

## RICHARD E. GILLILAN

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**Citations 2954 h-index 25 i10-index 44. (Google Scholar 12/2022)**

### 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

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

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**

CHES User Mtg. Poster: "High-Throughput BioSAXS: disposable tip pipetting and quick-change capillary flow cells" S. Neilsen, M. Moller, R. Gillilan (**1<sup>st</sup> 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):**

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](https://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](https://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-seeks-answers-to-early-life-beginnings](https://www.newswise.com/articles/high-pressure-biology-seeks-answers-to-early-life-beginnings))

**Workshops/Conferences Organized (recent)**

"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", CHES **Jul 15-16, 2021**

"High Pressure Biology with hands-on data collection", CHES **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 (selected)**

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)**

"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", 10<sup>th</sup> Asian Conference on High Pressure Research (S. Korea, virtual) Nov 2021

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

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

Binghamton University  
Chem 583P-01 (Structural Biology) Fall 2020, Fall 2022  
BCHM403 (S. Solmaz Biochemistry Class), Spring 2021  
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", *Département 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 (selected)**

"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<sup>st</sup> 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

### **Peer review activities (recent)**

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

- Miller, R. C., Cummings, C., Huang, Q., Ando, N. & **Gillilan, R. E.** Inline small-angle X-ray scattering-coupled chromatography under extreme hydrostatic pressure. *Protein Science* **31**, e4489 (2022).
- **Gillilan, R. E.** High-pressure SAXS, deep life, and extreme biophysics. in *Methods in Enzymology* (Academic Press, 2022). doi:[10.1016/bs.mie.2022.08.025](https://doi.org/10.1016/bs.mie.2022.08.025).
- Zhang, S., McCallum, S. A., **Gillilan, R. E.**, Wang, J. & Royer, C. A. High Pressure CPMG and CEST Reveal That Cavity Position Dictates Distinct Dynamic Disorder in the PP32 Repeat Protein. *J. Phys. Chem. B* (2022) doi:[10.1021/acs.jpcc.2c05498](https://doi.org/10.1021/acs.jpcc.2c05498).
- Trewhella, J. *et al.* 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* **78**, (2022)
- Allsopp, R. *et al.* Antimicrobial Peptide Mechanism Studied by Scattering-Guided Molecular Dynamics Simulation. *J. Phys. Chem. B* (2022) doi:[10.1021/acs.jpcc.2c03193](https://doi.org/10.1021/acs.jpcc.2c03193).
- Lokareddy, R. K. *et al.* Terminase Subunits from the Pseudomonas-Phage E217. *Journal of Molecular Biology* **434**, 167799 (2022).
- Florio, T. J., Lokareddy, R. K., Yeggoni, D. P., Sankhala, R. S., Ott, C. A., **Gillilan, R. E.** & Cingolani, G. (2022). *Nature Communications*. **13**, 1207.
- Doll, S. G. *et al.* Recognition of the TDP-43 nuclear localization signal by importin  $\alpha 1/\beta$ . *Cell Reports* **39**, 111007 (2022).
- Zovo, K., Pupart, H., Van Wieren, A., **Gillilan, R. E.**, Huang, Q., Majumdar, S. & Lukk, T. (2022). *ACS Omega*. **7**, 6184-6194.
- Li Y, **Gillilan R**, Abbaspourrad A. 2021. Tuning C-Phycocyanin Photoactivity via pH-Mediated Assembly Disassembly. *Biomacromolecules* 22(12):5128-5138
- 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(12):2592-98
- Rai, D.K., **Gillilan, R.E.**, Huang, Q., Miller, R., Ting, E., Lazarev, A., Tate, M.W., Gruner, S.M., 2021. High-pressure small-angle X-ray scattering cell for biological solutions and soft materials. *Journal of Applied Crystallography* 54, 111-122. <https://doi.org/10.1107/S1600576720014752>
- Ando, N., Barquera, B., Bartlett, D.H., Boyd, E., Burnim, A.A., Byer, A.S., Colman, D., **Gillilan, R.E.**, Gruebele, M., Makhatadze, G., Royer, C.A., Shock,

E., Wand, A.J., Watkins, M.B., 2021. The Molecular Basis for Life in Extreme Environments. Annu. Rev. Biophys. <https://doi.org/10.1146/annurev-biophys-100120-072804>

- Coombs, S.E., Banjade, S., Kriksunov, K., Clemente, N., Zhao, J., Wang, C., **Gillilan, R.E.**, Oswald, R.E., 2020. In Vitro Effects of (+)MK-801 (dizocilpine) and Memantine on  $\beta$ -Amyloid Peptides Linked to Alzheimer's Disease. Biochemistry 59, 4517-4522. <https://doi.org/10.1021/acs.biochem.0c00813>
- Biophysical analysis of Pseudomonas-phage PaP3 small terminase suggests a mechanism for sequence-specific DNA binding by lateral interdigitiation  
Niazi, Marzia; Florio, Tyler; Yang, Ruoyu; Lokareddy, Ravi; Swanson, Nicholas; **Gillilan, Richard**; Cingolani, Gino, Nucleic Acids Research (2020 online <https://doi.org/10.1093/nar/gkaa866>)
- Structure and function of the juxtamembrane GAF domain of potassium biosensor KdpD  
S Kumar, RE Gillilan, DA Yernool Protein Science 29 (9), 2009-2021 2020
- Quantitative measure of the size dispersity in ultrasmall fluorescent organic-inorganic hybrid core-shell silica nanoparticles by small-angle X-ray scattering  
KP Barteau, K Ma, FFE Kohle, TC Gardinier, PA Beaucage, RE Gillilan, ... Chemistry of Materials 31 (3), 643-657 2019
- Molecular architecture of the inositol phosphatase Siw14  
TJ Florio, RK Lokareddy, RE Gillilan, G Cingolani Biochemistry 58 (6), 534-545. 2018
- Predicting data quality in biological X-ray solution scattering. Wang C, Lin Y, Bougie D, **Gillilan RE**. Acta Crystallogr D Struct Biol. 2018 Aug 1;74(Pt 8):727-738.
- The consequences of cavity creation on the folding landscape of a repeat protein depend upon context. Jenkins KA, Fossat MJ, Zhang S, Rai DK, Klein S, Gillilan R, White Z, Gerlich G, McCallum SA, Winter R, Gruner SM, Barrick D, Royer CA., Proc Natl Acad Sci U S A. 2018 Aug 28;115(35):E8153-E8161
- Sankhala RS, Lokareddy RK, Begum S, Pumroy RA, **Gillilan RE**, Cingolani G. Three-dimensional context rather than NLS amino acid sequence determines importin  $\alpha$  subtype specificity for RCC1. Nature Communications. 2017; Vol 8 (1):979.
- Hopkins. J. B., **Gillilan, R. E.**, Skou, S. "BioXTAS RAW: improvements to a free open-source program for small-angle X-ray scattering data reduction and analysis." J. Appl. Cryst. , 50, 2017.
- Lorenzo Alamo, Natalia Koubassova, Antonio Pinto, **Richard Gillilan**, Andrey Tsaturyan, Raúl Padrón. Lessons from a tarantula: new insights into muscle thick filament and myosin interacting-heads motif structure and function.

Biophys Rev Vol 9 (5) 461-480 (2017).

- [Extended low-resolution structure of a Leptospira antigen offers high bactericidal antibody accessibility amenable to vaccine design](#), Ching-Lin Hsieh Christopher P Ptak Andrew Tseng Igor Massahiro de Souza Suguiura Sean P McDonough Tepyuda Srirakul Ting Li Yi-Pin Lin **Richard E Gillilan** Robert Oswald, *eLife* 2017;6:e30051 DOI: 10.7554/eLife.30051
- Lorenzo Alamo James S Ware Antonio Pinto **Richard E Gillilan** Jonathan G Seidman Christine E Seidman Raúl Padrón. [Effects of myosin variants on interacting-heads motif explain distinct hypertrophic and dilated cardiomyopathy phenotypes](#), *eLife* 2017;6:e24634 DOI: 10.7554/eLife.24634
- Schormann N1, Zhukovskaya N2, Bedwell G3, Nuth M2, **Gillilan R4**, Prevelige PE3, Ricciardi RP2,5, Banerjee S6, Chattopadhyay D1. [Poxvirus uracil-DNA glycosylase-An unusual member of the family I uracil-DNA glycosylases](#), *Protein Sci.* 2016 Dec;25(12):2113-2131. doi: 10.1002/pro.3058. Epub 2016 Nov 2.
- Lukk T, **Gillilan RE**, Szebenyi DM, Zipfel WR. [A visible-light-excited fluorescence method for imaging protein crystals without added dyes](#). *J Appl Crystallogr.* 2016 Feb 1;49(Pt 1):234-240. eCollection 2016 Feb 1.
- Alamo L, Qi D, Wriggers W, Pinto A, Zhu J, Bilbao A, **Gillilan RE**, Hu S, Padrón R. "[Conserved Intramolecular Interactions Maintain Myosin Interacting-Heads Motifs Explaining Tarantula Muscle Super-Relaxed State Structural Basis](#)." *J Mol Biol.* 2016 Feb 2.
- Tondnevis F, **Gillilan R**, Bloom L, McKenna R, "[Solution study of the Escherichia coli DNA polymerase III clamp loader reveals the location of the dynamic  \$\psi\chi\$  heterodimer](#)," *Structural Dynamics* **2(054701)**, (2015).
- Acerbo, A. S., Cook, M. J., & **Gillilan, R. E.** (2015). Upgrade of MacCHESS facility for X-ray scattering of biological macromolecules in solution. *Journal of Synchrotron Radiation*, 22(1), 180-186.
- Huang R, Szebenyi T, Pfeifer M, Woll A, Smilgies D-M, Finkelstein K, Dale D, Wang Y, Vila-Comamala J, **Gillilan R**, Cook M, Bilderback DH, "[Application of CHESS single-bounce capillaries at synchrotron beamlines](#)," *J. Phys.: Conf. Ser.* **493(1)**, 012034 (2014).
- Skou, S., **R. E. Gillilan** and N. Ando (2014). "Synchrotron-based small-angle X-ray scattering of proteins in solution." *Nature Protocols* **9(7)**: 1727-1739.
- Skou, M., S. Skou, T. G. Jensen, B. Vestergaard and **R. E. Gillilan** (2014). "In situ microfluidic dialysis for biological small-angle X-ray scattering." *Journal of Applied Crystallography* **47(4)**: 1355-1366.
- **Gillilan R.**, C. M., Temnykh G., Møller M., Nielsen S. . CHIPS AND ROBOTS: SCREENING, MIXING, AND DIALYSIS ON BIOSAXS BEAMLINES. *Transactions of the ACA* **44**, 40-50 (2013).
- Møller, M. et al. 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, doi:10.1371/journal.pone.0074783

(2013).

- **Gillilan RE**, K. V., O'Neill-Hennessey E, Cohen C, Brown JH. X-Ray Solution Scattering of Squid Heavy Meromyosin: Strengthening the Evidence for an Ancient Compact off State. *PLoS One* **8**, doi:doi:10.1371/journal.pone.0081994 (2013).
- Kim, C. U., J. L. Wierman, **R. Gillilan**, E. Lima, and S. M. Gruner. "A high-pressure cryocooling method for protein crystals and biological samples with reduced background X-ray scatter" *J. Appl. Cryst.* 46:234-241 (2013)
- Khan, I., **R. Gillilan\***, I. Kriksunov, R. Williams, W. R. Zipfel, and U. English. 2012. *Confocal microscopy on the beamline: novel three-dimensional imaging and sample positioning*. *J. Appl. Cryst.* 45:936-943.  
**(\*) Corresponding author**
- Meisburger, S. P., M. Warkentin, H. M. Chen, J. B. Hopkins, **R. E. Gillilan**, L. Pollack, and R. E. Thorne. 2013. *Breaking the Radiation Damage Limit with Cryo-SAXS*. *Biophys. J.* 104:227-236.
- Nielsen, S. S., Moller, M. & **Gillilan, R. E.** "High-throughput biological small-angle X-ray scattering with a robotically loaded capillary cell" *J. Appl. Cryst.* 45 (2012)
- L. J. Koerner, **R. E. Gillilan**, K. S. Green, S. Wang and S. M. Gruner "Small-angle solution scattering using the mixed-mode pixel array detector" *J. Synchrotron Rad.* (2011). 18, 148-156
- Yennawar, H., Moller, M., Gillilan, R. & Yennawar, N. "X-ray crystal structure and small-angle X-ray scattering of sheep liver sorbitol dehydrogenase." *Acta Crystallographica Section D-Biological Crystallography* **67**, 440-446 (2011)
- **Gillilan, R. E.**, Cook, M. J., Cornaby, S. W. & Bilderback, D. H. Microcrystallography using single-bounce monocapillary optics *J. Synchrotron Rad.* 17, 227-236 (2010)
- Cornaby S, Szebenyi DME, Smilgies DM, Schuller DJ, **Gillilan R**, Hao Q, Bilderback DH, "Feasibility of one-shot-per-crystal structure determination using Laue diffraction", *ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY*, Vol 66, 2-11 (2010)
- Vadim Cherezov, Nicole Höfer Doletta M. E. Szebenyi, **Richard Gillilan**, Vasundara Srinivasan, Christopher P. Jaroniec and Martin Caffrey, "Insights into the Mode of Action of a Putative Zinc Transporter CzcB in *Thermus thermophilus*", **(Cover article)** *Structure* Vol 16, 1378-1388 10 Sept 2008
- Donald H. Bilderback, Alexander Kazimirov, **Richard Gillilan**, Sterling Cornaby, Arthur Woll, Chang-Sheng Zha, and Rong Huang, "Optimizing Monocapillary Optics for Synchrotron X-ray Diffraction, Fluorescence Imaging, and Spectroscopy Applications", *AIP Conf. Proc.* 879, 758 (2007)
- Stuart B. Krasnoff, Ivan Keresztes, **Richard E. Gillilan**, Doletta M.E. Szebenyi, Bruno G.G. Donzelli, Alice C.L. Churchill, Donna M. Gibson. "Serinocylins A and B, Cyclic Heptapeptides from *Metarhizium anisopliae*"

- **Richard E. Gillilan**, Stephen D. Ayers and Noa Noy, "Structural Basis for Activation of Fatty Acid-binding Protein 4" *J. Mol. Biol.* (2007) 372, 1246-1260
- Nicle Hofer, Olga Kolaj, Hui Li, Vadim Cherezov, **Richard Gillilan**, J. Gerard Wall, and Martin Caffrey "Crystallization and preliminary X-ray diffraction analysis of a soluble domain of the putative zinc transporter CzcB from *Thermus thermophilus*" *Acta Cryst* (2007). F63, 673-677
- Stephen D. Ayers, Katherine L. Nedrow, **Richard E. Gillilan**, and Noa Noy\* "Continuous Nucleocytoplasmic Shuttling Underlies Transcriptional Activation of PPAR by FABP4" *Biochemistry*, 46 (23), 6744 -6752, 2007
- Joseph E. Wedekind, **Richard Gillilan**, Alena Janda, Jolanta Krucinska, Jason D. Salter, Ryan P. Bennett, Jay Raina, and Harold C. Smith "Nanostructures of APOBEC3G Support a Hierarchical Assembly Model of High Molecular Mass Ribonucleoprotein Particles from Dimeric Subunit" *J. Biol. Chem.*, Dec 2006; 281: 38122 - 38126
- Yevgeniy Kalinin, Jan Kmetko, Adam Bartnik, Andrew Stewart, **Richard Gillilan** and Emil B. Lobkovsky, Robert E. Thorne. "A new sample mounting technique for room-temperature macromolecular crystallography" *J. Appl. Cryst.* (2005). 38, 333-339
- **R. Gillilan**, R. Lilien, "Optimization and Dynamics of Protein-Protein Complexes Using B-Splines", *Journal of Computational Chemistry* 25: 1630-1645 (2004)
- L. You, **R. Gillilan**, T. Huffaker, "A model for the yeast cofactor A-Beta-Tubulin complex based on computational docking and mutagenesis", *Journal of Molecular Biology*, 341 (5) 1343-1354 (2004)
- R.E. Thorne, Z. Stum, J. Kmetko, K. O'Neill and **R. Gillilan**, "Microfabricated mounts for high-throughput macromolecular cryocrystallography", *Journal of Applied Crystallography* 36, 1455-1460 (2003)
- Budhu A, **Gillilan R**, Noy N. "Localization of the RAR interaction domain of cellular retinoic acid binding protein-II", *Journal of Molecular Biology*, 305 (4): 939-949 Jan 26 (2001)
- Trevor Hart, **Richard Gillilan**, Ryan Lilien, Steven Ness and Randy Read, "Molecular docking with a view: the integration of a Monte Carlo docking program into a virtual reality environment" in High Performance Computing Systems and Applications. Kluwer Academic Publisher (Summer 1998).
- **R.E. Gillilan**, *Scientific Applications of Virtual Reality* in Applied Virtual Reality, SIGGRAPH 98 Course 15 Notes, Los Angeles 1998 pp 8-2 to 8-17.
- M.A. Cunningham, L. Lawrence Ho, D.T. Nguyen, **R.E. Gillilan**, and P.A. Bash, Simulation of the Enzyme Reaction Mechanism of Malate Dehydrogenase, *Biochemistry* 36 (16) pp 4800-4816 1997

- F. Wood, D. Brown, R. Amidon, J. Alferness, B. Joseph, **R. Gillilan**, and C. Faerman, WorkSpace and the Study of Chagas' Disease IEEE Computer Graphics and Applications Vol 16, (4) pp 72-78 July 1996
- D.R. Ripoll, C.H. Faerman, **R.E. Gillilan**, I. Silman, J.L. Sussman, Electrostatic Properties of Human Acetylcholinesterase in Enzymes of the Cholinesterase Family}, D.M. Quinn et al. ed. Plenum Press, New York, 1995; pp 67-70
- **R.E. Gillilan** and F. Wood, Visualization, Virtual Reality, and Animation within the Data Flow Model of Computing, Computer Graphics, 29, 55-58 (1995).
- **R. Gillilan** and B. Land, *Scientific Visualization of Chemical Systems* Proc. IEEE Supercomputing '93, pp 296-301, Los Alamitos, CA, 1993
- Y.J. Yan, B. Kohler, **R.E. Gillilan**, R. M. Whitnell, K.R. Wilson and S. Mukamel Molecular Control Spectrometer Ultrafast Phenomena VIII; ed. J.-L. Martin, A. Migus, G.A. Mourou, A.H. Zewail Berlin Heidelberg:Springer-Verlag, 1993; p.8.
- Y.J. Yan, **R.E. Gillilan**, R.M. Whitnell, K.R. Wilson and S. Mukamel Optical Control of Molecular Dynamics: Liouville-Space Theory J. Phys. Chem. 97, 2320. (1993)
- **R.E. Gillilan** and K.R. Wilson. *Shadowing, Rare Events and Rubber Bands: a Variational Verlet Algorithm for Molecular Dynamics* J. Chem. Phys. 97 (3) pp 1757-1772 (1992)
- **R.E. Gillilan** and G.S. Ezra. Transport and Turnstiles in Multidimensional Hamiltonian Mappings for Unimolecular Fragmentation: Application to Van der Waals Predissociation. J. Chem. Phys. 95 (1991)
- **R.E. Gillilan**. Invariant Surfaces and Phase Space Flux in Three Dimensional Surface Diffusion. J. Chem. Phys. 93 (7) pp 5300-5314 (1990)
- **R.E. Gillilan** and W.P. Reinhardt. Barrier Recrossing in Surface Diffusion: A Phase Space Perspective. Chem. Phys. Lett. 156, pp 478-482 (1988)
- **R.E. Gillilan**, Ph.D. Thesis, Flux and Turnstiles in Three Dimensional Surface Diffusion. University Microfilms Inc. (1988)
- R.L. Waterland, J. Yuan, C.C. Martens, **R.E. Gillilan** and W.P. Reinhardt. Quantum-Classical Correspondence in the Presence of Global Chaos. Phys. Rev. Lett. 61, 2733-2736 (1988)
- W.P. Reinhardt and **R.E. Gillilan**, Semi-classical Quantization on Adiabatically Generated Tori, or Einstein on the Brink. Path Integrals from meV to MeV}, edited by M.C. Gutzwiller et al. World Scientific, Singapore and Philadelphia pp 154-172 (1986)
- **R.E. Gillilan**, T.M. Pohl and D.L. Whalen. alpha and beta Deuterium Isotope Effects in the Hydrolysis of Naphthalene Tetrahydro Epoxides: Rate-Limiting Hydrogen Migration in the Spontaneous Hydrolysis of 6-Methoxy-1,2,3,4-tetrahydronaphthalene Oxide.

J. Am. Chem. Soc. 104, 4482-4484 (1982)

- **R.E. Gillilan**, T.M. Pohl and D.L. Whalen. 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 (1982)

#### **Meeting and Research Reports (pre-2015)**

**GillilanRE**, 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 Reflexions (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 Synchrotron Radiation and Structural Proteomics (26 pages), Pan Stanford Series on Nanobiotechnology New York 2010

"Daniel C. Dennett" (biography) in ICONS of UNBELIEF: Atheists, Agnostics, and Secularists, **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 Kongsaree, 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) <i>Scientific Applications of Virtual Reality</i>	1998,1997
VR Expo '96, New Delhi, India <i>Molecular Modeling and Virtual Reality</i>	1996
NCI-Frederick Cancer Research and Development Center <i>Visualization, Animation and Virtual Reality for Chemistry and Biology</i>	1996
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 Woodlands, Texas	1995

**Continuing Education (courses and schools attended)**

DataCol 99 (synchrotron diffraction data collection) Brookhaven, NY	1999
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. Les Houches, France	1989

**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

**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) 1985

University of Maryland, Baltimore County 1980-1982  
Undergraduate Research Assistant in Organic Chemistry

University of Maryland, Baltimore County  
Teaching assistant in Introductory Chemistry 1981

*\*I moved with W.P. Reinhardt's group to UPenn in 1984*