

DAVID FOUTCH

Graph-Based AI for Structural Biology

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Summary

Structural Bioinformatics & Graph ML Specialist with 5 years of experience modeling protein systems, developing interactive visualization tools, and extracting structural features that drive biological function. Skilled in building graph-based models that integrate molecular biology with modern machine learning.

Work Experience

Blind Lab, Vanderbilt University Medical Center *Computational Biologist* May 2023–Present

- **Drug Screening Strategy:** Designed a novel graph-theoretical approach to identify structural mechanisms underlying differential free energy in LRH-1 ligand-bound proteins, informing molecular screening strategies.
- **Protein Structure Network Analysis Plugin:** Developed a PyMOL plugin integrating NetworkX and RING to build residue interaction networks, identifying structural features modulating protein function and ligand binding.
- **Interactive Protein Structure Network Explorer:** Built an interactive Dash/Flask web app to visualize protein structure networks using Python in 2D/3D with centrality metrics and sequence mapping.
- **GraphSAGE Workflow:** Embeds residue networks for predicting free energy differences and identifying functional structural variants.

Center for Precision Medicine, Vanderbilt University Medical Center *Statistical Analyst* May 2021–May 2023

- **Knowledge Graph for Clinical Phenotypes:** Built Dash/Flask web app linked to a cloud-hosted Neo4j Aura graph database connecting ICD, CPT, and CUI codes to clinical phenotypes.
- **Clinical Phenotyping:** Developed phenotypes for maternal opioid use, JIA, cognitive decline (MMSE), and ER-to-ICU outcomes in infants for the CPM team.
- **scRNA-Seq Pulmonary Fibrosis Analysis:** Analyzed single-cell RNA-Seq data (GSE136831), identifying cell-type-specific expression signatures and enriched pathways in fibrotic disease phenotypes.

Nexus Information Systems *Consultant* July 2020–May 2021

Delivered cross-disciplinary talks on MRI physics, CNNs, network neuroscience, and fMRI (SPM, MATLAB). Supported research efforts at Wake Forest School of Medicine and ORNL.

Selected Presentations

Stanford AI Show-and-Tell Series (2025)

- Built an 8-head GAT ($8 \times 16 \rightarrow 128$ -d) with AdamW, LayerNorm, residuals, Xavier init, and dropout to classify LRH-1 low vs. high free-energy conformations.
 - Used early stopping (patience=15) to stabilize convergence on modest graph datasets.
 - Applied Integrated Gradients to map residue-level importance onto 3D structure: LOW states showed pocket-mouth concentration; HIGH states showed distributed flexibility.
 - Validated robustness across graph constructions (7.0 Å vs. 4.5 Å): Spearman $\rho = 0.63$ ($p < 0.001$); Top-K Jaccard = 0.54.
 - Designed reproducible ROI masks via distance+SASA filters; applied BH-FDR corrections to generate testable allosteric hypotheses.
 - All modeling and analysis executed on a custom-designed and self-built AI workstation (Dual Xeon Silver, RTX 3090, 256GB ECC RAM, Ubuntu 22.04), enabling full local GNN training, inference, and structural visualization workflows.
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Education

- **MS, Genome Science and Technology** *University of Tennessee, Knoxville, May 2020*
- **Plant Systems Biology (ABT)** *Southern Illinois University, Carbondale, May 2015*
- **BS, Mathematics; BA, Experimental Psychology** *Southern Illinois University, Carbondale, May 2013*

Certifications

Stanford University Professional Certificate in AI:

- **XCS224W—Machine Learning with Graphs (Completed, June 2025):** Graph Neural Networks, node/edge/graph embeddings, message passing, graph generative models, link prediction, node classification.
 - **XCS224N—Natural Language Processing with Deep Learning (In Progress, 2025):** Dependency parsing, RNNs/LSTMs, word embeddings, sequence-to-sequence models, attention, transformer architectures, neural machine translation.
 - **XCS236—Deep Generative Models (Jan 26-Apr 5, 2026):** Variational autoencoders, diffusion models, normalizing flows, energy-based models, latent-variable modeling, probabilistic generative modeling for high-dimensional data.
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Publications

- **Foutch D**, Blind R.D. *“PDB2Graph: Protein Structure Network Analysis”* (in preparation)
- Haratipour H, **Foutch D**, Blind R.D. *“Heuristic of Rigid Docking Scores”*, 2024
- Pham B, Cheng Z, Lopez D, Lindsay RJ, **Foutch D**, Majors RT, Shen T. *“Statistical Analysis of Protein-Ligand Interaction Patterns”*, 2022
- **Foutch D**, Pham B, Shen T. *“Protein Conformational Switch Discerned”*, 2021