

Gregory W. Kyro

Computational Biophysical Chemistry PhD Student at Yale University

Fellow of the National Science Foundation

Founder & President of the Yale University Chapter of the Biophysical Society

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Other:  [LinkedIn](#) |  [Google Scholar](#) |  [GitHub](#)

TL;DR

I am a Chemistry PhD Student at Yale, Fellow of the National Science Foundation, and Founder and President of the Yale University Chapter of the Biophysical Society. My research pertains to the development of deep learning methods for modeling protein-small molecule interactions.

During the first year of my PhD, I created [HAC-Net](#) — a deep learning model that, at the time, was the state of the art for predicting protein-ligand binding affinity — which was used to identify a potential [inhibitor of a G protein-coupled receptor](#) whose overexpression leads to cancer, diabetes, and multiple sclerosis, as well as a potential [antivirulence drug for drug-resistant staphylococcal infections](#). During the second year of my PhD, I created [ChemSpaceAL](#) — the first active learning methodology for fine-tuning a molecular generative model toward a specified protein target — which is being utilized in collaboration with experimental biochemists at Brown University to design small-molecule binders to the HNH domain of CRISPR-Cas9 to enhance its specificity for target DNA sequences. During the third year of my PhD, I created [CardioGenAI](#) — a generative deep learning framework for re-engineering drugs for reduced hERG-related cardiotoxicity while preserving their primary pharmacology — which I applied to specific programs within Pfizer R&D that were dealing with hERG liabilities. During the fourth and last year of my PhD, I developed [T-ALPHA](#) — the current state-of-the-art deep learning model for predicting protein-ligand binding affinity — which incorporates an uncertainty-aware self-learning method for protein-specific alignment.

In addition, I developed a [method for describing intraprotein information transfer](#) as the propagation of electrostatic couplings throughout a secondary structure element-based network, which has led to valuable insights into the allosteric mechanisms of multiple important biological systems such as [CRISPR-Cas9](#), [imidazole glycerol phosphate synthase](#), and [D-dopachrome tautomerase](#). Moreover, I developed software for PROTACs screening at OpenEye Scientific, aided in the development of quantum computing-based methods for studying small molecules in collaboration with NVIDIA and Moderna, and contributed to the fine-tuning of OpenAI's large language models.

I co-developed an AI-based rapid synthesis framework that was acquired by Merck Group and is currently being integrated across multiple teams within the company. I have also published numerous [papers](#) in top-tier academic journals, won first place at highly selective and competitive [competitions](#), presented my work at several conferences, created multiple [Python packages](#), and established various collaborations with labs around the world. For these reasons, I have received numerous highly prestigious awards and appeared in Yale News multiple times.

Education

Yale University

05/23 – 05/25

PhD in Computational Biophysical Chemistry

Advisor: Prof. Victor S. Batista

Yale University

09/21 – 12/23

MS in Computational Biophysical Chemistry

GPA: 4.0 / 4.0

SUNY Binghamton

09/16 – 05/21

BS in Chemistry, Minors in Biology & Mathematics

Major GPA: 4.0 / 4.0

Research Experience

Laboratory of Prof. Victor S. Batista, Yale University

09/21 – Present

National Science Foundation Graduate Research Fellow, PhD Candidate

- Developed numerous state-of-the-art deep learning methods for modeling protein-small molecule interactions which have been applied to successfully identify multiple small-molecule drug candidates that are currently being pursued as therapeutics
- Developed statistical methods predicated on concepts from graph theory and information theory to characterize information transfer in proteins which have been applied to derive quantitative insights into the allosteric mechanisms of multiple biologically significant systems

Pfizer Research & Development

05/24 – 12/24

Computational Safety Sciences Intern

- Developed a generative deep learning framework for re-engineering drug candidates for reduced hERG liability while preserving their primary pharmacology, and applied it to internal drug development programs dealing with hERG-related challenges

OpenAI (via Scale AI)

03/24 – 06/24

Fine-tuning Prompt Engineer

- Contributed to the fine-tuning of OpenAI's large language models by crafting scientifically rigorous Q&A-based prompts pertaining to mathematics, physics, and chemistry to enhance the models' scientific domain expertise

OpenEye Scientific

05/23 – 08/23

Scientific Software Developer Intern

- Led the development of a deep learning model for classifying protein-protein interaction interfaces which was integrated into the company's virtual screening pipeline for PROTACs

NASA (via PreScouter)

06/21 – 09/21

Science & Technology Consultant

- Consulted for NASA on cutting-edge advancements pertaining to energy storage, privacy-preserving networks, image detection, aerial surveillance, and aerodynamic levitation

Laboratory of Prof. Alistair J. Lees, SUNY Binghamton

08/17 – 06/21

Undergraduate Researcher

- Revealed insights into excited-state mechanisms in binuclear rhenium(I)-based organometallic systems using computational methods (quantum chemistry calculations) and experimental spectroscopy (NMR, UV-Vis, fluorescence, and IR spectroscopy), ultimately leading to anion sensor-based applications

Innovations Acquired by Pharma

- **Innovation:** SAGE – a platform that incorporates AI, cutting-edge reactions, and automated synthesis to reduce attrition in early-stage drug discovery | **Acquired by:** Merck Group, 08/24

Selected Awards, Scholarships, & Honors

- *First Place, Merck Innovation Cup* | Merck Group 07/24
- *Graduate Research Fellowship* | National Science Foundation 03/23
- *Conference Travel Fund* | Yale University 02/23
- *Award No. 5T32GM008283-35* | National Institutes of Health 09/22
- *Biophysical Training Grant* | National Institutes of Health 08/21
- *Stanley K. Madan Award in Inorganic Chemistry* | SUNY Binghamton 05/21
- *Honors Thesis in Chemistry* | SUNY Binghamton 05/21
- *Summer Scholars Program Award* | SUNY Binghamton 06/21
- *SUNY Binghamton Undergraduate Research Award for Spring 2020* | SUNY Binghamton 01/20
- *SUNY Binghamton Undergraduate Research Award for Fall 2019* | SUNY Binghamton 09/19
- *Research Conference Travel Fund* | SUNY Binghamton 03/19
- *SUNY Binghamton Undergraduate Research Award for Spring 2019* | SUNY Binghamton 01/19
- *SUNY Binghamton Undergraduate Research Award for Fall 2018* | SUNY Binghamton 09/18
- *SUNY Binghamton Undergraduate Research Award for Spring 2018* | SUNY Binghamton 01/18
- *SUNY Binghamton Undergraduate Research Award for Fall 2017* | SUNY Binghamton 09/17

Selected Publications

- [18] **Kyro, GW**; Wong, G; Batista, VS. "Data Augmentation via Combinatorial Subset Sampling for Enhanced Ranking of Protein-Ligand Binding Affinities". [In Progress].
- [17] **Kyro, GW**; Qiu, T; Batista, VS. "A Model-Centric Review of Deep Learning for Protein Design". *Chemical Review* [Under Review]. DOI: [10.48550/arXiv.2502.19173](https://doi.org/10.48550/arXiv.2502.19173)
- [16] **Kyro, GW**; Smaldone, AM; Shee, Y; Xu, T; Batista, VS. "T-ALPHA: A Hierarchical Transformer-Based Deep Neural Network for Protein-Ligand Binding Affinity Prediction with Uncertainty-Aware Self-Learning for Protein-Specific Alignment". *Journal of Chemical Information and Modeling*. 2025. DOI: [10.1021/acs.jcim.4c02332](https://doi.org/10.1021/acs.jcim.4c02332)
- [15] **Kyro, GW**; Batista, VS. "Hierarchical Cross-Scale Transformer Architecture for Bottom-Up Reasoning". *TechRxiv*. 2024. DOI: [10.36227/techrxiv.173121338.85984992/v1](https://doi.org/10.36227/techrxiv.173121338.85984992/v1)
- [14] Smaldone, AM; Shee, Y; **Kyro, GW**; Farag, MH; Chandani, Z; Kysoeva, E; Batista, VS. "A Hybrid Transformer Architecture with a Quantized Self-Attention Mechanism Applied to Molecular Generation". *Journal of Chemical Theory and Computation* [Under Review]. DOI: [10.48550/arXiv.2502.19214](https://doi.org/10.48550/arXiv.2502.19214)
- [13] Smaldone, AM; **Kyro, GW**; Shee, Y ; Batista, VS. "Quantum Machine Learning in Drug Discovery: Applications in Academia and Pharmaceutical Industries". *Chemical Reviews* [Accepted]. DOI: [10.48550/arXiv.2409.15645](https://doi.org/10.48550/arXiv.2409.15645)
- [12] **Kyro, GW**; Martin, MT ; Watt, ED; Batista, VS. "CardioGenAI: A Machine Learning-based Framework for Re-engineering Drugs for Reduced hERG Liability". *Journal of Cheminformatics* [Accepted]. DOI: [10.48550/arXiv.2403.07632](https://doi.org/10.48550/arXiv.2403.07632)

- [11] **Kyro, GW**; Morgunov, A ; Brent, RI; Batista, VS. "ChemSpaceAL: An Efficient Active Learning Methodology Applied to Protein-Specific Molecular Generation". *Journal of Chemical Information and Modeling*. 2024, 64, 3, 653-665. DOI: [10.1021/acs.jcim.3c01456](https://doi.org/10.1021/acs.jcim.3c01456)
- [10] **Kyro, GW**; Brent, RI; Batista, VS. "HAC-Net: A Hybrid Attention-based Convolutional Neural Network for Highly Accurate Protein-Ligand Binding Affinity Prediction". *Journal of Chemical Information and Modeling*. 2023, 63, 7, 1947-1960. DOI: [10.1021/acs.jcim.3c00251](https://doi.org/10.1021/acs.jcim.3c00251)
- [9] Maschietto, F; Allen, B; **Kyro, GW**; Batista, VS. "MDiGest: A Python Package for Describing Allostery from Molecular Dynamics Simulations". *Journal of Chemical Physics*. 2023, 158, 215103. DOI: [10.1063/5.0140453](https://doi.org/10.1063/5.0140453)
- [8] Smaldone, AM; **Kyro, GW**; Batista, VS. "Quantum Convolutional Neural Networks for Multi-Channel Supervised Learning". *Quantum Machine Intelligence*. 2023, 5, 41. DOI: [10.1007/s42484-023-00130-3](https://doi.org/10.1007/s42484-023-00130-3)
- [7] Yang, KR; **Kyro, GW**; Batista, VS. "The Landscape of Computational Approaches for Artificial Photosynthesis". *Nature Computational Science*. 2023, 3, 504-513. DOI: [10.1038/s43588-023-00450-1](https://doi.org/10.1038/s43588-023-00450-1)
- [6] Chen, E; Widjaja, V; **Kyro, GW**; Allen, B; Das, P; Bhandari, V; Lolis, EJ; Batista, VS; Lisi, GP. "Mapping N- to C-terminal Allosteric Coupling Through Disruption of the Putative CD74 Activation Site in D-Dopachrome Tautomerase". *Journal of Biological Chemistry*. 2023, 299, 6, 104729. DOI: [10.1016/j.jbc.2023.104729](https://doi.org/10.1016/j.jbc.2023.104729)
- [5] Maschietto, F; Morzan, U; Tofoleanu, F; Gheereart, A; Chaudhuri, A; **Kyro, GW**; Nekrasov, P; Brooks, B; Loria, JP; Rivalta, I; Batista, VS. "Turning Up the Heat Mimics Allosteric Signaling in Imidazole-Glycerol Phosphate Synthase". *Nature Communications*. 2023, 14, 2239. DOI: [10.1038/s41467-023-37956-1](https://doi.org/10.1038/s41467-023-37956-1)
- [4] Maschietto, F; **Kyro, GW**; Allen, B; Batista, VS. "Electrostatic Networks for Characterization of Allosteric Pathways in Cas9 Apo, RNA- and DNA-Bound Forms". *Biophysical Journal*. 2023, 122 (3). DOI: [10.1016/j.bpj.2022.11.389](https://doi.org/10.1016/j.bpj.2022.11.389)
- [3] Wang, J; Arantes, PR; Ahsan, M; Sinha, S; **Kyro, GW**; Maschietto, F; Allen, B; Skeens, E; Lisi, GP; Batista, VS; Palermo, G. "Twisting and Swiveling Domain Motions in Cas9 to Recognize Target DNA Duplexes, Make Double-Strand Breaks, and Release Cleaved Duplexes". *Frontiers in Molecular Biosciences*. 2023, 9. DOI: [10.3389/fmolb.2022.1072733](https://doi.org/10.3389/fmolb.2022.1072733)
- [2] Wang, J; Skeens, E; Arantes, P; Maschietto, F; Allen, B; **Kyro, GW**; Lisi, GP; Palermo, G; Batista, VS. "Structural Basis for Reduced Dynamics of Three Engineered HNH Endonuclease Lys-to-Ala Mutants for the Clustered Regularly Interspaced Short Palindromic Repeat (CRISPR)-Associated 9 (CRISPR/Cas9) Enzyme". *Biochemistry*. 2022, 61 (9), 785-794. DOI: [10.1021/acs.biochem.2c00127](https://doi.org/10.1021/acs.biochem.2c00127)
- [1] **Kyro, GW**; Lees, AJ. "Photophysics of Rhenium(I) Polypyridyl-based Complexes and Their Employment as Highly Sensitive Anion Sensors". 2021. DOI: [10.13140/RG.2.2.29980.56962](https://doi.org/10.13140/RG.2.2.29980.56962)

Selected Presentations & Lectures

- [28] "Quantum-Classical Machine Learning Methods for Optimizing Drug Toxicity". Invited Research Talk at *QuantumCT Industry Collaboration Forum, Yale Ventures* (2025).
- [27] "Current State-of-the-Art Deep Learning Models for Protein Design". Invited Research Talk at *Biophysical Chemistry Seminar, Yale University* (2025).
- [26] "Introduction to Deep Learning for Biochemistry". Invited Guest Lecture at *CHEM 584: Machine Learning and Quantum Computing, Yale University* (2025).

- [25] "Transformers for Modeling Protein-Ligand Interactions". Poster Presentation at *Chemical Research Symposium, Yale University* (2025).
- [24] "A Hybrid Quantum-Classical Transformer Architecture with a Quantized Self-Attention Mechanism Applied to Molecular Generation". Poster Presentation at *Chemical Research Symposium, Yale University* (2025).
- [23] "Machine Learning for Modeling Cardiac Ion Channels". Invited Research Talk at *Scientific Seminar, Novartis Institutes for Biomedical Research* (2025).
- [22] "T-ALPHA: A Hierarchical Transformer-Based Deep Neural Network for Protein-Ligand Binding Affinity Prediction with Uncertainty-Aware Self-Learning for Protein-Specific Alignment". Invited Research Talk at *10th Annual Biophysics and Structural Biology Research Symposium, Yale University* (2025).
- [21] "Assessment of Different Machine Learning Architectures for hERG Activity Prediction". Poster Presentation at *Computational Medicinal Chemistry School, Novartis Institutes for Biomedical Research* (2024).
- [20] "Some of the Problems with Public Datasets for Protein-Ligand Binding Affinity Prediction". Invited Research Talk at *Computational Biophysics and Drug Design Meeting, Bernal Institute at the University of Limerick* (2024).
- [19] "Generative AI Methods for Lead Optimization in Drug Discovery". Poster Presentation at *Chemical Research Symposium, Yale University* (2024).
- [18] "CardioGenAI: A Machine Learning-based Framework for Re-engineering Drugs for Reduced hERG Liability". Invited Research Talk at *Innovation Cup Alumni Symposium, Merck Group* (2024).
- [17] "A Machine Learning-based Framework for Re-engineering Drugs for Reduced hERG Liability". Invited Research Talk at *Global Discovery Investigative Toxicology and Translational Sciences—Computational Safety Sciences Town Hall, Groton Laboratories at Pfizer Research & Development* (2024).
- [16] "CardioGenAI: A Machine Learning-based Framework for Re-engineering Drugs for Reduced hERG Liability". Poster Presentation at *Summer Intern Poster Session, Groton Laboratories at Pfizer Research & Development* (2024).
- [15] "A Generative AI-based Framework for Toxicity Applications in Early-Stage Drug Development". Poster Presentation at *9th Annual Biophysics and Structural Biology Research Symposium, Yale University* (2024).
- [14] "A Hybrid Quantum-Classical Machine Learning Framework for Drug Toxicity Applications". Invited Research Talk at *QuantumCT Industry Collaboration Forum, Yale West Campus* (2024).
- [13] "Generative Machine Learning and Active Learning Methods for Hit Identification in Drug Discovery". Poster Presentation at *Sterling Chemistry Laboratory 101st Anniversary Symposium, Yale University* (2024).
- [12] "CardioGenAI: A Machine Learning-based Framework for Re-engineering Drugs for Reduced hERG Liability". Poster Presentation at *19th Annual Drug Discovery Chemistry Conference* (2024).
- [11] "ChemSpaceAL: An Efficient Active Learning Methodology Applied to Protein-Specific Molecular Generation". Invited Research Talk at *Annual Biophysical Society Meeting* (2024).

- [10] "Machine Learning and Statistical Methods for Modulating Protein Function with Small Molecule Inhibitors". Invited Research Talk at *National Institutes of Health Biophysics Seminar, Yale University* (2023).
- [9] "HAC-Net: A Hybrid Attention-based Convolutional Neural Network for Highly Accurate Protein-Ligand Binding Affinity Prediction". Poster Presentation at *Annual Biophysical Society Meeting* (2023).
- [8] "Introduction to Deep Learning for Chemistry". Invited Guest Lecture at *CHEM 584: Machine Learning and Quantum Computing, Yale University* (2022).
- [7] "Photophysics of Binuclear Rhenium (I) Tricarbonyl Complexes and Their Employment as Anion Sensors Through Charge-Mediated Hydrogen Bonding". Poster Presentation at *261st American Chemical Society National Meeting & Exposition* (2021).
- [6] "Variable Anion Recognition Sites in Phosphorescent Rhenium (I) Polypyridyl-based Sensors". Poster Presentation at *259th American Chemical Society National Meeting & Exposition* (2020).
- [5] "Photophysics of Polypyridyl-based Rhenium (I) Complexes and Their Employment as Highly Sensitive Anion Sensors". Poster Presentation at *3rd SUNY Binghamton Conference in Chemistry Research* (2020).
- [4] "Highly Sensitive Rhenium (I) Sensors for Anions Through Amide Hydrogen Bonding". Poster Presentation at *Undergraduate Research Conference, SUNY Binghamton* (2020).
- [3] "Amide Protons as Binding Groups in a Polypyridyl-based Rhenium (I) Anion Sensor" Poster Presentation in Poster Presentations at *257th American Chemical Society National Meeting & Exposition* (2019).
- [2] "Excited-State Properties of Rhenium (I)-based Anion Sensors". Poster Presentation at *2nd SUNY Binghamton Conference in Chemistry Research* (2019).
- [1] "Organometallic Complexes as Anion Sensors: a Highly Sensitive Rhenium (I) Complex for Cyanide and Halide Anions". Poster Presentation at *1st SUNY Binghamton Conference in Chemistry Research* (2018).

Professional & Leadership Experience

- | | |
|---|-----------------|
| • <i>Founder & President</i> Yale University Chapter of the Biophysical Society | 01/24 – Present |
| • <i>Scientific Reviewer</i> Journal of Chemical Theory and Computation | 10/22 – Present |
| • <i>Scientific Reviewer</i> Journal of Molecular Modeling | 02/25 – Present |
| • <i>Biophysics Research Seminar Organizer</i> Yale University | 08/22 – 05/24 |
| • <i>Founder, Mentor & Tutor</i> Illuminating Minds Academy | 09/23 – 01/24 |
| • <i>Scientific Blog Writer</i> Biophysical Society | 02/23 – 04/23 |
| • <i>STEM Tutor</i> Transformation Tutoring | 12/21 – 12/22 |
| • <i>Research Ambassador</i> Undergraduate Research Center at SUNY Binghamton | 8/19 – 06/21 |
| • <i>Network and Computer Systems Intern</i> Rapid Access Communications Inc. | 11/19 – 02/20 |

Teaching Experience

- *Teaching Fellow* | Advanced General Chemistry II | Yale University 01/25 – Present
- *Teaching Fellow* | General Chemistry I | Yale University 08/24 – 12/24
- *Teaching Fellow* | Matrix Methods in Quantum Mechanics | Yale University 10/23 – 12/23
- *Teaching Fellow* | Machine Learning & Quantum Computing | Yale University 03/23 – 06/23
- *Teaching Assistant* | Inorganic Chemistry Fall 2020 | SUNY Binghamton 09/20 – 12/20
- *Teaching Assistant* | Chemical Principles I Fall 2020 | SUNY Binghamton 09/20 – 12/20
- *Teaching Assistant* | Inorganic Chemistry Fall 2019 | SUNY Binghamton 09/19 – 12/19
- *Teaching Assistant* | Chemical Principles II Spring 2019 | SUNY Binghamton 01/19 – 05/19
- *Teaching Assistant* | Introduction to Chemistry Fall 2017 | SUNY Binghamton 09/17 – 12/17

Technical Skills

- **Deep Learning Architectures:** transformers, diffusion models, GANs, autoencoders, RNNs, LSTMs, GRUs, CNNs, GNNs, LLMs and more
- **Machine Learning Architectures:** linear regression, logistic regression, decision trees, random forests, support vector machines, gradient boosting machines, and more
- **Machine Learning Techniques:** active learning, reinforcement learning, transfer learning, feature engineering, dimensionality reduction, regularization, hyperparameter optimization, ensemble methods, cross-validation, clustering, data preprocessing and more
- **Python Software Packages:** PyTorch, TensorFlow, Scikit-Learn, XGBoost, PyG, RDKit, BioPython, MDAnalysis, PyMOL, Open Babel, ProLIF, OpenMM, PDBFixer, Optuna, SciPy, NumPy, Pandas, Matplotlib, Seaborn, and more
- **Cheminformatics:** molecular property prediction, molecular interaction analysis, molecular modeling, virtual screening, ligand-based drug design, structure-based drug design, Molecular Dynamics simulation analysis, molecular feature representations, quantitative structure-activity relationship modeling, molecular similarity analysis, conformational analysis, protein visualization, molecular mechanical calculations, quantum chemistry calculations, and more
- **Data Analysis:** statistical and mathematical modeling, time series analysis, visualization, network analysis, optimization techniques, and more
- **Quantum Computing:** quantum machine learning, quantum circuit construction, quantum algorithms, and more

Foundational Skills

- **Problem Solving & Critical Thinking:** first-principles reasoning, creativity skills, optimization, and more
- **Leadership & Project Management:** idea generation, time management, multitasking, strategic thinking, mentorship, and more
- **Communication & Collaboration:** public speaking, technical writing, interpersonal skills, and more
- **Adaptability & Execution:** extreme discipline, versatility, curiosity, sangfroid, growth mindset, and more

Selected GitHub Repositories

- [6] **T-ALPHA:** github.com/gregory-kyro/T-ALPHA
- [5] **CardioGenAI:** github.com/gregory-kyro/CardioGenAI
- [4] **ChemSpaceAL:** github.com/gregory-kyro/ChemSpaceAL
- [3] **HAC-Net:** github.com/gregory-kyro/HAC-Net
- [2] **molecular_dynamics_analyses:** github.com/gregory-kyro/molecular_dynamics_analyses
- [1] **eigenvector_centrality:** github.com/gregory-kyro/eigenvector_centrality

Professional Development

Massachusetts Institute of Technology, edX

- Machine Learning With Python 06/22
- Biochemistry: Biomolecules, Methods & Mechanisms 05/22
- Computational Thinking Using Python 07/21

Harvard University, edX

- Principles of Biochemistry 05/22
- Using Python for Research 07/21

Selected Coursework

Yale University

Machine Learning & Computational Modeling:	Machine Learning & Quantum Computing, Computational Chemistry, Computer Science & The Modern Intellectual Agenda
Quantum Physics & Statistics:	Advanced Quantum Mechanics, Statistical Mechanics I and II, Quantum Mechanics I and II
Biophysics:	Biochemical Rates & Mechanisms I and II, Quantitative Biochemical Imaging, Biophysical Optical Spectroscopy

SUNY Binghamton

Quantum Systems & Chemical Dynamics:	Quantum Chemistry, Physical Chemistry, Molecular Photochemistry
Molecular Biophysics & Biochemistry:	Biophysical Chemistry, Molecular Biology, Molecular Genetics
Chemistry Principles:	Intermediate Inorganic Chemistry, Chemical Principles I and II, Transition Metal Chemistry, Organic Chemistry I and II, Analytical Chemistry
Mathematical, Physical & Data Science Principles:	Infinite Series, Integration Techniques & Application, Integral Calculus, Differential Calculus, General Physics I and II, Biostatistics
Biological Systems:	Organismal Biology, Evolutionary Biology, Human Biology & Health

Current Research Collaborations

Industry Collaborations

- Pfizer (Drug Safety and Toxicology)
- NVIDIA (Quantum Algorithm Engineering)
- Moderna (Computational Protein Design and Modeling)
- Novartis (Preclinical Safety)
- Boehringer Ingelheim (Computational Antibody and Protein Engineering)

Academic Collaborations

- Yale School of Medicine (Schwartz Lab, Cardiology)
- Yale School of Medicine (Hafler Lab, Neuroimmunology)
- Yale School of Medicine (Hafler Lab, Pulmonology)
- Brown University (Lisi Lab, Molecular Biology & Biochemistry)
- University of California, Riverside (Palermo Lab, Bioengineering)
- Yale University (Loria Lab, Chemistry & Biophysics)

Selected Media Coverage

- Featured by [Merck Group](#) for winning first place at the 2024 Merck Innovation Cup
- Featured in the [Yale Alumni Magazine](#) for sharing insights on biochemistry research
- Featured in [Yale News](#) for becoming a National Science Foundation fellow
- Featured by the [Yale University Chapter of the Biophysical Society](#) for contributing to quantum machine learning in drug discovery
- Featured in the [Biophysical Society Blog](#) for sharing opinions about work presented at the 2023 Biophysical Society Annual Meeting

Professional Memberships

- QuantumCT
- American Chemical Society
- Biophysical Society
- OpenLabs at Yale

Volunteer Activities

- | | |
|--|-----------------|
| • <i>Scientific Speaker</i> Yale Pathways to Science | 12/23 – Present |
| • <i>Outreach Volunteer</i> American Chemical Society | 06/19 – 06/20 |
| • <i>Medical Volunteer</i> Long Island Jewish Medical Center | 06/17 – 01/19 |
| • <i>Patient Care Volunteer</i> Ronalds McDonald House Charities | 06/17 – 12/18 |
| • <i>Gift of Sight Volunteer</i> Luxottica Group S.p.A. | 05/16 – 08/16 |
| • <i>Special Education Volunteer</i> Merillon Little League Baseball | 06/15 – 08/15 |

Additional Achievements

- Scored a perfect 28/28 in the New York State School Music Association guitar competition at level 4 when I was 8 years old
- Have done a high-intensity workout at least once every day since 2010 (no exceptions)
- 2944 puzzle rating (99.9th percentile) and 1999 bullet rating (99.8th percentile) on chess.com
- Five-sport athlete in high school (baseball, wrestling, basketball, track, football)

References

Victor S. Batista, Yale University

- Position: John Gamble Kirkwood Professor of Chemistry
- Relationship: PhD Advisor
- Email: victor.batista@yale.edu

Matthew T. Martin, Pfizer R&D

- Position: Executive Director, Global Head of Computational Safety Sciences
- Relationship: Research Supervisor
- Email: matthew.martin@pfizer.com

J Patrick Loria, Yale University

- Position: Professor of Chemistry & Biophysics, Director of Graduate Studies
- Relationship: Research Collaborator and Thesis Committee Member
- Email: patrick.loria@yale.edu

Vishal Vaidya, Pfizer R&D

- Position: Vice President, Chief Toxicology Scientist
- Relationship: Research Collaborator and Career Mentor
- Email: vishal.vaidya@pfizer.com

Alistair J. Lees, SUNY Binghamton

- Position: Professor of Chemistry
- Relationship: Undergraduate Research Advisor
- Email: alees@binghamton.edu

Tianyu Zhu, Yale University

- Position: Professor of Chemistry
- Relationship: Research Collaborator and Thesis Committee Member
- Email: tianyu.zhu@yale.edu

John R. Swierk, SUNY Binghamton

- Position: Professor of Chemistry
- Relationship: Undergraduate Academic Advisor and Honors Thesis Committee Member
- Email: jswierk@binghamton.edu

Christof T. Grewer, SUNY Binghamton

- Position: Professor of Biological and Physical Chemistry
- Relationship: Professor and Honors Thesis Committee Member
- Email: cgrewer@binghamton.edu