
PRAC- Hierarchical molecular dynamics sampling for assessing pathways and free energies of RNA catalysis, ligand binding, and conformational change

NSF ACI-1515572 (PI: Cheatham; co-PIs Simmerling, York, Walker, Roitberg) 08/01/15 -07/31/18
PRAC- Ensembles of molecular dynamics engines for assessing force fields, conformational change, and free energies of proteins and nucleic acids

The COVID-19 High Performance Computing Consortium MCB200069 (PI Ramanathan) *Artificial intelligence driven integrative biology for accelerating therapeutic discovery against SARS-CoV-2*

COMPLETE LISTS OF PUBLISHED WORK

`http://www.ncbi.nlm.nih.gov/sites/myncbi/1lq0lNg9li-Qk/bibliography/48048182/public/`

`https://scholar.google.com/citations?user=KFOBbygAAAAJ`

PUBLICATIONS (reverse chronological order)

Citation statistics as of October 2021: Total citations = 43,140; H-Index = 56; I-10 = 114)

1. Zou, J., Li, Z., Liu, S., Peng, C., Fang, D., Wan, X., Lin, Z., Lee, T., Raleigh, D., Yang, M., and Simmerling, C.*, *Scaffold Hopping Transformations Using Auxiliary Restraints for Calculating Accurate Relative Binding Free Energies.* J. Chem. Theory Comput. 2021, 17, 6, 3710–3726
2. Zou, J., Xiao, S., Simmerling, C., and Raleigh, D., *Quantitative Analysis of Protein Unfolded State Energetics: Experimental and Computational Studies Demonstrate That Non-Native Side-*

Chain Interactions Stabilize Local Native Backbone Structure., J. Phys. Chem. B, 2021, 125, 13, 3269–3277

3. Casalino, L., Dommer, A., Gaieb, Z., Barros, E., Sztain, T., Ahn, S., Trifan, A., Brace, A., Bogetti, A., Ma, H., Lee, H., Turilli, M., Khalid, S., Chong, L., Simmerling, C., Hardy, D., Maia, J., Phillips, J., Kurth, T., Stern, A., Huang, L., McCalpin, J., Tatineni, M., Gibbs, T., Stone, J., Jha, S., Ramanathan, A., Amaro, R., *AI-Driven Multiscale Simulations Illuminate Mechanisms of SARS-CoV-2 Spike Dynamics.* International Journal of High Performance Computing Applications, in press 2021
4. Fallon, L., Raguette, L., Wang, Y., Corbo, C., Stepanenko, D., Cuomo, A., Guerra, J., Budhan, S., Varghese, S., Rizzo, R., Simmerling, C., *Free Energy Landscapes for RBD Opening in SARS-CoV-2 Spike Glycoprotein Simulations Suggest Key Interactions and a Potentially Druggable Allosteric Pocket.* J. Am. Chem. Soc., 2021, 143, 30, 11349–11360
5. Brini, E., Simmerling, C., Dill, K. *Protein Storytelling through Physics,* Science 370:6520 (2020)
6. Barros, E. P., Casalino, L., Gaieb, Z., Dommer, A. C., Wang, Y., Fallon, L., Raguette, L., Belfon, K., Simmerling, C., Amaro, R. E. *The Flexibility of ACE2 in the Context of SARS-CoV-2 Infection.* Biophysical Journal Special Issue on COVID-19, in press 2020
7. Kasavajhala, Koushik; Lam, Kenneth; Simmerling, Carlos. *Exploring Protocols to Build Reservoirs to Accelerate Temperature Replica Exchange MD Simulations.* Journal of Chemical Theory & Computation, 16 (12), 7776-7799 (2020)
8. Iuliano, J., Jinnette Tolentino Collado, Agnieszka A. Gil, Pavithran T. Ravindran, Andras Lukacs, SeungYoun Shin, Helena A. Woroniecka, Katrin Adamczyk, James M. Aramini, Uthama R. Edupuganti, Christopher R. Hall, Gregory M. Greetham, Igor V. Sazanovich, Ian P. Clark, Taraneh Daryaee, Jared E. Toettcher, Jarrod B. French, Kevin H. Gardner, Carlos L. Simmerling*, Stephen R. Meech*, and Peter J. Tonge, *Unraveling the Mechanism of a LOV Domain Optogenetic Sensor: A Glutamine Lever Induces Unfolding of the Jα Helix*, ACS Chem. Biol. 2020, 15, 10, 2752–2765 DOI: 10.1021/acschembio.0c00543
9. Crooks, E., B. Irizarry, M. Ziliox, T. Kawakam, T. Victor, F. Xu, H. Hojo, K. Chiu, C. Simmerling, W. Van Nostrand, S. Smith and L. Miller, "*Copper stabilizes antiparallel β-sheet fibrils of the amyloid β40 (Aβ40)-Iowa variant*", J. Biol. Chem., 295:8914-8927, (2020) DOI: 10.1074/jbc.RA119.011955
10. Tian, C., Kasavajhala, K., Belfon, K., Raguette, L., Huang, H., Miguez, A., Bickel, J., Wang, Y., Pincay, J., Wu, Q., Simmerling, C. "*ff19SB: Amino-Acid Specific Protein Backbone Parameters Trained Against Quantum Mechanics Energy Surfaces in Solution*", Journal of Chemical Theory and Computation, 2020, 16, 1, 528-552, DOI:10.1021/acs.jctc.9b00591
11. Zou, J., Simmerling, C.*, Raleigh, D.*, *"Dissecting the Energetics of Intrinsically Disordered Proteins via a Hybrid Experimental and Computational Approach"*, J. Phys. Chem. B 123 (49), 10394-10402, 2019, DOI:10.1021/acs.jpcb.9b08323
12. Ghoreishi, D., Cerutti, D., Fallon, Z., Simmerling, C., Roitberg, A., "*A Fast Implementation of the Nudged Elastic Band Method in AMBER*", Journal of Chemical Theory and Computation, 2019, DOI: 10.1021/acs.jctc.9b00329
13. Zou, J., Tian, C., Simmerling, C., "*Blinded Prediction of Protein-Ligand Binding Affinity Using Amber Thermodynamic Integration for the 2018 D3R Grand Challenge 4*", Journal of Computer Aided Molecular Design (2019), DOI:10.1007/s10822-019-00223-x
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