Dr. Alan Grossfield

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Current as of: 5/25/22

Research Interests

- Molecular simulation and statistical mechanics of biological systems
- G protein-coupled receptor structure and function
- Aggregation of alpha-synuclein and amyloid formation
- Phase separation of lipid membranes
- New treatments for opioid-induced respiratory depression and addiction
- Developing new tools to perform and analyze molecular simulations

Research Experience and Education

- Associate Professor, Department of Biochemistry and Biophysics
  University of Rochester Medical Center
  March 2014 - present
- Assistant Professor, Department of Biochemistry and Biophysics
  University of Rochester Medical Center
  October 2007- March 2014
- Research Staff Member, IBM T. J. Watson Research Center
  Biomolecular Dynamics and Scalable Modeling, Blue Gene Project
  Group Leader: Dr. Michael Pitman
  September 2004 – September 2007
  Molecular dynamics simulations of rhodopsin
- Post-doctoral fellow, Washington University Medical School
  Department of Biochemistry
  Adviser: Dr. Jay Ponder
  May 2000 – August 2004
  Ion solvation thermodynamics, polarizable force field thermodynamics
- Graduate Student, Johns Hopkins Medical School
  Department of Biophysics and Biophysical Chemistry
  Adviser: Dr. Thomas Woolf
  August 1994 – May 2000
  Thesis title: Computer simulation of membrane-protein interactions
- Undergraduate Student, Cornell University
  Physics major, concentration in Biology
  September 1990 – May 1994
- Undergraduate Research, Cornell University
  Adviser: Dr. P. A. Karplus
  Summer, 1993

- Visiting Research Student, CIBA-Geigy
  Summers 1990 – 1992

Teaching

- IND 408: 3–4 lectures/year (Protein Folding, Thermodynamics, Molecular simulation, Protein structure prediction), 2008-
- BCH 412: 3 lectures/year (Membrane Structure, NMR, Ligand binding calculation), 2008-
- BPH 509:
  - 7–9 lectures (Statistical mechanics, advanced simulation methods), 2009-2015 biannually, each lecture 2 hrs
  - Course director starting in 2017-
  - 15-18 lectures (Statistical mechanics, advanced simulation methods), 2019-, course is now an annual ½ semester course
- BPH 411: 1 lecture (Solid state NMR), 2010-2018 biannually
- BCH 517: (facilitated student interactions with seminar speakers and student discussion of speaker papers), 2010, 2012
- IND 501: (facilitated small-group ethics discussion), 2008, 2009, 2011-present

Lab Members

- Postdocs: Dr. Tod D. Romo, 2008-2018 (now staff scientist)
- Graduate Students
  - Joshua N. Horn, 2008-2013 (defended Aug 14, 2013): Neuman Award (2012), Student seminar award in Biophysics (2010, 2011), CIRC Retreat Best Poster (2012), RIT Graduate Research Symposium Best Presentation (2012), Supported by T32 Training Grant in Cellular, Biochemical and Molecular Sciences (2011)
  - Nicholas Leioatts, 2009-2014: Elon Huntington Hooker Fellowship (2013-2014), Neuman Award (2013), Student seminar award in Biophysics (2011, 2012), Biochemistry Retreat Best Poster Award (2012), Departmental Travel Award (2011), Supported by T32 Training Grant in Cellular, Biochemical and Molecular Sciences (2012)
  - Dejun Lin, 2010-2016: Leon L. Miller Fellowship (2011), Student seminar award in Biophysics (2012), Neuman Travel Award (2012, 2013), Wallace O. Fenn thesis award (2016)
  - Letty Leslie Ann Salas Estrada, 2013-2020: Leon L. Miller Fellowship (2013), Beca Complemento Scholarship for Graduate Students in a Foreign Country (2015, 2018), International Fellowship American Association of University Women (2016), Elena Gilde Grossfield Trainee Presentation Award (2016), Best Biophysics Student Seminar Award (2016, 2018), Elon Huntington Hooker Fellowship (2017), Joan Write Goodman Dissertation Fellowship (2018), Newman Award (2019), George V. Metzger Award (2020)
  - Sreyoshi Sur, 2013-2020: Dept. of Chemistry National Travel Award (2016), Elena Gilde Grossfield Trainee Presentation Award (2017), Graduate Student Association Travel Award (2019)

    - Ashlin James Poruthoor, 2018-: Newman Travel Award (2020, 2021)
    - Emily Robinson: 2019-: Newman Travel Award (2021)
- Undergraduates and High School Students
    - Megan Jenkins (2008)
    - Kevin Hu (high school student, summer 2010)
    - Jesse Sengillo (2010-2011)
    - Colin Desrosiers (2010-2011)
    - Larry Gersz (Tulane undergrad, summer 2011)
    - David Toomey (2011)
    - Ta-chun "Eric" Kao (2011-2012)
    - Ahsum Khan (2011-2012)
    - Hanna Shebert (high school student, summer 2012)
    - Aaron Cravens (2012-2013, presented at National Conferences for Undergraduate Research in 2013)
    - Poojah Suresh (2013-2015, presented poster at Biophysical Society in 2015)
    - Nicholas Yeager (2014)
    - Kimberly Bogardus (summer 2013, Goldwater Fellowship winner from Hamilton College)
    - Christopher Langfield (2016-2017)
    - Anthony Pane (2017-2019)
    - Brian Fan (2018-2019)
    - Shivali Singh (2018)
    - Natalie Ramesh (2020-2021)
    - Marlen Toktomamatov (2020-2022)
    - Teddy Miller (2022-)

Funding

- Current
    - NIH R21GM138970, "Developing computational methods to determine the thermodynamics of lipid phase coexistence", 8/2020-7/2022, sole PI, 35% effort, ~$122,000 ADC
    - NIH U01DA051373, "Optimization of novel thioesters as a therapeutic strategy for combatting opioid overdoses and abuse", 9/2020-8/2023, subcontract-PI (PI:Dr. Stephen Lewis, Case Western Reserve University), 20% effort, ~$58,000 ADC
    - NIH R01NS117968, "Exploiting new fibril structures to understand the biophysical basis for oligomerization and toxicity of alpha-synuclein", subcontract-PI (PI:Dr. Jonathan Sachs, University of Minnesota), 9/2020-8/2024, 20% effort, ~$63,000 ADC
- Concluded awards
    - DOE R1039934, "Photosynthesis protein collective vibrations role in energy transfer and dissipation", 8/2018-7/2021, co-investigator (PI: Dr. Andrea Markelz, University at Buffalo), 5% effort, ~$27,000 ADC
    - NSF MCB 1817862, "Light-induced protein quake of visual rhodopsin investigated by femtosecond time-resolved X-ray scattering", 3/2018-9/2021, co-

investigator (PI: Dr. Michael Brown, University of Arizona), 5% effort, ~$25,000 ADC

- NIH GM095496, "Multiscale modeling of GPCRs", 2011-2016, sole PI, $170,000/year direct costs, 50% salary support
- NIH T32 GM068411 student support
  - Joshua Horn (2011)
  - Nicholas Leioatts (2012)
  - Emily Robinson (2022)
- NIH National Research Service Award (1 F32 NS42975) 2001-2004**,** postdoctoral fellowship (Grossfield)

Consulting

- Moderna Therapeutics, 12/2020-present

Awards and Service

- Graduate Student Society Mentoring Award, 2019 (Med School wide)
- Outstanding Graduate Student Teacher Award, 2013 (Med School wide)
- Teaching Award in Biophysics, 2008, 2009, 2013, 2014, 2016, 2017, 2018, 2020, 2022
- Study sections and grant review
  - DOE Early Career Research Program, 11/2009
  - ACS Petroleum Research Fund, 9/2012
  - Ad-hoc, NIH BCMB-W study section, 6/2014
  - Netherlands Organization for Scientific Research, 6/2015
  - Ad-hoc, NIH BPNS study section, 7/2015
  - Wellcome Trust/DBT India Alliance. 7/2015
  - DOE 7/2017
  - Ad-hoc, NIH BCMB study section, 1/2018
  - NSF CTMC study section, 1/2018
  - National Academies Committee- Molecular Dynamics (Anton), 6/2018
  - Ad-hoc, NIH BBM study section, 1/2019
  - NSF Molecular Biophysics CAREER panel, 9/2019
  - Ad-hoc, NIH BCMB study section, 3/2020
  - Ad-hoc, NIH AUD study section, 2/2021, 5/2022
- Editorial boards
  - Biophysical Journal, 2018-
  - Chemistry and Physics of Lipids, 2018-2020
  - Proteins:Structure, Function and Bioinformatics, acting editor, 2017-2020
  - Invited guest editor for special issue of Chemistry and Physics of Lipids, 2013
- Annual Presentation skills workshop
  - Created and ran workshop to train students to give better scientific talks

  - 10-20 students attend each year
  - Runs 1 day each summer, 2017- present
- Student committees (incomplete)
  - Dilnoza Amirkulova (Chemical Engineering, Andrew White)
  - Paul Black (Biophysics, William Bernhard)
  - Chapin Cavender (Biophysics, David Mathews)
  - Dhrubo Jyoti Basu Roy (Biophysics, Benjamin Miller)
  - Stanislav Bellaousov (Chemistry, David Mathews)
  - Laura DiChiacchio (Biophysics, David Mathews)
  - Rozzy Finn (Biochemistry, David Pearce)
  - Yinghan Fu (Biophysics, David Mathews)
  - Keedakkatt Puth, Anees Mohammed (Chemistry, David Mathews)
  - Joohyun Lee (Chemistry, David McCammant)
  - Colleen Maillie (undergrad Biology, Anne Meyer)
  - Sayan Mondal (Biophysics, Cornell-Weill Medical College, Harel Weinstein)
  - Mukta Palshikar (Biophysics, Juilee Thakar)
  - Min Sun Park (Biophysics, Harry Stern)
  - Evan Ranken (Physics)
  - Brendaliz Santiago (Microbiology and Immunology, Robert Quivey)
  - James Seuch (Biophysics, David Mathews)
  - Mallory Scott (Biophysics, Paul Kammermeier)
  - Karl Smith (Biophysics, James McGrath)
  - Louis Smith (Biophysics, David Mathews)
  - Jason Tubbs (Chemistry, Doug Turner)
  - Keith VanNostrand (Biophysics, David Mathews)
  - Ethan Walker (Biochemistry, Sina Ghaemmaghami)
  - Zhenjiang Xu (Biophysics, David Mathews)
- Program in Biophysics, Structural and Computational Biology
  - Steering Committee, 2008-
  - Education Director, Program in Biophysics, 2011-2012
  - Admissions Committee, Program in Biophysics, Structural and Computational Biology, 2008-present
  - Director of Admissions, Program in Biophysics, Structural and Computational Biology, 2012-present
  - BSCB retreat organizer: 2010, 2011, 2017, 2019
- University of Rochester Health Sciences Center for Computational Innovation, Research Advisory Roundtable, 2009-2011
- University of Rochester Medical Center Faculty Council, 2009-2015
- Dean's Committee on Graduate Admissions, 2012
- Graduate Education Strategy Workgroup, 2012
- Steering Committee for Ethics Training, 2011-
- Pittsford Schools Summer Internship Program, 2010, 2012
- Referee for Proteins, Biophysical Journal, BBA Biomembranes, Structure, J. Phys. Chem. B, J. of Mol. Biol., J. Mol. Graphics Model., J. Comput. Chem., J. Chem. Phys., Biochemistry, J. Mem. Biol., PLOS, J. Amer. Chem. Soc., J. Med. Chem.,

PNAS, Nature Chemistry, J. Chem. Theor. Comput., J. Chem Inf. Model.

Invited Seminars since Fall 2007

- 2022
  - Tinker Developers Conference (6/2022)
  - Sante Fe Meeting on Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment
- 2021
  - University of Pittsburgh (virtual)
- 2020
  - University of Southampton, UK (virtual)
  - Biological Physics symposium (virtual)
  - CECAM Workshop on simulation of GPCRS (postponed due to COVID)
  - MolSSI Workshop on Rare Event Sampling (postponed due to COVID)
  - Tinker Developers Conference (postponed due to COVID)
- 2019
  - ACS Spring National Meeting
  - ACS Fall National Meeting
  - MolSSI Workshop on Interoperability in Molecular Simulation
  - SUNY Oswego
  - Sante Fe Meeting on Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment
  - University of Illinois
  - Virginia Tech
- 2018
  - University of Guelph (Ontario, CA)
- 2017
  - ACS Spring National Meeting
  - SUNY Brockport
  - FASEB TWS Program Directors' Meeting
  - Illinois Institute of Technology
  - MolSSI Workshop on Best Practices in Molecular Simulation
  - Sante Fe Meeting on Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment
  - University of Pennsylvania
- 2016
  - University of Akron
  - SUNY Geneseo
  - University of Vermont
  - University of Maryland
- 2015
  - SUNY Buffalo, Dept. of Physics
  - CUNY Workshop on GPCRs
  - Rochester Institute of Technology
  - Telluride Meeting on Biological Membranes and Membrane Proteins: Challenges

for Theory and Experiment

- 2014
  - Gordon Conference on Computational Chemistry (also spoke at Gordon Research Symposium)
  - Gibbs Conference on Biothermodynamics
  - Houghton College
  - McMaster University (Ontario, CA)
- 2013
  - University of Illinois Urbana-Champaign, Biophysics Symposium
  - University of West Virginia, Dept. of Chemistry
  - Ursinus College, Dept. of Chemistry
  - Wells College, Dept. of Chemistry
  - Telluride Conference on Membrane Protein Folding and Function
  - Delaware Membrane Protein Symposium
  - Rochester Institute of Technology, Dept. of Physics
  - Biophysical Society National Meeting, Subgroup Meeting on Membrane Structure
  - University of Chicago James Franck Institute
  - University of North Carolina-Wilmington, Dept. of Chemistry
  - University of Pittsburgh, Dept. of Computational and Systems Biology
- 2012
  - University of Toronto/Sick Kid's Hospital
  - Cornell University Biophysics Colloquium
  - American Chemical Society National Meeting
  - Arizona State Membrane Biophysics Conference
  - Membrane Protein Biophysics FASEB Meeting (Snowmass)
- 2011
  - American Chemical Society National Meeting
  - University of Southern Florida, Dept. of Physics
  - Cornell University, Dept. of Chemical Engineering
- 2010
  - SUNY Potsdam, Dept. of Physics
  - Allegheny College, Dept. of Physics
  - Wells College, Dept. of Physics
  - University of Texas-Austin, Dept. of Biomedical Engineering
- 2009
  - Cornell University Biophysics Colloquium
  - 31st IEEE-Engineering in Medicine and Biology Conference, Minneapolis, Minnesota
  - Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment", Telluride, CO
  - University of Minnesota, Dept. of Chemistry
  - SUNY Binghamton Dept. of Physics
- 2008
  - Cornell High Energy Synchrotron Center

- Rochester Institute of Technology
- Session Chair, Computational Chemistry Gordon Research Conference
- "Fukuoka Symposium on Molecular Soft Interactions at the Biomembrane Interface", Kyushu University, Fukuoka, Japan
- University of Western Ontario, Dept. of Physics

- 2007
  - "Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment", Park City, Utah

Publicly Distributed Software

- LOOS, a C++ library for rapidly implementing new molecular simulation analysis techniques, cited >140 times, https://github.com/GrossfieldLab/loos
- WHAM, a commonly used implementation of the weighted histogram analysis method for analyzing umbrella sampling free energy calculations, cited > 700 times, http://membrane.urmc.rochester.edu/content/wham
- Contributor to simulation packages Tinker, WESTPA, and OpenMM

Professional Societies

- Biophysical Society: 1996-
- American Association for the Advancement of Science: 2002-
- American Chemical Society, 2014-

Publications: H-index = 35 (Google Scholar)

https://scholar.google.com/citations?user=VZI-Aj8AAAAJ&hl=en
https://orcid.org/0000-0002-5877-2789
https://www.ncbi.nlm.nih.gov/myncbi/1zSCqhw7ZCn5Y/bibliography/public/

1. Sur S., and Grossfield A., Effects of cholesterol on the mechanism of fengycin, a biofungicide, Biophys. J., 2022, 121, 1963-1974
2. Onukwufor J.O., et al, Grossfield A., Wojtovich, A. P., **A reversible mitochondrial complex I thiol switch mediates hypoxic avoidance behavior in C. elegans,** Nat. Comm., 2022, 13, 2403
3. Seckler J. M., Grossfield A., May W. J., Getsy P. M., Lewis S. J., **Nitrosyl factors play a vital role in the ventilatory depressant effects of fentanyl in unanesthetized rats**, Biomed. Pharmacother., 2022, 146, 112571
4. Grossfield, A., **How to be a good member of a scientific software community [Article v1.0]**, Liv. J. Comput. Mol. Sci., 2022, 3
5. Gaston, B., Baby, S., May, W., Young, A., Grossfield, A., Bates, J., Seckler, J., Wilson, C., and Lewis, S., **D-Cystine di(m)ethyl ester reverses the deleterious effects of morphine on ventilation and arterial blood gas chemistry while promoting analgesia**, Sci. Rep., 2021, 11, 10038
6. Romo, T. D., Grossfield, A., and Markelz, A. G., **Persistent protein motions in a rugged energy landscape revealed by normal mode ensemble analysis**, J. Chem. Inf. Model., 2020, 60, 6419-6426

7. Maji, D., Grossfield, A., and Kielkopf, C. L, **Structures of SF3b1 reveal a dynamic Achilles heel of spliceosome assembly: Implications for cancer-associated abnormalities and drug discovery,** BBA Gene Regulatory Mechanisms, 2019, 1862, 194440
8. Smith, L. G., Tan, Z., Spasic, A., Dutta, D., Salas-Estrada, L. A., Grossfield, A., and Mathews, D. H., **Chemically accurate relative folding stability of RNA hairpins from molecular simulations**, J. Chem. Theor. Comput**.**, 2018, 14, 6598-6612
9. Grossfield, A., Patrone, P. N., Roe, D. R., Schultz, A. J., Siderius, D. W., and Zuckerman, D. M., **Best practices for quantification of uncertainty and sampling quality in molecular simulations**, Living Journal of Computational Molecular Science, 2018, 1, 1-24
10. Sur, S., Romo, T. D., and Grossfield, A., **Selectivity and mechanism of fengycin, an antimicrobial lipopeptide, from molecular dynamics**, J. Phys. Chem. B, 2018, 122, 2219-2226
11. Salas-Estrada, L. A., Leioatts, N., Romo, T. D., and Grossfield, A., "**Lipids Alter Rhodopsin Function via Ligand-like and Solvent-like Interactions,** Biophys. J., 2018, 114, 355-367
12. Thompson, J. L., Zhao, Y., Stathopulos, P. B., Grossfield, A., and Shuttleworth, T. J., **Phosphorylation-mediated structural changes within the SOAR domain of STIM1 enable specific activation of distinct Orai channels**, J. Biol. Chem., 2018, 293, 3145-31552018
13. Romo, T. D., Lewis, A. K., Braun, A. B., Grossfield, A., and Sachs, J. N., **Minimal nucleation state of α-synuclein is stabilized by dynamic threonine-water networks**, ACS Chemical Neuroscience, 2017, DOI: 10.1021/acschemneuro.7b00171
14. Aytenfisu, A. H., Spasic, A., Grossfield, A., Stern, H. A., Mathews, D. H., **Revised RNA dihedral parameters for the Amber force field improve RNA molecular dynamics**, J. Chem. Theor. Comput., 13, 2017, 900-915
15. Lin, D., **Generalized and efficient algorithm for computing multipole energies and gradients based on Cartesian tensors**, J. Chem. Phys., 2015, 143, 114115
16. Lin, D. and Grossfield, A., **Thermodynamics of micelle formation and membrane fusion modulate antimicrobial lipopeptide activity**, Biophys. J., 2015, 108, 750-759
17. Leioatts, N., Romo, T. D., Danial, S. A., and Grossfield, A., **Retinal conformation changes rhodopsin's dynamic ensemble**, Biophys. J., 2015, 109, 608-617
18. Romo, T. D., Leioatts, N. and Grossfield, A., **Lightweight object-oriented structure analysis: Tools for building tools to analyze molecular dynamics simulations**, J. Comput. Chem., 2014, 35, 2305-2318
19. Lin, D., and Grossfield, A., **Thermodynamics of antimicrobial lipopeptide binding to membranes: Origins of affinity and selectivity**, Biophys. J., 2014, 107, 1862-1872
20. Leioatts, N., Suresh, P., Romo, T. D., and Grossfield A., **Structure-based simulations reveal concerted dynamics of GPCR activation**, Proteins: Struc. Func. Bioinf., 2014
21. Romo, T. D. and Grossfield, A., **How fast is your camera? Timescales for molecular motion and their role in restraining molecular dynamics**, Biophysical Journal, 2014, 106, 2549-2551
22. Romo, T. D. and Grossfield, A., **Unknown Unknowns: the Challenge of Systematic and Statistical Error in Molecular Dynamics Simulations**, Biophysical Journal**,** 2014, 106, 1553-1554, PMC4008789

23. Horn, J. N., Kao, T.-C., and Grossfield, A., **Coarse-grained molecular dynamics provides insight into the interactions of lipids and cholesterol with rhodopsin**, in Computational Approaches to G Protein-Coupled Receptor Modeling and Simulation in Support of Rational Drug Discovery, ed. Marta Filizola, *Adv. Exp. Med. Biol.*, 2014, 796:75–94, PMC40344522
24. Leioatts, N., and Grossfield, A. **Molecular dynamics simulations of membranes and membrane proteins**, in Molecular modeling at the atomic scale - Methods and applications in quantitative biology, ed. Ruhong Zhou, Taylor and Francis, 2014
25. Leioatts, N., Mertz, B., Martínez-Mayorga, K., Romo, T. D., Pitman, M. C., Feller, S. E., Grossfield, A., and Brown, M. F., **Retinal ligand mobility explains internal hydration and reconciles active rhodopsin structures**, Biochemistry, 2013, 53, 376-385, PMC4096112
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27. Horn, J. N., Cravens, A., and Grossfield A., **Interactions between fengycin and model bilayers quantified by coarse-grained molecular dynamics**, Biophysical Journal, 2013, 105, 1612-1623
28. Horn, J. N., and Grossfield, A., **Simulating the mechanism of antimicrobial lipopeptides with all-atom molecular dynamics**, Biochemistry, 2013, 52, 5604-5610
29. Leioatts, N., and Grossfield, A. **Molecular dynamics simulations of membranes and membrane proteins**, in Molecular modeling at the atomic scale - Methods and applications in quantitative biology, ed. Ruhong Zhou, Taylor and Francis, to be published in 2013
30. Seckler, J. M., Leioatts, N., Miao, H., and Grossfield, A. **The interplay of structure and dynamics in the function of HIV-1 reverse transcriptase**, Proteins: Struc. Func. Bioinf., 2013, 81, 1792-1801
31. Horn, J. N., Kao, T.-C., and Grossfield, A., **Coarse-grained molecular dynamics provides insight into the interactions of lipids and cholesterol with rhodopsin**, in Computational Approaches to G Protein-Coupled Receptor Modeling and Simulation in Support of Rational Drug Discovery, ed. Marta Filizola, Springer, *Adv. Exp. Med. Biol.*, 2014, 796:75–94
32. Leioatts, N., Romo, T. D., and Grossfield, A., **Elastic Network Models are Robust to Variations in Formalism**, J. Chem. Theor. Comput., 2012, 8, 2424-2434, NIHMS383307
33. Olausson, B., Grossfield, A., Pitman, M., Brown, M., Feller, S., Vogel, A., **Molecular dynamics simulations reveal specific interactions of post-translational palmitoyl modifications with rhodopsin in membranes**, J. Am. Chem. Soc., 2012, 134, 4234-4331
34. Horn, J. N., Sengillo, J. D., Lin, D., Romo, T. D., and Grossfield, A., **Characterization of a potent antimicrobial lipopeptide via coarse-grained molecular dynamics**, Biochim. Biophys. Acta, 2012, 1818, 212-218
35. Romo, T. D., and Grossfield, A. **Block covariance overlap method and convergence in molecular dynamics simulation**, J. Chem. Theor. Comput., 2011, 7, 2464-2472
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37. Grossfield, A., **Recent progress in the study of G protein-coupled receptors with molecular dynamics computer simulations**, Biochim. Biophys. Acta, 2011, 1808, 1868-1878
38. Romo, T. D. and Grossfield, A., **Validating and enhancing elastic network models using molecular dynamics simulations**, Proteins, 2011, 79, 23-34
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C., and Reggio, P. H., **A lipid pathway for ligand binding is necessary for a cannabinoid G protein-coupled receptor**, J. Biol. Chem., 2010, 285, 17954-17964, PMID: 20220143
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41. Grossfield, A., and Zuckerman, D. M. **Quantifying uncertainty and sampling quality in biomolecular simulations,** Annual Reports in Computational Chemistry, 2009, 5, 23-48, NIHMS155855
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43. Romo, T. D., Grossfield, A., **LOOS: an extensible platform for the structural analysis of simulations**, Proceedings of 31st IEEE-Engineering in Medicine and Biology Conference, 2009, 2332-2335
44. Grossfield, A. **Implicit modeling of membranes**, in "Computational Modeling of Membranes", ed Scott Feller, Current Topics in Membranes 2008, 60, 131-157
45. Grossfield, A., Pitman, M. C., Feller, S. E., Soubias, O., and Gawrisch, K. **Internal Hydration Increases during Activation of the G-Protein-Coupled Receptor Rhodopsin**, J. Mol. Biol. 2008, 381, 478-486
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47. O'Neil, L. L., Grossfield, A., Wiest, O. **Computational Investigation of the Base Flipping of the Thymine Dimer in Duplex DNA**, J. Phys. Chem. B, 2007, 111, 11843-11849
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52. Grossfield, A., Feller, S. E., Pitman, M. C., **A role for direct interactions in the modulation of rhodopsin by omega-3 polyunsaturated lipids**, Proc. Nat. Acad. Sci. USA, 2006, 103, 4888-4893
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55. Fitch, B. G., Rayshubskiy, A., Eleftheriou, M, Ward, T.J.C., Giampapa, M., Zhestkov, Y., Pitman, M. C., Suits, F., Grossfield, A., Pitera, J., Swope, W., Zhou, R., Feller, S., and

Germain. R. S., **Blue Matter: Strong scaling of molecular dynamics on Blue Gene/L**. Research Report RC23688, IBM Research Division, 2005.
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