RICHARD E. GILLILAN

Cornell High Energy Synchrotron Source 200L Wilson Lab Ithaca, NY 14853

Work phone: (607)255-7163

email: reg8@cornell.edu

Citations 3604 h-index 28 i10-index 54. (Google Scholar 6/14/2024)

Education

Ph.D. in Chemistry, University of Pennsylvania 1988 Advisor: William P. Reinhardt

B.A. in Chemistry (Honors) and Mathematics 1983 University of Maryland, Baltimore County

Positions

Visiting Scientist Cornell High-Energy Synchrotron Source, Cornell 2024-present

Beamline Scientist (Senior Research Associate-II), Cornell High-Energy Synchrotron Source, Cornell 2000-2024

Visualization Specialist/Research Scientist/Sr Tech Advisor 1992-2000 Cornell Theory Center (CTC), Cornell University, Ithaca NY

Postgraduate Research Chemist for Kent R. Wilson 1990-1992 Department of Chemistry, University of California, San Diego

Postdoctoral Research Associate for Gregory S. Ezra 1988-1990 Department of Chemistry, Cornell University

Awards, Professional Activities (recent)

Fellow of the American Crystallographic Association (elected 2021)

DOE Beamline Review Panel (APS) Nov 2022 DOE BER (ALS) Renewal Review Panel Apr 2022 NSF (CHRNS) Renewal Review Panel, March 2020 NIH (APS) P41 Scientific Advisory Committee 2019, **Chair** 2020-2022 DOE BER (ALS) Renewal Review Panel Nov 2018 DOE (APS) Scientific Advisory Committee Beamline Review April 2018 NIH (APS) P41 Review Panel July 2015 NCNR Future Directions August 2014

Thesis Committee for Robert Miller Cornell Department of Chemistry 2022

External Examiner, Dissertation Committee for Thomas Grant SUNY Buffalo/HWI Jan 2013

Proposal Evaluator, Vinnova (Sweden's Innovation Agency), industrial beamtime proposals, appointed 2019

Chair, Small Angle Scattering Scientific Interest Group, American Crystallographic Association, elected 2012

CHESS User Mtg. Poster: "High-Throughput BioSAXS: disposable tip pipetting and quick-change capillary flow cells" S. Neilsen, M. Moller, R. Gillilan (1st Prize, Best Technical Achievement) 2011

Chair, Oxford Cryosystems Poster Prize Committee American Crystallographic Association 2008

Chair, Synchrotron Scientific Interest Group, American Crystallographic Association, elected 2006

Postdoctoral researchers supervised:

Durgesh Rai Jesse Hopkins Alvin Acerbo Soren Skou

Press Releases (recent):

Physics Magazine Viewpoint 2024 Placing a Full Protein Library Under Pressure; https://physics.aps.org/articles/v17/132

Pysics.org (JHU): With AI, extreme microbe reveals how life's building blocks adapt to high pressure; https://phys.org/news/2024-09-ai-extreme-microbe-reveals-life.html

Physics Today: Deep-sea comb jellies' cells are primed to withstand
pressure July 10, 2024
(https://pubs.aip.org/physicstoday/online/43489/Deep-sea-comb-jelliescells-are-primed-to)

ScienceDaily "Researcher uses pressure to understand RNA dynamics"
https://www.sciencedaily.com/releases/2023/06/230622182820.htm
June 22, 2023

Cornell Chronicle: Wild blue wonder: X-ray beam explores food color protein **Dec 2, 2021** (news.cornell.edu/stories/2021/12/wild-blue-wonder-x-ray-beam-explores-food-color-protein)

AIP/ACA: X-Ray Scattering Facility for Extreme Biology Opens for Research July 28, 2020 (www.newswise.com/articles/x-ray-scattering-facility-for extreme-biology-opens-for-research)

AIP/ACA: High-Pressure Biology Seeks Answers to Early Life Beginnings, July 18, 2019 (www.newswise.com/articles/high-pressure-biology-seeksanswers-to-early-life-beginnings)

Workshops/Conferences Organized

"High Pressure Structural Biology and Extreme Biophysics Workshop", Cornell University, (with C. Royer, S. Gruner, N. Ando) **April 7-10, 2022**

"Biology Under Extreme Conditions: 2030 and Beyond", CHESS Jul 15-16, 2021

"High Pressure Biology with hands-on data collection", CHESS April 2021

ACA WK.01: Applications of Small Angle Scattering to Structural Biology: An Introduction (co-organized with J. Hopkins and K. Gupta) Online **Jul 2020**

ACA WK.04 "Applications of Small Angle Scattering to Structural Biology: An Introduction" (co-organized with K. Gupta, J. Hopkins ...)**Jul 2018**

International Small Angle Scattering Meeting (SAS2018) "BioSAS: Advanced Applications" course (Co-organized with J. Hopkins, E. Brooks et al) Oct 2018

"BioSAXS Essentials" training workshops (annual), Wilson Lab, Cornell March 2011, May 2011, Feb 2012, March 2013, Oct 2014, May 2017, Apr 2018

ACA WK.04: Small Angle Scattering: Structural Biology and Soft Matter, Philadelphia, PA, July 2015

ACA WK.01 Biological Small Angle Solution Scattering: Theory & Practice National-level training workshop held in conjunction with the annual ACA meeting, Honolulu, HI, **July 2013**

Professional Meeting Sessions Organized/Chaired (recent)

ACA Session "Phase Separation and Aggregation of Biomolecular Systems and Intrinsically Disordered Proteins", co-organized with Y. Liu (Aug 2, 2022)

Co-organized/ran ACA Session-1-1-1 "Macromolecular Structure Under Physiological Conditions" (July 21, 2019)

BioMolecules Under Pressure (co-organized with Rai and Gruner), Cornell (June July 2019)

ACA Transactions Symposium: Neutron & Synchrotron Sources: Crystallography Session I - Small Angle Scattering (July 2013)

ACA 13.14: Microcrystal Session **chair** (ACA 13.14, June 5, 2008) (selected speakers, ran meeting, managed funds, wrote meeting report)

"Frontier Applications of X-ray Science in Biology: The Energy Recovery Linac X-ray Source" (Summer ERL meeting series, Cornell) June 2006

Invited Lectures (recent)

"Structural change under pressure across the whole proteome: Lessons from scattering and limited proteolysis" Neutrons and Food 7, University of Delaware, Newark, DE June 11, 2024

"Introduction to BioSAS", Binghamton University BCHM508, February 26, 2024

"High-pressure limited proteolysis uncovers widespread and functionally important conformational dynamics on the whole proteome scale" Plots and Scotch - CMU Biophysics Seminar Series, January 25, 2024 "High-pressure limited proteolysis uncovers widespread and functionally important conformational dynamics on the whole proteome scale" Cornell Biophysics Colloquium (Cornell) Nov 29, 2023

"Hiding in the crowd: how hydrostatic pressure reveals hidden states and sensitive structures" Pittsburgh Diffraction Conference (Wyndham University Center, Pittsburgh) Oct 17, 2023

"Biological X-ray Scattering Under Intense Pressure: A Quick HOW-TO", High Pressure MX Workshop 2023 (CHESS, Cornell) Jun 10,2023.

"SAXS Overview", Everything BioSAXS 9 (Advanced Photon Source) Feb 2023

"The Scattering Profile" $13^{\rm th}$ Annual SIBYLS BioSAXS Workshop, Advanced Light Source, Berkeley Aug 2022

Advanced Photon Source/Angonne National Lab, Everything BioSAXS 8: "SAXS Overview" 3/2022

"BioSAXS/HP-Bio: from biomolecules to extreme biophysics and beyond", Small-angle Scattering Seminar Series (SAXS-SIG, Advanced Photon Source) Jan 2022

"High Pressure Cold Dissociation of a Protein Complex Characterized by Chromatography-Coupled X-ray Scattering",10th Asian Conference on High Pressure Research (S. Korea, virtual) Nov 2021

SUNY UpState Medical University course B666 (Protein Structure): 2012, 2016, 2018, 2020, 2022 (alt years)

Advanced Photon Source/Angonne National Lab, Everything BioSAXS 7: "SAXS Overview" 3/2021

Cornell University Chem 7889 (Ando) Fall 2023

Binghamton University Chem 583P-01(Structural Biology) Fall 2020, Fall 2022 BCHM403 (S. Solmaz Biochemistry Class), Spring 2021, Spring 2023 BCHM403 (L. Musselman Biochemistry Class), Fall 2021

"BioSAXS Essentials", Methods in Biophysics class, RPI, Troy NY Nov. 2018

"BioSAXS Essentials", CHM 515 Princeton University Oct 2015

"Une introduction pratique à BioSAXS : acquisition de données et d'analyse", Départment de Biochimie, Université de Montréal, Canada, Jan 16-17m 2013

"Amazing things behind the beamstop: what small-angle x-ray scattering tells us about proteins in solution", University of Alabama, Birmingham, May 16-18, 2012

SUNY UpState Medical University Lecture/lab session for Course GS 632, Dec 2011 Cornell Biophysics Colloquium, "Shapes from solutions: high-throughput x-ray solution scattering for molecule biology". Sept. 2010

Cornell Biophysics Colloquium, "New Opportunities for Structural Biology with Cornell's Energy Recovery Linac" Apr. 2006

NY Structural Biology Group, "New Opportunities for Structural Biology with Cornell's Energy Recovery Linac" 1/24/06 Manhattan

Recent Contributed Lectures

"A Structural Proteomic Survey of *Thermus thermophilus Under Deep Ocean Pressure"*, Astrobiology Science Conference (AbSciCon 2024), Providence, RI May 6, 2024

"Biological X-ray scattering under intense pressure: what we can learn", 2023 Extreme Biophysics and Biology Conference (Scripps Institute of Oceanography, San Diego) April 29, 2023

"Biological X-ray scattering under intense pressure: what we can learn", 2023 Extreme Biophysics and Biology Conference, April 28-May1, 2023

"Solution Scattering and High Pressure Biology" in Mapping Free Energy Landscape of Molecular Machines ACA session 1.1.2, July 2021

"HP-Bio: High Pressure BioSAXS for Deep Life and Extreme Biophysics" in Frontiers in SAS ACA session July 2020

"Structural Biology in the Abyss: SEC-SAXS at Deep Ocean Pressures" in Crystallography at Extreme Conditions ACA session 1.2.2, July 2019

"MacCHESS: The Macromolecular Diffraction Facility at the Cornell High-Energy Synchrotron Source" (July 2010 Chicago)

MacCHESS Workshop (June 10, 2009) "Young Again at 70: SAXS and Biology in the $21^{\rm st}$ Century"

American Crystallographic Association (ACA Knoxville TN, 2008) "The State of Microcrystallography" (Microcrystal session) R. E. Gillilan

Microscopy and Microanalysis 2008 (Albuquerque, NM, Aug 2008) "Using Molecular Envelope Information Derived from SAXS and EM for Crystallographic Phasing" Quan Hao, Xinguo Hong, and Qun Liu (presented by Richard Gillilan)

American Crystallographic Association (Salt Lake City, 2007) "Microcrystals and Microbeams at MacCHESS" R. E. Gillilan, M. J. Cook, S. Cornaby, Detlef Smilgies, T..A. Szebenyi and D. H. Bilderback

Pittsburgh Diffraction Conference (Buffalo, 10/25/07-10/27/07) "How to Get Diffraction from Almost Nothing: Microcrystals and Microbeams at MacCHESS", R. E. Gillilan, M. J. Cook, S. Cornaby, Detlef Smilgies, T..A. Szebenyi and D. H. Bilderback

Current Peer review activities

Astrobiology, Molecular Pharmacology (ACS), Journal of Synchrotron Radiation, Journal of Applied Crystallography, Protein Science, Biophysical Reviews, IUCr Journal, Journal of Molecular Biology, Biopolymers, X-Ray Optics and Instrumentation, ACTA D

Peer-reviewed publications

1. Yuan G, Salipante PF, Hudson SD, Gillilan RE, Huang Q, Hatch HW, Shen VK, Grishaev AV, Pabit S, Upadhya R, et al. (2024) Flow Activation Energy of High-Concentration Monoclonal Antibody Solutions and Protein-Protein Interactions Influenced by NaCl and Sucrose. Mol. Pharmaceutics [Internet]. Available from: https://doi.org/10.1021/acs.molpharmaceut.4c00460

2. Winnikoff JR, Milshteyn D, Vargas-Urbano SJ, Pedraza-Joya MA, Armando AM, Quehenberger O, Sodt A, Gillilan RE, Dennis EA, Lyman E, et al. (2024) Homeocurvature adaptation of phospholipids to pressure in deep-sea invertebrates. Science 384:1482-1488.

3. Moran HM, Manriquez-Sandoval E, Sharma P, Fried SD, Gillilan RE (2024) Proteome-Wide Assessment of Protein Structural Perturbations under High Pressure. PRX Life 2:033011.

4. Ko Y-H, Lokareddy RK, Doll SG, Yeggoni DP, Girdhar A, Mawn I, Klim JR, Rizvi NF, Meyers R, Gillilan RE, et al. (2024) Single Acetylation-mimetic Mutation in TDP-43 Nuclear Localization Signal Disrupts Importin $\alpha 1/\beta$ Signaling. Journal of Molecular Biology 436:168751.

5. Zhang M, Liu Y, Zuo X, Qian S, Pingali SV, Gillilan RE, Huang Q, Zhang D (2023) pH-Dependent Solution Micellar Structure of Amphoteric Polypeptoid Block Copolymers with Positionally Controlled Ionizable Sites. Biomacromolecules 24:3700-3715.

6. Wang J, Koduru T, Harish B, McCallum SA, Larsen KP, Patel KS, Peters EV, Gillilan RE, Puglisi EV, Puglisi JD, et al. (2023) Pressure pushes tRNALys3 into excited conformational states. Proceedings of the National Academy of Sciences 120:e2215556120.

7. Li Y, Li Q, Gillilan RE, Abbaspourrad A (2023) Reversible disassemblyreassembly of C-phycocyanin in pressurization-depressurization cycles of high hydrostatic pressure. International Journal of Biological Macromolecules 253:127623.

8. Illava G, Gillilan R, Ando N (2023) Development of in-line anoxic small-angle X-ray scattering and structural characterization of an oxygen-sensing transcriptional regulator. J Biol Chem:105039.

9. Ford RR, Gilbert PH, Gillilan R, Huang Q, Donnelly R, Qian KK, Allen DP, Wagner NJ, Liu Y (2023) Micelle Formation and Phase Separation of Poloxamer 188 and Preservative Molecules in Aqueous Solutions Studied by Small Angle X-ray Scattering. Journal of Pharmaceutical Sciences 112:731-739.

10. Chowdhury AA, Manohar N, Lanzaro A, Kimball WD, Witek MA, Woldeyes MA, Majumdar R, Qian KK, Xu S, Gillilan RE, et al. (2023) Characterizing Protein-Protein Interactions and Viscosity of a Monoclonal Antibody from Low to High Concentration Using Small-Angle X-ray Scattering and Molecular Dynamics Simulations. Mol. Pharmaceutics [Internet]. Available from: https://doi.org/10.1021/acs.molpharmaceut.3c00484

11. Biswas S, Hecht AL, Noble SA, Huang Q, Gillilan RE, Xu AY (2023) Understanding the Impacts of Molecular and Macromolecular Crowding Agents on Protein-Polymer Complex Coacervates. Biomacromolecules [Internet]. Available from: https://doi.org/10.1021/acs.biomac.3c00545

12. Zovo K, Pupart H, Van Wieren A, Gillilan RE, Huang Q, Majumdar S, Lukk T (2022) Substitution of the Methionine Axial Ligand of the Tl Copper for the Fungal-like Phenylalanine Ligand (M298F) Causes Local Structural Perturbations that Lead to Thermal Instability and Reduced Catalytic Efficiency of the Small Laccase from Streptomyces coelicolor A3(2). ACS Omega 7:6184-6194.

13. Zhang S, McCallum SA, Gillilan RE, Wang J, Royer CA (2022) High Pressure CPMG and CEST Reveal That Cavity Position Dictates Distinct Dynamic Disorder in the PP32 Repeat Protein. J. Phys. Chem. B [Internet]. Available from: https://doi.org/10.1021/acs.jpcb.2c05498

14. Trewhella J, Vachette P, Bierma J, Blanchet C, Brookes E, Chakravarthy S, Chatzimagas L, Cleveland TE IV, Cowieson N, Crossett B, et al. (2022) A round-robin approach provides a detailed assessment of biomolecular small-angle scattering data reproducibility and yields consensus curves for benchmarking. Acta Crystallographica Section D [Internet] 78. Available from: https://doi.org/10.1107/S2059798322009184

15. Miller RC, Cummings C, Huang Q, Ando N, Gillilan RE (2022) Inline smallangle X-ray scattering-coupled chromatography under extreme hydrostatic pressure. Protein Science 31:e4489.

16. Lokareddy RK, Hou C-FD, Doll SG, Li F, Gillilan RE, Forti F, Horner DS, Briani F, Cingolani G (2022) Terminase Subunits from the Pseudomonas-Phage E217. Journal of Molecular Biology 434:167799.

17. Gillilan RE High-pressure SAXS, deep life, and extreme biophysics. In: Methods in Enzymology. Academic Press; 2022. Available from: https://www.sciencedirect.com/science/article/pii/S0076687922003500

18. Florio TJ, Lokareddy RK, Yeggoni DP, Sankhala RS, Ott CA, Gillilan RE, Cingolani G (2022) Differential recognition of canonical NF- κ B dimers by Importin α 3. Nature Communications 13:1207.

19. Doll SG, Meshkin H, Bryer AJ, Li F, Ko Y-H, Lokareddy RK, Gillilan RE, Gupta K, Perilla JR, Cingolani G (2022) Recognition of the TDP-43 nuclear localization signal by importin $\alpha 1/\beta$. Cell Reports 39:111007.

20. Allsopp R, Pavlova A, Cline T, Salyapongse AM, Gillilan RE, Di YP, Deslouches B, Klauda JB, Gumbart JC, Tristram-Nagle S (2022) Antimicrobial Peptide Mechanism Studied by Scattering-Guided Molecular Dynamics Simulation. J. Phys. Chem. B 126:6922-6935.

21. Rai DK, Gillilan RE, Huang Q, Miller R, Ting E, Lazarev A, Tate MW, Gruner SM (2021) High-pressure small-angle X-ray scattering cell for biological solutions and soft materials. Journal of Applied Crystallography 54:111-122.

22. Li Y, Gillilan R, Abbaspourrad A (2021) Tuning C-Phycocyanin Photoactivity via pH-Mediated Assembly-Disassembly. Biomacromolecules 22:5128-5138.

23. Harish B, Gillilan RE, Zou J, Wang J, Raleigh DP, Royer CA (2021) Protein unfolded states populated at high and ambient pressure are similarly compact. Biophysical Journal 120:2592-2598.
24. Ando N, Barquera B, Bartlett DH, Boyd E, Burnim AA, Byer AS, Colman D, Gillilan RE, Gruebele M, Makhatadze G, et al. (2021) The Molecular Basis for Life in Extreme Environments. Annu. Rev. Biophys. 50:343-372.

25. Niazi M, Florio TJ, Yang R, Lokareddy RK, Swanson NA, Gillilan RE, Cingolani G (2020) Biophysical analysis of Pseudomonas-phage PaP3 small terminase suggests a mechanism for sequence-specific DNA-binding by lateral interdigitation. Nucleic Acids Res 48:11721-11736.

26. Kumar S, Gillilan RE, Yernool DA (2020) Structure and function of the juxtamembrane GAF domain of potassium biosensor KdpD. Protein Sci 29:2009-2021.

27. Coombs SE, Banjade S, Kriksunov K, Clemente N, Zhao J, Wang C, Gillilan RE, Oswald RE (2020) In Vitro Effects of (+)MK-801 (dizocilpine) and Memantine on β -Amyloid Peptides Linked to Alzheimer's Disease. Biochemistry 59:4517-4522.

28. Florio TJ, Lokareddy RK, Gillilan RE, Cingolani G (2019) Molecular Architecture of the Inositol Phosphatase Siw14. Biochemistry 58:534-545.

29. Barteau KP, Ma K, Kohle FFE, Gardinier TC, Beaucage PA, Gillilan RE, Wiesner U (2019) Quantitative Measure of the Size Dispersity in Ultrasmall Fluorescent Organic-Inorganic Hybrid Core-Shell Silica Nanoparticles by Small-Angle X-ray Scattering. Chem. Mater. 31:643-657.

30. Wang C, Lin Y, Bougie D, Gillilan RE (2018) Predicting data quality in biological X-ray solution scattering. Acta Crystallographica Section D 74:727-738.

31. Jenkins KA, Fossat MJ, Zhang S, Rai DK, Klein S, Gillilan R, White Z, Gerlich G, McCallum SA, Winter R, et al. (2018) The consequences of cavity creation on the folding landscape of a repeat protein depend upon context. PNAS 115:E8153-E8161.

32. Alamo L, Pinto A, Sulbarán G, Mavárez J, Padrón R (2018) Lessons from a tarantula: new insights into myosin interacting-heads motif evolution and its implications on disease. Biophys Rev 10:1465-1477.

33. Sankhala RS, Lokareddy RK, Begum S, Pumroy RA, Gillilan RE, Cingolani G (2017) Three-dimensional context rather than NLS amino acid sequence determines importin α subtype specificity for RCC1. Nature Communications 8:979.

34. Hsieh C-L, Ptak CP, Tseng A, Suguiura IM de S, McDonough SP, Sritrakul T, Li T, Lin Y-P, Gillilan RE, Oswald RE, et al. (2017) Extended low-resolution structure of a Leptospira antigen offers high bactericidal antibody accessibility amenable to vaccine design Dötsch V, editor. eLife 6:e30051.

35. Hopkins JB, Gillilan RE, Skou S (2017) BioXTAS RAW: improvements to a free open-source program for small-angle X-ray scattering data reduction and analysis. Journal of Applied Crystallography 50:1545-1553.

36. Alamo L, Ware JS, Pinto A, Gillilan RE, Seidman JG, Seidman CE, Padrón R (2017) Effects of myosin variants on interacting-heads motif explain distinct hypertrophic and dilated cardiomyopathy phenotypes Robbins J, editor. eLife 6:e24634.

37. Schormann N, Zhukovskaya N, Bedwell G, Nuth M, Gillilan R, Prevelige PE, Ricciardi RP, Banerjee S, Chattopadhyay D (2016) Poxvirus uracil-DNA glycosylase-An unusual member of the family I uracil-DNA glycosylases. Protein Science 25:2113-2131.

38. Lukk T, Gillilan RE, Szebenyi DME, Zipfel WR (2016) A visible-light-excited fluorescence method for imaging protein crystals without added dyes. J Appl Crystallogr 49:234-240.

39. Alamo L, Qi D, Wriggers W, Pinto A, Zhu J, Bilbao A, Gillilan RE, Hu S, Padrón R (2016) Conserved Intramolecular Interactions Maintain Myosin Interacting-Heads Motifs Explaining Tarantula Muscle Super-Relaxed State Structural Basis. Journal of Molecular Biology 428:1142-1164.

40. Acerbo AS, Cook MJ, Gillilan RE (2015) Upgrade of MacCHESS facility for X-ray scattering of biological macromolecules in solution. J Synchrotron Radiat 22:180-186.

41. Skou S, Gillilan RE, Ando N (2014) Synchrotron-based small-angle X-ray scattering of proteins in solution. Nat Protoc Nat Protoc 9:1727-1739.

42. Skou M, Skou S, Jensen TG, Vestergaard B, Gillilan RE (2014) In situ microfluidic dialysis for biological small-angle X-ray scattering. J Appl Crystallogr 47:1355-1366.

43. Huang R, Szebenyi T, Pfeifer M, Woll A, Smilgies D-M, Finkelstein K, Dale D, Wang Y, J Vila-Comamala J, Gillilan R, et al. (2014) Application of CHESS single-bounce capillaries at synchrotron beamlines. Journal of Physics: Conference Series 493:012034.

44. Møller M, Nielsen SS, Ramachandran S, Li Y, Tria G, Streicher W, Petoukhov MV, Cerione RA, Gillilan RE, Vestergaard B (2013) Small angle X-ray scattering studies of mitochondrial glutaminase C reveal extended flexible regions, and link oligomeric state with enzyme activity. PLoS One 8:e74783.

45. Meisburger SP, Warkentin M, Chen H, Hopkins JB, Gillilan RE, Pollack L, Thorne RE (2013) Breaking the radiation damage limit with Cryo-SAXS. Biophys J 104:227-236.

46. Kim CU, Wierman JL, Gillilan R, Lima E, Gruner SM (2013) A high-pressure cryocooling method for protein crystals and biological samples with reduced background X-ray scatter. J Appl Crystallogr 46:234-241.

47. Gillilan RE, Kumar VSS, O'Neall-Hennessey E, Cohen C, Brown JH (2013) X-Ray Solution Scattering of Squid Heavy Meromyosin: Strengthening the Evidence for an Ancient Compact off State. PLOS ONE 8:e81994.

48. Gillilan R, Temnykh CM, Møller M, Nielsen S CHIPS AND ROBOTS: SCREENING, MIXING, AND DIALYSIS ON BIOSAXS BEAMLINES. In: Transactions of the ACA. Vol. 44. American Crystallographic Association; 2013. pp. 40-50.

49. Nielsen SS, Moller M, Gillilan RE (2012) High-throughput biological smallangle X-ray scattering with a robotically loaded capillary cell. Journal of Applied Crystallography 45:213-223. 50. Khan I, Gillilan R, Kriksunov I, Williams R, Zipfel WR, Englich U (2012) Confocal microscopy on the beamline: novel three-dimensional imaging and sample positioning. J Appl Crystallogr 45:936-943.

51. Yennawar H, Møller M, Gillilan R, Yennawar N (2011) X-ray crystal structure and small-angle X-ray scattering of sheep liver sorbitol dehydrogenase. Acta Crystallogr D Biol Crystallogr 67:440-446.

52. Koerner LJ, Gillilan RE, Green KS, Wang S, Gruner SM (2011) Small-angle solution scattering using the mixed-mode pixel array detector. J Synchrotron Radiat 18:148-156.

53. Gillilan RE, Cook MJ, Cornaby SW, Bilderback DH (2010) Microcrystallography using single-bounce monocapillary optics. J Synchrotron Radiat 17:227-236.

54. Cornaby S, Szebenyi DME, Smilgies D-M, Schuller DJ, Gillilan R, Hao Q, Bilderback DH (2010) Feasibility of one-shot-per-crystal structure determination using Laue diffraction. Acta Crystallogr D Biol Crystallogr 66:2-11.

55. Cherezov V, Höfer N, Szebenyi DME, Kolaj O, Wall JG, Gillilan R, Srinivasan V, Jaroniec CP, Caffrey M (2008) Insights into the mode of action of a putative zinc transporter CzrB in Thermus thermophilus. Structure 16:1378-1388.

56. Krasnoff SB, Keresztes I, Gillilan RE, Szebenyi DME, Donzelli BGG, Churchill ACL, Gibson DM (2007) Serinocyclins A and B, cyclic heptapeptides from Metarhizium anisopliae. J Nat Prod 70:1919-1924.

57. Höfer N, Kolaj O, Li H, Cherezov V, Gillilan R, Wall JG, Caffrey M (2007) Crystallization and preliminary X-ray diffraction analysis of a soluble domain of the putative zinc transporter CzrB from Thermus thermophilus. Acta Crystallogr Sect F Struct Biol Cryst Commun 63:673-677.

58. Gillilan RE, Ayers SD, Noy N (2007) Structural basis for activation of fatty acid-binding protein 4. J Mol Biol 372:1246-1260.

59. Bilderback DH, Kazimirov A, Gillilan R, Cornaby S, Woll A, Zha C, Huang R (2007) Optimizing Monocapillary Optics for Synchrotron X-ray Diffraction, Fluorescence Imaging, and Spectroscopy Applications. AIP Conference Proceedings 879:758-763.

60. Ayers SD, Nedrow KL, Gillilan RE, Noy N (2007) Continuous nucleocytoplasmic shuttling underlies transcriptional activation of PPARgamma by FABP4. Biochemistry 46:6744-6752.

61. Wedekind JE, Gillilan R, Janda A, Krucinska J, Salter JD, Bennett RP, Raina J, Smith HC (2006) Nanostructures of APOBEC3G support a hierarchical assembly model of high molecular mass ribonucleoprotein particles from dimeric subunits. J Biol Chem 281:38122-38126.

62. Kalinin Y, Kmetko J, Bartnik A, Stewart A, Gillilan R, Lobkovsky E, Thorne R (2005) A new sample mounting technique for room-temperature macromolecular crystallography. Journal of Applied Crystallography 38:333-339.

63. You L, Gillilan R, Huffaker TC (2004) Model for the yeast cofactor A-betatubulin complex based on computational docking and mutagensis. J Mol Biol 341:1343-1354. 64. Gillilan RE, Lilien RH (2004) Optimization and dynamics of protein-protein complexes using B-splines. J. Comput. Chem. 25:1630-1646.

65. Thorne RE, Stum Z, Kmetko J, O'Neill K, Gillilan R (2003) Microfabricated mounts for high-throughput macromolecular cryocrystallography. Journal of Applied Crystallography 36:1455-1460.

66. Budhu A, Gillilan R, Noy N (2001) Localization of the RAR interaction domain of cellular retinoic acid binding protein-II. J Mol Biol 305:939-949.

67. Hart TN, Gillilan RE, Lilien R, Ness SR, Read RJ Molecular Docking with a View: The Integration of a Monte Carlo Docking Program into a Virtual Reality Environment. In: Schaeffer J, editor. High Performance Computing Systems and Applications. Boston, MA: Springer US; 1998. pp. 309-322. Available from: https://doi.org/10.1007/978-1-4615-5611-4_30

68. Gillilan R Scientific Applications of Virtual Reality. In: Applied Virtual Reality. Vol. 14. Orlando, Florida: SIGGRAPH; 1998. p. https://history.siggraph.org/wp-content/uploads/2021/09/1998-14-Contents-Applied-Virtual-Reality.pdf.

69. Cunningham MA, Ho LL, Nguyen DT, Gillilan RE, Bash PA (1997) Simulation of the Enzyme Reaction Mechanism of Malate Dehydrogenase. Biochemistry 36:4800-4816.

70. F. Wood, D. Brown, R. A. Amidon, J. Alferness, B. Joseph, R. E. Gillilan, C. Faerman (1996) WorkSpace and the study of Chagas' disease. IEEE Computer Graphics and Applications 16:72-78.

71. Ripoll DR, Faerman CH, Gillilan R, Silman I, Sussman JL Electrostatic Properties of Human Acetylcholinesterase. In: Quinn DM, Balasubramanian AS, Doctor BP, Taylor P, editors. Enzymes of the Cholinesterase Family. Boston, MA: Springer US; 1995. pp. 67-70. Available from: <u>https://doi.org/10.1007/978-1-</u> 4899-1051-6 16

72. Gillilan RE, Wood F (1995) Visualization, virtual reality, and animation within the data flow model of computing. SIGGRAPH Comput. Graph. 29:55-58.

73. Yan YJ, Gillilan RE, Whitnell RM, Wilson KR, Mukamel S (1993) Optical control of molecular dynamics: Liouville-space theory. J. Phys. Chem. 97:2320-2333.

74. R. E. Gillilan, B. R. Land Scientific visualization of chemical systems. In: Supercomputing '93:Proceedings of the 1993 ACM/IEEE Conference on Supercomputing. ; 1993. pp. 296-301.

75. Yan YJ, Kohler B, Gillilan RE, Whitnell RM, Wilson KR, Mukamel S Molecular Control Spectrometer. In: Ultrafast Phenomena VIII. Antibes Juan-Les-Pins, France: Springer; 1992.

76. Gillilan RE, Wilson KR (1992) Shadowing, rare events, and rubber bands. A variational Verlet algorithm for molecular dynamics. The Journal of Chemical Physics 97:1757-1772.

77. Gillilan RE (1990) Invariant surfaces and phase space flux in three-dimensional surface diffusion. The Journal of Chemical Physics 93:5300-5314.

78. Gillilan RE, Reinhardt WP (1989) Barrier recrossing in surface diffusion: A phase-space perspective. Chemical Physics Letters 156:478-482.

79. Waterland RL, Yuan J-M, Martens CC, Gillilan RE, Reinhardt WP (1988) Classical-Quantum Correspondence in the Presence of Global Chaos. Phys. Rev. Lett. 61:2733-2736.

80. Gillilan RE (1988) Flux and Turnstiles in Three Dimensional Surface Diffusion.

81. Reinhardt WP, Gillilan RE Semi-classical Quantization on Adiabatically Generated Tori, or Einstein on the Brink. In: Path Integrals from meV to MeV. World Scientific; 1986.

82. Gillilan RE, Pohl TM, Whalen DL (1982) The .alpha.- and .beta.-deuterium isotope effects in the hydrolysis of tetrahydronaphthalene epoxides: ratelimiting hydrogen migration in the spontaneous hydrolysis of 6-methoxy-1,2,3,4tetrahydronaphthalene oxide. J. Am. Chem. Soc. 104:4482-4484.

83. Gillilan RE, Pohl TM, Whalen DL (1982) Substituent effects on rates and product distributions in the hydrolysis reactions of naphthalene tetrahydro epoxides. Models for tetrahydro epoxides of polycyclic aromatic hydrocarbons. J. Am. Chem. Soc. 104:4481-4482.

Meeting and Research Reports (pre-2015)

Gillilan RE, WK.04: Small Angle Scattering - Structural Biology and Soft Matter ACA RefleXions (workshop report), (Fall 2015)

Richard E. Gillilan, Søren S. Nielsen, X-Ray Lab-on-a-Chip: Sample Dialysis for Small-Angle X-Ray Solution Scattering (2011-2012 CNF Research Accomplishments Report)

R.E. Gillilan, S.S. Nielsen, "X-Ray Lab on a Chip: A Microfluidic Mixing System for Small-Angle X-ray Solution Scattering" (CNF Report 2011 #1940-10)

Richard E. Gillilan "Structures from Solutions: Biomolecular Small-Angle Solution Scattering at MacCHESS" Chess News Magazine (2009) pp 53-56

Richard Gillilan and Ruslan Sanishvili "Microcrystallography", ACA RefleXions, Fall 2008 pp 49-50

Richard Gillilan and Gerd Rosenbaum, "Microcrystals, Microbeams, and Multiple Crystals" ACA ReflecXions(American Crystallographic Association) Number 3, Fall 2007 p54

Richard Gillilan

CHESS User Meeting Workshop Report on the MacCHESS Workshop Synchrotron Radiation News, Vol. 18, No. 2, 2005

Book Chapters

"Single-bounce Monocapillary X-ray Optics: Design and Biological Applications" Richard E. Gillilan and Donald H. Bilderback, Chapter 2 in <u>Synchrotron Radiation</u> and <u>Structural Proteomics</u> (26 pages), Pan Stanford Series on Nanobiotechnology New York 2010

"Daniel C. Dennett" (biography) in <u>ICONS of UNBELIEF: Atheists, Agnostics, and</u> <u>Secularists</u>, **Richard Gillilan**, Ed. S.T. Joshi, GREENWOOD Icons series, pp 39-50, Greenwood Press, Westport, Connecticut 2008

"Visualizing Enzyme Electrostatics with IBM Visualization Data Explorer" **R.E. Gillilan** and D.R. Ripoll, , pp 61-81 in Data Visualization in Molecular Science Jack E. Bowie ed., Addison-Wesley, New York 1995

Film and video productions

Photoactive Yellow Protein (6:00) Paul Bash (Argonne National Laboratory), Richard Gillilan (CTC) video, music and narration, 1997

Computational Enzymology: The Reaction in Malate Dehydrogenase (5:44) Paul Bash (Argonne National Laboratory), Richard Gillilan (CTC) and T. Jackman (IBM)

video, music and narration, 1996

Chorismate Mutase (4:32) Angela Y. Lee, Ping Kongsaeree, Bruce Ganem, Jon Clardy (Cornell), Richard Gillilan and Wayne Lytle (CTC) video, music and narration, 1995

Select Modes of Filamentous Actin (5:17) Monique Tirion, Daniel Ben-Avraham (Clarkson University), Richard Gillilan (CTC) video, narration only, 1995

Acetylcholinesterase (4:00) Daniel Ripoll (CTC), Joel Sussman, Israel Silman (Weizmann Institute), Richard Gillilan (CTC) video, no sound, 1993

Visualization in Chemistry (2:50) Richard Gillilan (UCSD) 16mm film, music only, 1992

Solution Reaction Dynamics, The Movie Robert Whitnell, Richard Gillilan and Kent Wilson (UCSD) 16mm stereo film, music only, 1991

Film Appearances (work-related)

The Age of Viruses (Indaganda Producciones, New Atlantis, 2005)

Articles about my past visualization work written by others

"The Frontiers of Virtual Reality And Visualization in Biochemical Research", Scientific Computing and Automation July 96 pp 20-22

"Researchers Battle Disease in Cornell Theory Center's SC'95 I-WAY Demo", ForeFronts (Cornell Theory Center Magazine) Vol 10 (4) 1995

"Flickering on the CAVE Walls, Reality in Another Dimension", Washington Post Nov 28, 1994

"Data Explorer Hunts a Parasite", IBM Visions (2) 1995

"Acetylcholinesterase: Molecules Take Visual Forms", IBM Visions (3) 1993

Journal cover artwork (CTC era)

Chemistry and Biology (Clardy PBP Jan 2000) Structure (Clardy DHODH Jan 2000) Proteins Structure Function and Genetics, v34 #1 Jan 1999 IBM Visions, Issue 2 1995 IBM Systems Journal, Vol 34, (2) 1995 Chemistry and Biology, Vol 1 (2) Oct. 1994 In Chemistry, Vol 3, No. 4, 1993

Short courses and workshops organized (CTC era)

MacCHESS Annual User Meeting (co-organizer) Cornell University	2000
Flexible Ligand Docking II (workshop) Cornell Theory Center	1998
Flexible Ligand Docking (workshop) Cornell Theory Center	1997

Molecular Graphics and Animation (multiple 2-3 day workshops) Cornell Theory Center April 1994, October 1994 and June 1995

Visualization of Chemical Systems (one day course) SuperComputing 93 1993

Invited lectures (CTC era)

SIGGRAPH 98,97 Course 15 (Applied Virtual Reality) Scientific Applications of Virtual Reality 1998,1997

VR Expo '96, New Delhi, India Molecular Modeling and Virtual Reality 1996

NCI-Frederick Cancer Research and Development Center 1996 Visualization, Animation and Virtual Reality for Chemistry and Biology

New Trends in Bio-Pharmaceutical Discovery, IBM T.J. Watson Structure-Based Drug Design and Virtual Reality 1995

Visualization Technology to Find and Develop More Oil, (keynote speaker):Visualization and Virtual Reality 1995 Woodlands, Texas

Continuing Education (courses and schools attended)

DataCol 99 (synchrotron diffraction data collection)	1999
Brookhaven, NY	
Protein NMR (BioBM 730, audit)	1999
Protein-Nucleic Acid Interaction (BioMI 692, audit)	1998
Survey of Cell Biology (BIOBM 432, audit)	1997
Macromolecular Crystallography (BioBM 738 credit)	1997

NATO Advanced Study Institute LII: Chaos and Quantum Phys. 1989 Les Houches, France

Lectures and demonstrations given in various Cornell courses (CTC era)

• Protein Structure and Function (Bio631, 2 lectures+demo)	1997
• Freshman Engineering (170, 1 lecture)	1998
• Society for Humanities "Virtuality" (1 lecture/demo)	1999
• Science and Society (1 lecture/demo)	1999
	2000

Early Teaching Experience and research assistantships

Supervision of undergraduate and masters student independent study projects in computer science (CS490,CS790) 1995-1999 Mentor: NASA SHARP Plus Program for high school students 1999,2001 Employment of undergraduate, Masters and H.S. students 1995-1999 University of Pennsylvania^{*} (Physical Chemistry TA) 1983-1984 University of Colorado (Physical Chemistry TA) 1983-1984 University of Colorado (Physical Chemistry TA) 1980-1982 University of Maryland, Baltimore County 1980-1982 Undergraduate Research Assistant in Organic Chemistry University of Maryland, Baltimore County 1981 *I moved with W.P. Reinhardt's group to UPenn in 1984