Alexander Luke Perryman, Ph.D.

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Mission of the Perryman lab: we will develop a research approach that could best be framed as computational chemical biology, to bridge the gaps between ligands, targets, and cells, in order to advance compounds into *in vivo* studies. We will apply this cutting edge approach to help advance research against drug-resistant infectious diseases and emerging diseases. Our primary focus will be tuberculosis, but we will also help in the fight against the ESKAPE pathogens, and we will help guide the optimization of the chemical tools and drug leads that our collaborators are pursuing. We will create, validate, and apply new workflows that combine different types of computational techniques together (e.g., docking-based virtual screens + ligand-based machine learning models, or Molecular Dynamics + docking of pharmacophore-filtered libraries) to (a) enhance accuracy and efficiency while exploring vast areas of chemical space, and (b) to help shift the paradigm for antibacterial drug discovery. We will also continue to extend the OpenZika project on IBM's World Community Grid (of which I am Co-P.I.) and analyze its massive virtual screening results by using novel workflows to identify new inhibitors of Zika virus replication or infection. We will:

- create, improve, validate, & apply machine learning models (e.g., ligand-based Bayesian models that can be trained with data on whole-cell potency, target inhibition, or on ADMET properties)
- combine Bayesian models, docking, pharmacophores, binding site prediction, sequence analysis comparisons, homology modeling, and/or MD, depending on what the particular project needs
- develop novel workflows that harness the strengths of ligand-based, target-based, and cell-based approaches, while minimizing the weaknesses that can occur when these techniques are performed in isolation
- create virtual libraries of synthesizable analogs and filter them with Bayesian models and/or docking studies, to prioritize analogs for subsequent synthesis and assays
- increase the accuracy and efficiency of chemical tool and drug discovery, as part of multi-disciplinary collaborations
- help advance translational research in many therapeutic areas
- effectively communicate our research to non-computational collaborators and to the general public

The new *in silico* models we create and the novel workflows that will incorporate them will be honed by an iterative cycle: we will discover candidate compounds using computational techniques; collaborators will perform enzyme and cell-based *in vitro* evaluation of these candidates; validated hits will be optimized in conjunction with medicinal chemists (using a combination of computer-guided analog design and medicinal chemistry-based SAR principles) and new assay data; followed by eventual *in vivo* experiments of the best lead compounds. Simultaneously, applying and then re-training these models with new experimental data from these collaborations in hit discovery, hit-to-lead optimization, and lead development research will give us the opportunity to both improve our computational models and to discover novel chemical tools that can both help advance the research performed throughout the entire drug discovery community.

Education

2000 - 2005 Ph.D., Biomedical Sciences (Pharmacology Dept.), University of CA, San Diego's School of Medicine (UCSD); HHMI Predoctoral Fellow in Professor Andy McCammon's lab. Dissertation: "Computer-Aided Protein Structure Studies: Hunting Down the Hidden Secrets of HIV."

1996 - 2000 B.S., Biochemistry, *Summa Cum Laude*, University of Missouri-Columbia (MU)

Research and Professional Experience

Rutgers University-NJ Medical School; Associate Professor Joel S. Freundlich's lab **2013 - present**
Research Teaching Specialist III (staff position with research, supervisory, training, and administrative responsibilities); Center for Emerging & Re-emerging Pathogens; Department of Pharmacology, Physiology and Neuroscience

- Computational & biological techniques applied to targets from *Mycobacterium tuberculosis* (*Mtb*)
- Created & developed new workflows to combine target-based, ligand-based, and cell-based approaches to advance chemical tool discovery
- Performed virtual screens to discover novel inhibitors of *Mtb* InhA, an *Mtb* transpeptidase, and Zika virus NS3 helicase
- Expressed, purified, & performed enzyme inhibition studies with that *Mtb* transpeptidase
- Created machine-learning models to predict metabolic stability (using a new data "pruning" strategy that can create more accurate models), created Bayesian models to predict whole-cell activity against ESKAPE pathogens, created Bayesian models to predict mammalian cell cytotoxicity, & created Bayesian models to predict aqueous solubility
- Created virtual libraries of hundreds of thousands of synthetically accessible analogs of hits and leads; applied different machine learning models to prioritize them for synthesis; improved the metabolic stability, potency, and/or selectivity index of different series of compounds
- Co-P.I. of the OpenZika project on IBM's World Community Grid; designed and helped prepare the experiments; since May, 2016, we have submitted 3.5 billion docking jobs, to screen 6 million compounds against all of the Zika proteins (and targets from related flaviviruses); 2.6 billion results have been produced; prepared a new library of 30.2 million compounds, which is currently being docked against the protease class; discovered novel hits that inhibit ZIKV and/or Dengue virus replication
- Wrote and submitted two grant applications as the Principal Investigator
- Created and maintained group website = http://njms.rutgers.edu/departments/labs/freundlich

The Scripps Research Institute; Professor Arthur J. Olson's lab **2007 - 2013**
Research Associate, Dept. of Integrative Structural & Computational Biology

- Drug discovery, molecular modeling, structure analysis, and virtual high-throughput screening
- Managed & performed day-to-day duties for the "FightAIDS@Home" project on IBM's World Community Grid, designed & ran over 40 million AutoDock jobs, from 09/2007-08/2013
- Created new dynamic model of HIV integrase inhibition and drug resistance, in collaboration with Pfizer Global Research and Development, Sandwich, UK and HHMI/UCSD
- Helped invent new approach to fragment-based crystallographic screening
- Created, led, & performed day-to-day duties for "GO Fight Against Malaria" (GO FAM) project on IBM's World Community Grid, performed 1.16 billion Vina jobs from 11/2011-07/2013
- Created & maintained website for GO FAM = http://GOFightAgainstMalaria.scripps.edu
- Designed & performed virtual screens to discover new "hits" against targets from HIV, *Plasmodium falciparum*, & *Mycobacterium tuberculosis*

California Institute of Technology; Professor Stephen L. Mayo's lab **2005 - 2007**
Amgen Postdoctoral Fellow, Division of Biology

- Protein design and protein engineering applied to the optimization of antiviral proteins and to a DARPA project on biomolecular electronics
- Helped invent new method to prevent and treat enveloped viruses (US Patent 8,865,876)

Univ. of California, San Diego; Professor J. Andrew McCammon's lab **2000 - 2005**
H.H.M.I. Predoctoral Fellow and Palade Scholar, Dept. of Pharmacology/Biomedical Sciences Program

- Computational chemistry and structure-based drug design against HIV protease
- Discovered a mechanism of multi-drug-resistance for HIV protease using MD simulations
- Predicted existence of allosteric sites on HIV protease, from results of Molecular Dynamics
- Helped invent and automate the Relaxed Complex Scheme of computational drug discovery

University of Missouri-Columbia; Professor Thomas P. Quinn's lab **1998 - 2000**
Beckman Scholar/Intern, Department of Biochemistry, June 1998 - August 1999
Technical Research Assistant, Department of Biochemistry, September 1999 - June 2000

- Designed, modelled, synthesized, and evaluated biomolecular radiopharmaceuticals (radioactive metal-cyclized peptides) to detect and treat different cancers
- Derived and added parameters to Sybyl's Tripos force field to enable calculating charges and performing Molecular Dynamics simulations on Re and Tc-cyclized peptides

University of Missouri-Columbia; Assistant Professor Cleopas T. Samudzi's lab **1996 - 1998**
Student Research Assistant, (HHMI Express Program), Dept. of Biochemistry, June 1996 - August 1997
Research Intern, College of Ag., Food, & Nat. Res., Department of Biochemistry, Sep. 1997 - May 1998

- Expressed, purified (without affinity tags), and attempted to crystallize proteins
- Helped perform statistical analysis of Biological Macromolecular Crystallization Database (BMCD) to develop general guidelines to facilitate crystallizing proteins

Invited Presentations

2017 Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University, Columbus, Ohio. 1 hour seminar on "Novel computational approaches to chemical tool discovery and translational research for infectious diseases."

2016 Sokol Institute of Pharmaceutical Life Sciences, College of Science and Mathematics, Montclair State University, Montclair, New Jersey. 1 hour seminar on "Novel computational approaches to chemical tool discovery for *Mycobacterium tuberculosis* (and the ESKAPEES)."

2015 250th National Meeting of the American Chemical Society in Boston, MA, 20 min. oral presentation in the Computational Toxicology: From QSAR Models to Adverse Outcome Pathways session, on "Addressing a key hurdle in translational research: Predicting mouse liver microsomal stability using machine learning."

2014 Rutgers/Robert Wood Johnson Medical School 6th Annual National Postdoc Appreciation Day Symposium, Piscataway, NJ: 15 min. oral pres. (one of three) "Advancing drug discovery against TB: Novel Mtb InhA inhibitors identified through a new docking + machine-learning paradigm." https://ored.rutgers.edu/content/rwjms-hosts-successful-post-doc-symposium

2012 World Community Grid Lecture Series: World AIDS Day webcast on "FightAIDS@Home: Advancing the discovery of allosteric inhibitors." (15 min. webinar on recent progress and future plans, followed by 15 min. Q&A with the public), http://youtu.be/khFbQTcoqyI

2012 Cambridge Healthtech Institute's Drug Discovery Chemistry 2012, 7th annual Fragment-Based Drug Discovery conference, San Diego, CA: 30 min. oral pres. "Virtual Screens of fragments against a panel of HIV protease variants on FightAIDS@Home discovered two novel inhibitors."

2011 World Community Grid Lecture Series: World AIDS Day webcast on "FightAIDS@Home: Advancing drug discovery against superbugs of HIV." (15 min. seminar on recent progress and future plans, followed by 15 min. Q&A with the public), http://www.youtube.com/watch?v=62AtXdwriTc

2010 World Community Grid Lecture Series: World AIDS Day webcast on "FightAIDS@Home: Advancing drug discovery against HIV/AIDS." (15 min. seminar followed by 15 min. Q&A with the public), http://www.worldcommunitygrid.org/about_us/viewNewsArticle.do?articleId=147

2009 Division of Mechanics, Center for Applied Sciences, and Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan. 1 hour seminar on "A dynamic model of HIV integrase inhibition and drug resistance."

2009 School of Pharmacy, National Taiwan University, Taipei, Taiwan. 1 hour seminar on a "Fragment-based screen against HIV protease: Crystallographic evidence for two allosteric binding sites."

2008 Scripps/Pfizer Joint Scientific Meeting, Pfizer Global Research & Development, Sandwich, UK, poster and 1 hour seminar to the Computational Chemistry group on "Computational modeling of the catalytic domain of HIV integrase with a closed loop and two magnesiums."

2005 7th Beckman Scholars Symposium, 45 min. oral presentation on "Computer-aided protein structure studies: Hunting down the hidden secrets of HIV." Two Nobel Laureates were among the 17 invited speakers.

2004 227th American Chemical Soc. National Meeting in Anaheim, CA, 30 min. oral pres. in the Rational Drug Design section, "HIV-1 protease MD of a wild-type and of the V82F/I84V mutant: Possible contributions to drug resistance and a potential new target site for drugs."

2003 Gordon Research Conference on Proteins, poster titled "Computer-aided discovery of HIV protease inhibitors that target drug-resistant mutants: 17 ns of MD on a w.t. and a mutant with preliminary Relaxed Complex studies."

2000 221st American Chemical Society's National Meeting in San Diego, CA, 30 min. oral pres. in the Advances in 3-D Searching and Pharmacophores section, "Using Molecular Dynamics to explain and predict the differences in affinities of two series of radiometal-cyclized hormone analogs."

1999 13th International Symposium on Radiopharmaceutical Chemistry, 15 min. oral presentation, "Design and synthesis of technetium and rhenium-cyclized somatostatin analogs."

Peer-Reviewed Publications: 29 papers published; 10 as 1st author + 2 as co-1st author
(***** indicates corresponding author, @ = contributed equally, # of citations from Google Scholar)
Total # of citations for all papers = 1,516

29) Inoyama, D., Paget, S., Russo, R., Kandasamy, S., Kumar, P., Singleton, E., Occi, J., Tuckman, M., Zimmerman, M., Ho, H., **Perryman, A. L**., Dartois, V., Connell, N., and Freundlich, J.S. "Novel pyrimidines as antitubercular agents." *Antimicrobial Agents & Chemotherapy*, (in press, 2017).

28) Stratton, T. P.,@ **Perryman, A. L.,**@ Vilchèze, C., Russo, R., Li, S. G., Patel, J. S., Singleton, E., Ekins, S., Connell, N., Jacobs, W. R. Jr., and Freundlich, J. S. "Addressing the metabolic stability of antituberculars through machine learning." *ACS Medicinal Chemistry Letters*, 8(10): 1099-1104 (2017).

27) Mottin, M., Braga, R. C., da Silva, R. A., Martins da Silva, J. H., **Perryman, A. L**., Ekins, S. E., & Horta Andrade, C. "Molecular Dynamics simulations of Zika Virus NS3 helicase: Insights into RNA binding site activity." *Biochemical and Biophysical Research Communications*, 492(4): 643-651 (2017). (1 citation)

26) Sukheja, P., Kumar, P., Mittal, N., Li, S. G., Singleton, E., Russo, R., **Perryman, A. L**., Shrestha, R., Awasthi, D., Husain, S., Soteropoulos, P., Brukh, R., Connell, N., Freundlich, J. S., & Alland, D. "A novel small-molecule inhibitor of the Mycobacterium tuberculosis demethylmenaquinone methyltransferase MenG is bactericidal to both growing and nutritionally deprived persister cells." *MBio*, 8(1): e02022-16 (2017). (1 citation)

25) Kumar, P., Kaushik, A., Lloyd, E. P., Li, S. G., Mattoo, R., Ammerman, N. C., Bell, D. T., **Perryman, A. L.,** Zandi, T. A., Ekins, S., Ginell, S. L., Townsend, C. A., Freundlich, J. S., & Lamichhane, G. "Non-classical transpeptidases yield insight into new antibacterials." *Nature Chemical Biology*, 13(1): 54-61 (2016). (9 citations)

24) Ekins, S.,***** **Perryman, A. L.,*** & Horta Andrade, C.***** "OpenZika: an IBM World Community Grid project to accelerate Zika Virus drug discovery." *PLoS Neglected Tropical Diseases*, 10(10): e0005023 (2016). (3 citations; viewed 4,916 times)

23) Ekins, S.,@ **Perryman, A. L.,**@ Clark, A. M., Reynolds, R. C., & Freundlich, J. S. "Machine learning model analysis and data visualization with small molecules tested in a mouse model of *Mycobacterium tuberculosis* infection (2014-2015)." *J. Chemical Information and Modeling*, 56(7): 1332-1343 (2016). (5 citations)

22) **Perryman, A. L**., Stratton, T. P., Ekins, S., & Freundlich, J. S. "Predicting mouse liver microsomal stability with "pruned" machine-learning models and public data." *Pharmaceutical Research*, 33: 433-449 (2016). (13 citations)

21) **Perryman, A. L**.,*[@] Yu, W.,[@] Wang, X., Ekins, S., Forli, S., Li, S. G., Freundlich, J. S., Tonge, P. J., & Olson, A. J. "A virtual screen discovers novel, fragment-sized inhibitors of *Mycobacterium tuberculosis* InhA." *J. Chemical Information and Modeling*, 55(3): 645-659 (2015). (16 citations)

20) Deng, N., Forli, S., He, P., **Perryman, A**., Wickstrom, L., Vijayan, R. S. K., Tiefenbrunn, T., Stout, D., Gallicchio, E., Olson, A. J., and Levy, R. M. "Distinguishing binders from false positives by free energy calculations: Fragment screening against the flap site of HIV protease." *J. Physical Chemistry B*, 119(3): 976-988 (2015). (20 citations)

19) Al Olaby, R. R., Cocquerel, L., Zemla, A., Saas, L., Dubuisson, J., Vielmetter, J., Marcotrigiano, J., Khan, A. G., Vences Catalan, F., **Perryman, A. L**., Freundlich, J. S., Forli, S., Levy, S., Balhorn, R., & Azzazy, H. M. "Identification of a novel drug lead that inhibits HCV infection and cell-to-cell transmission by targeting the HCV E2 glycoprotein." *PLoS One*, 9(10): e111333 (2014). (11 citations)

18) Stec, J., Vilchèze, C., Lun, S., **Perryman, A. L.**, Wang, X., Freundlich, J. S., Bishai, W., Jacobs, W. R. Jr., & Kozikowski, A. P. "Biological evaluation of potent triclosan-derived inhibitors of the enoyl-acyl carrier protein reductase InhA in drug-sensitive and drug-resistant strains of *Mycobacterium tuberculosis*." *ChemMedChem*, 9(11): 2528-2537 (2014). (11 citations)

17) Mobley, D. L., Liu, S., Lin, N. M., Wymer, K. L., **Perryman, A. L**., Forli, S., Deng, N., Su, J., Branson, K., & Olson, A. J. "Blind prediction of HIV integrase binding from the SAMPL4 challenge." *J. Computer Aided Molecular Design*, 28(4): 327-345 (2014). (25 citations)

16) Gallicchio, E., Deng, N., He, P., Wickstrom, L., **Perryman, A. L**., Santiago, D. N., Forli, S., Olson, A. J., & Levy, R. M. "Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge." *J. Computer Aided Molecular Design*, 28(4): 475-490 (2014). (35 citations)

15) **Perryman, A. L.,**[@] Santiago, D. N.,[@] Forli, S., Santos-Martins, D., & Olson A. J. "Virtual screening with AutoDock Vina and the common pharmacophore engine of a low diversity library of fragments and hits against the three allosteric sites of HIV integrase: participation in the SAMPL4 protein-ligand binding challenge." *J. Computer Aided Molecular Design*, 28(4): 429-441 (2014). (23 citations)

14) Tiefenbrunn, T., Forli, S., Baksh, M. M., Chang, M. W., Happer, M., Lin, Y.-C., **Perryman, A. L**., Rhee, J.-K., Torbett, B. E., Olson, A. J., Elder, J. H., Finn, M. G., & Stout, C. D. "Small molecule regulation of protein conformation by binding in the flap of HIV protease." *ACS Chemical Biology*. 8(6): 1223-1231 (2013). (27 citations)

13) Wang, J. C., Lin, Y. H., Chen, C. M., **Perryman, A. L**., & Olson, A. J.. "Robust scoring functions for protein-ligand interactions with Quantum Chemical charge models." *J. Chemical Information and Modeling*, 51(10): 2528-2537 (2011). (36 citations)

12) Lin, Y.-C., **Perryman, A. L**., Olson, A. J., Torbett, B. E., Elder, J. H., & Stout, C. D. "Structural basis for drug and substrate specificity exhibited by FIV encoding a chimeric FIV/HIV protease." *Acta Crystallographica,* D67: 540-548 (2011). (6 citations)

11) Cosconati, S., Forli, S., **Perryman, A. L**., Harris, R., Goodsell, D. S., & Olson, A. J. "Virtual Screening with AutoDock: Theory and practice." *Expert Opinion on Drug Discovery*, 5(6): 597-607 (2010). (226 citations)

10) **Perryman, A. L**., Zhang, Q., Soutter, H. H., Rosenfeld, R., McRee, D. E., Olson, A. J., Elder, J. E., & Stout, C. D. "Fragment-based screen against HIV protease," *Chemical Biology & Drug Design*, 75(3): 257-268 (2010). (69 citations)

9) **Perryman, A. L**., Forli, S., Morris, G. M., Burt, C., Cheng, Y., Palmer, M. J., Whitby, K., McCammon, J. A., Phillips, C., & Olson, A. J. "A dynamic model of HIV integrase inhibition and drug resistance," *Journal of Molecular Biology*, 397(2): 600-615 (2010). (59 citations)

8) **Perryman, A. L**.,* Lin, J. H., & McCammon, J. A. "Optimization and computational evaluation of a series of potential active site inhibitors of the V82F/I84V drug-resistant mutant of HIV-1 protease: An application of the Relaxed Complex method of structure-based drug design," *Chemical Biology & Drug Design*, 67(5): 336-345 (2006). (25 citations)

7) **Perryman, A. L**.,* Lin, J. H., & McCammon, J. A. "Restrained molecular dynamics simulations of HIV-1 protease: The first step in validating a new target for drug design," *Biopolymers*, 82(3): 272-284 (2006). (58 citations)

6) **Perryman, A. L**.,* Lin, J. H., & McCammon, J. A. "HIV-1 protease molecular dynamics of a wild-type and of the V82F/I84V mutant: Possible contributions to drug resistance and a potential new target site for drugs," *Protein Science*, 13 (4): 1108-1123 (2004). (223 citations)

5) Lin, J. H., **Perryman, A. L.,** Schames, J. R., & McCammon, J. A. "The Relaxed Complex method: Accommodating receptor flexibility for drug design with an improved scoring scheme," *Biopolymers*, 68 (1): 47-62 (Peter Kollman memorial issue, 2003). (168 citations)

4) **Perryman, A. L**.* & McCammon, J. A. "AutoDocking dinucleotides to the HIV-1 integrase core domain: Exploring possible binding sites for viral and genomic DNA," *J. Medicinal Chemistry* (Letter), 45 (26): 5624-5627 (2002). (41 citations)

3) Lin, J. H., **Perryman, A. L.**, Schames, J. R., & McCammon, J. A. "Computational drug design accommodating receptor flexibility - the Relaxed Complex scheme," *J. American Chemical Society* (Communication), 124 (20): 5632-5633 (2002). (385 citations)

2) **Perryman, A. L**., Cheng, Z., Jurisson, S. S., & Quinn, T. P. "Design and synthesis of technetium and rhenium-cyclized somatostatin analogs," *J. Labelled Compounds and Radiopharmaceuticals*, vol. 42, supplement 1, p. S156-157 (1999). (1 citation)

1) Farr, R. G. Jr., **Perryman, A.L**., & Samudzi, C. T. "Re-clustering the database for crystallization of macromolecules," *J. Crystal Growth*, 183 (4): 653-668 (1998). (20 citations)

News Videos

1) "Anyone with a computer can now help scientists find a cure for the Zika virus," FiOS1 News, reported by Raven Santana, May 19, 2016;
http://www.fios1news.com/newjersey/zika-research-app#.Vz4hBMj3aJI

2) "Rutgers University scientists want public to help with Zika research," News12 New Jersey, reported by Christopher Keating, May 20, 2016; http://newjersey.news12.com/news/rutgers-university-scientists-want-public-to-help-with-zika-research-1.11816750

3) "OpenZika project uses public to help find Zika virus cure," NJTV News (PBS), reported by Michael Hill, May 25, 2016;
http://www.njtvonline.org/news/video/openzika-project-uses-public-help-find-zika-virus-cure/

News Radio Clips

1) "Rutgers researchers seek computing help in quest for Zika treatment," WHYY (NPR) radio, reported by Taunya English, May 31, 2016; http://www.newsworks.org/index.php/local/healthscience/94185-rutgers-researchers-seek-computing-help-in-quest-for-zika-treatment

2) "Discovery May Lead to New Class of AIDS Drugs," KPBS-FM radio, reported by Tom Fudge; Feb. 04, 2010; http://www.kpbs.org/news/2010/feb/04/discovery-may-lead-new-class-aids-drugs/

News Articles

1) "Rutgers researchers using power of Web to help stop Zika," *Bergen Record*, by Lindy Washburn, May 19, 2016. http://www.northjersey.com/news/rutgers-researchers-using-power-of-web-to-help-stop-zika-1.1601659

2) "Rutgers scientists aiding in Zika research project," *Washington Times*, by the Associated Press, May 19, 2016; http://www.washingtontimes.com/news/2016/may/19/rutgers-scientists-aiding-in-zika-research-project/

3) "How you and your laptop can help Rutgers tackle the Zika virus," *Star-Ledger*, by Kathleen O'Brien, May 19, 2016; http://www.nj.com/healthfit/index.ssf/2016/05/how_you_and_your_laptop_can_help_rutgers_tackle_th.html

4) "Fighting the Zika virus with the power of supercomputing," *World Pharma News*, May 19, 2016; http://www.worldpharmanews.com/development/3485-fighting-the-zika-virus-with-the-power-of-supercomputing

5) "Fight Zika by making your smartphone into a supercomputer," *CNBC*, by Dan Mangan, May 19, 2016; http://www.cnbc.com/2016/05/18/fight-zika-by-making-your-smartphone-into-a-supercomputer.html

6) "OpenZika project uses supercomputing power to identify potential drug candidates to cure Zika virus," *News-Medical.Net*, May 19, 2016; http://www.news-medical.net/news/20160519/OpenZika-project-uses-supercomputing-power-to-identify-potential-drug-candidates-to-cure-Zika-virus.aspx

7) "'Everyone Wants to Contribute:' Rutgers Scientists Aid in Zika Research," *NBC10 Philadelphia*, May 20, 2016; http://www.nbcphiladelphia.com/news/health/Rutgers-Scientists-Aid-Zika-Research-380098801.html

8) "International Business Machines Corp Jumps to Fight Zika Virus; Here's How," *Business Finance News*, by Raheel Farooq, May 20, 2016; http://www.businessfinancenews.com/29055-international-business-machines-jumps-to-fight-zika-virus-heres-how/

9) "GO Fight Against Malaria," *Citizen Science, Scientific American* (12/2011), http://www.scientificamerican.com/citizen-science/project.cfm?id=go-fight-against-malaria

10) "Simulations Find Possible HIV Achilles' Heel," by Louisa Dalton. *Biomedical Computation Review*, 2(4):2 (2006). http://www.biomedicalcomputationreview.org/content/simulations-find-possible-hiv-achilles'-heel

Press Releases

1) "Post grid calculations continue to yield progress and inspire new methods against deadly diseases," by Dr. Alexander L. Perryman. http://www.worldcommunitygrid.org/about_us/viewNewsArticle.do?articleId=433

2) "GO Fight Against Malaria update: Promising early findings for malaria & drug-resistant tuberculosis," by Dr. Alexander L. Perryman. http://www.worldcommunitygrid.org/about_us/viewNewsArticle.do?articleId=373

3) "*Jeopardy!* winnings spur IBM and Scripps Research collaboration to fight malaria," by Mika Ono, *TSRI "News & Views*", http://www.scripps.edu/newsandviews/e_20111212/malaria.html (12/12/2011)

4) "I'll take 'Curing Malaria' for $1,000, Alex," by Alex L. Perryman, guest contributor for the "*Citizen IBM*" blog, http://citizenibm.com/2011/11/ill-take-curing-malaria-for-1000-alex.html (11/16/2011)

5) "Two compounds discovered that pave the way for new class of AIDS drug: IBM World Community Grid computing strength powers breakthrough research that will guide their development," by Sandra Dressel, http://www-03.ibm.com/press/us/en/pressrelease/29568.wss (03/02/2010).

6) "Scientists find two compounds that lay the foundation for a new class of AIDS drug," by Mika Ono, *TSRI "News & Views*", 10(5), http://www.scripps.edu/newsandviews/i_20100208/hiv.html and http://www.eurekalert.org/pub_releases/2010-02/sri-srs020310.php (02/08/2010).

7) "Getting into a flap: A new theory about the dynamics of protease may lead to treatment options," by Chael Needle. *Art and Understanding* ("America's AIDS Magazine"), 15(4): 36 (2006). http://www.aumag.org/lifeguide/THApril06.html

8) "Computer simulation hints at new HIV drug target," *Howard Hughes Medical Institute*, (3/10/2006). http://www.hhmi.org/news/computer-simulation-hints-new-hiv-drug-target

9) "SDSC resources help scientists identify possible source of HIV drug resistance," *San Diego Supercomputer Center*, (3/25/2004). http://www.sdsc.edu/News%20Items/PR032504.html

10) "UCSD scientists create new computational method that could shorten time to develop new drugs," *National Partnership for Advanced Computational Infrastructure*, (5/22/2002). http://www.sdsc.edu/News Items/PR052202.html

Patents and Inventions

1) Co-Inventor of new approach to fragment-based crystallographic screening, to facilitate discovery of allosteric inhibitors. See Publication (10).

2) United States Patent 8,865,876, approved 10/21/2014, "Engineered Lectin Oligomers with Antiviral Activity," by Stephen L. Mayo, Jennifer R. Keeffe, and Alexander L. Perryman.

3) Co-Inventor of the "Relaxed Complex Scheme" (RCS) of *in silico* structure-based drug design; one of the 1st approaches to incorporate target flexibility in docking. See publications (3) and (5).

Peer Review Activities (peer reviewed for 24 different journals)

Expert Opinion on Drug Discovery; Scientific Reports (Nature Publishing Group)*; Journal of the American Chemical Society; Journal of Medicinal Chemistry; PROTEINS: Structure, Function, and Bioinformatics; Chemical Biology & Drug Design* (over 20 papers reviewed*); Advances in Pharmacology; Journal of Molecular Biology*; *Journal of Chemical Information & Modeling; Journal of Physical Chemistry; Journal of Molecular Graphics and Modelling; Biopolymers; Journal of Computer-Aided Molecular Design*; *Journal of Computational Chemistry*; *Bioorganic & Medicinal Chemistry Letters*; *Bioinformatics*; *European Journal of Medicinal Chemistry*; *Journal of Chemical Theory and Computation*; *Journal of Molecular Modeling*; *Journal of Theoretical & Computational Chemistry*; *BMC Structural Biology*; *Protein Science*; *SpringerPlus*; and *Drug Discovery Today.*

Awards and Honors

2016	Appointed to Advisory Board of Montclair State University's NSF TUES Type 1 grant: Incorporation of Research Skills into the Undergraduate Biochemistry Curriculum to Create Extraordinary Scientists for the Modern Research Environment
2005 – 2007	Amgen Postdoctoral Fellowship, Div. of Biology, California Institute of Technology
2000 – 2005	Howard Hughes Medical Institute Predoctoral Fellowship, Univ. of CA, San Diego
2000 – 2005	George E. Palade Scholar, Univ. of CA, San Diego
2004	CCG Graduate Excellence Award for the 227th American Chemical Society's National Meeting, by the ACS Div. of Computers in Chem. & by the Chemical Computing Group
2000	Top Senior Award from Phi Lambda Upsilon (Honorary Chemical Society), MU
1999 – 2000	Barry Goldwater Scholar (from U.S. Congress)

1998 – 1999 Beckman Scholar, internship from the Arnold and Mabel Beckman Foundation

1996 – 2000 National Merit Scholar

Teaching and Leadership Experience

2002 Head T.A. for Professor Mauricio Montal's "Introduction to Structural Biochemistry" class (BIBC100) at UCSD; quoting from Professor Montal's T.A. evaluation form of me, I was "Outstanding. Among the best head T.A.'s I have had in the past 10 years. Enthusiastic, committed, knowledgeable, reliable. Alex should be complimented."

2008 - 2012 Instructor for NBCR Summer Institute (National Biomedical Computation Resource); Virtual Screening & Computer Aided Drug Design; UCSD/TSRI; La Jolla, CA, USA

2013 - present Mentoring Ph.D. candidate Xin Wang (leading our project on *Mycobacterium tuberculosis* InhA and teaching him about molecular modeling), Dr. Nisha Mittal (taught her how to perform a nitrocefin-based activity assay for an *Mtb* transpeptidase), Dr. Daigo Inoyama (teaching him how to perform Bayesian modeling), M.D./Ph.D. student Jimmy S. Patel (taught him how to perform the nitrocefin-based activity assay and am teaching him Bayesian modeling), Masters student Fahid Naseer (taught him Bayesian modeling), and M.D./Ph.D. student Hoa M. Pham (teaching him Bayesian modeling)

2015 - 2017 Taught sections of Professor Joel S. Freundlich's graduate student class on "Critical Readings in the Chemical Biology of Pathogens" at the Rutgers University-NJ Medical School. I became the Co-Instructor in 2016.

Molecular Artwork

1) Created cover image for *Journal of Molecular Biology* (March 26, 2010), with Stefano Forli, Ph.D.
2) Created cover images for *Chemical Biology & Drug Design* (August, 2006, and March, 2010)
3) Created all ribbon models for the textbook ***Molecules that Changed the World***, by Prof. K.C. Nicolaou and Dr. Tamsyn Montagnon, WILEY-VCH GmbH & Co. KGaA, (2008)
4) Created cover images for *Biopolymers* (March, 2002, and June 15, 2006)
5) Created cover image for *Protein Science* (April 2004)

References (see http://www.linkedin.com/in/AlexLPerryman for several recommendations)

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Dissertation advisor and Co-Inventor of Relaxed Complex Scheme
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The Scripps Research Institute.
Postdoctoral advisor (previous) (858) 784-9702 olson@scripps.edu

Sean Ekins, Ph.D., D.Sc., Founder and CEO, Collaborations Pharmaceuticals, Inc., Fuquay-Varina, NC, and CEO, Phoenix Nest, Inc., Brooklyn, NY.
Collaborator on machine-learning models, *Mtb* InhA, and *Mtb* transpeptidase projects. Co-P.I .of OpenZika (215) 687-1320 collaborationspharma@gmail.com

Garrett M. Morris, D. Phil., Associate Professor, Systems Approaches to Biomedicine, and Director of the Systems Approaches to Biomedical Science Centre for Doctoral Training, University of Oxford, UK.
Co-P.I. of HIV Integrase project & collaborator on FightAIDS@Home and GO Fight Against Malaria projects. +44 1865-281770 garrett.morris@stats.ox.ac.uk