

## **Publications**

- [10] **Kyro, GW** et al. "HAC-Net: A Hybrid Attention-Based Convolutional Neural Network for Highly Accurate Protein-Ligand Binding Affinity Prediction" *Nat. Commun.* [Submitted] (2022).
- [9] Maschietto, F; **Kyro, GW** et al. "MDiGest: A Comprehensive Toolkit for Detection of Allosteric Communication From Molecular Dynamics Simulations of Biochemical Systems" *J. Chem. Phys.* [Submitted] (2022).
- [8] Yang, KR; **Kyro, GW** et al. "Unlocking Unlimited Sustainable Energy: Computational Approaches to Modeling Artificial Photosynthesis" *Nat. Comput. Sci.* [Submitted] (2022).
- [7] **Kyro, GW** et al. "Electrostatic Networks for Characterization of Allosteric Communication in the Cas9 Enzyme" [In Preparation] (2022).
- [6] Wang, J; Skeens, E; Arantes, P; Maschietto, F; **Kyro, GW** et al. "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, 785-794.
- [5] Morzan, U; Tofoleanu, F; **Kyro, GW** et al. "The Heat is On: Temperature Increase Mimics Allosteric Signaling in Imidazole-Glycerol Phosphate Synthase" *Nat. Commun.* [Submitted] (2022).
- [4] Chen, E; Widjaja, V; **Kyro, GW** et al. "Mapping N- to C-terminal Allosteric Coupling Through Disruption of the Putative CD74 Activation Site in D-Dopachrome Tautomerase" *Biochemistry* [Submitted] (2022).
- [3] Wang, J; Arantes, R; **Kyro, GW** et al. "Structural and Dynamic Insights into Cas9: How It Recognizes Target DNA Duplex, Makes Double-Strand Breaks, and Releases Cleaved Duplexes" *ACS Chem. Bio.* [Submitted] (2022).
- [2] **Kyro, GW** "Hac-Net v1.0.0" GitHub (2022) doi: <https://doi.org/10.5281/zenodo.7168142>.
- [1] **Kyro, GW** et al. "Photophysics of Rhenium(I) Polypyridyl-Based Complexes and Their Employment as Highly Sensitive Anion Sensors" [Preprint] (2021) doi: <http://dx.doi.org/10.13140/RG.2.2.29980.56962>.