HECTOR ALBERTO CHAIRES

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GitHub: QuantaQuaestio **Website:** https://quantaquaestio.github.io/assets/personalwebsite/index.html

EDUCATION

Rice University

BS in Biochemistry and Cell Biology (Distinction in Research and Creative Work) May 2019

EXPERIENCE

Novartis

Research Scientist II (Protein Sciences/Discovery Sciences) Jun 2025- Present

- Applied MD-derived residence time analysis to rationalize SPR kinetic differences across ligands differing by single functional group modifications.
- Solved co-crystal structures using seeding to elucidate SAR of a cryptic binding pocket.
- Collaborated with medicinal chemists to understand SAR and guide compound design by solving crystal structures of key ligands and running glide docking and co-folding using Boltz-2.

Relay Therapeutics

Research Associate II (Structural Biologist and Protein Engineer) Aug 2022- Apr 2025

- Designed libraries of primary amines from the top 70 nitrogen heterocycles most frequently found in FDA-approved drugs through 2024. Used this library to enumerate modifications on a lead compound. Employed docking, Amber MD stability simulations, and FEP analyses to prioritize designs, resulting in compounds with 5-fold improvement in potency confirmed by SPR.
- Managed 2 FTEs at a CRO for protein production, purification, and characterization (LC-MS, SDS-PAGE, nDSF, SEC-MALS, FSEC) for assay development, hit-finding, and structural biology across three projects.
- Enabled crystal system and performed fragment based screening to identify cryptic pocket on an undruggable transcription factor.
- Developed novel X-ray crystal systems to enable structure-based medicinal chemistry against two novel protein targets leading to identification of cryptic allosteric pockets.
- Developed an aggregation based light scattering assay to measure protein stabilization. Onboarded and trained team members on nDSF, DLS, and SLS using the Uncle from Unchained Labs.
- Implemented Boltz-1 and Chai-1 for construct design, VHH epitope prediction, and to predict protein-protein interactions.

Researcher in the Fraser Lab at UCSF

Junior Specialist II (University of California San Francisco, J. S. Fraser Lab) May 2019- Jul 2020

- Solved X-ray crystal structures of protein-ligand complexes to understand binding interactions of novel streptogramin analogs that overcome resistance in S. aureus by inhibiting acetyltransferase VatA. Used cryo-EM to analyze the binding mode of streptogramin analogs to *P. falciparum* and *O. cuniculus* ribosomes.

HHMI Exceptional Research Opportunities Program May-Aug 2017, 2018

Research Assistant (Harvard Medical School, S. C. Harrison Lab)

- Solved an X-ray crystal structure of a Fab from primary B-cells derived from *Rhesus macaque*s immunized with Influenza A, H1N1 to understand affinity maturation. Used phage display to affinity mature a broadly neutralizing antibody against novel circulating strains of Influenza A.

PUBLICATIONS

Li Q*, Pellegrino J*, Lee DJ, Tran AA, **Chaires HA,** Wang R, Park JE, Ji K, Chow D, Zhang N, Brilot AF, Biel JT, van Zundert G, Borrelli K, Shinabarger D, Wolfe C, Murray B, Jacobson MP, Fraser JS, Seiple IB. Synthetic group A streptogramin antibiotics that overcome Vat resistance. *Nature* 586**,** 145–150 (2020)

Chaires, H. A., Bajic, G., Moody, M., & Harrison, S. C. (2018). Structure of influenza hemagglutinin antibody from *Rhesus Macaque* with disulfide bond in its CDRH3. *ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY*, *256*.

Chaires, H. A., Fraser J.S. Crystal structure of streptogramin A acetyltransferase VatA from *Staphylococcus aureus* in complex with streptogramin analog F0224 (46) PDB: **6X3J**
Chaires, H. A., Fraser J.S. Crystal structure of streptogramin A acetyltransferase VatA from *Staphylococcus aureus* in complex with streptogramin analog F1037 (47) PDB: **6X3C**

TECHNICAL SKILLS

Programming: Python, C, HTML/CSS/JavaScript
Systems/Cloud/Version Control: Linux, AWS (user), Jupyter
Software/Tools: Maestro, cryoSPARC, OpenMM, OpenFE, PyMOL, Boltz-2, Prism, Phenix, Coot, LiveDesign