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## Area of Expertise

My lab is broadly interested in the development and application of computational methods to solve problems in pharmaceutical sciences. We integrate pharmaceutical sciences with computer sciences, chemistry, biology, and physics to develop new biotechnologies, understand molecular mechanisms underlying diseases, and design new drugs. Specifically, we are interested in protein allostery study, computer-aided drug design, CRISPR-Cas9 technology improvement, artificial intelligence (AI) for drug discovery, and big data analysis of health disparity diseases. We extensively engage in dynamic collaborations with various experimental labs with a goal to bridge the interface of computational, experimental, and clinical research.

## Qualifications

PhD in Chemistry, Ohio State University  
BS in Chemistry, Peking University

## Recent Publications

### **Sparse group selection and analysis of function-related residue for protein-state recognition**

Bai, F., Puk, K. M., Liu, J., Zhou, H., Tao, P., Zhou, W. & Wang, S., 30 Jul 2022, In: Journal of Computational Chemistry. 43, 20, p. 1342-1354 13 p.

### **Rational Engineering of CRISPR-Cas9 Nuclease to Attenuate Position-Dependent Off-Target Effects**

Zuo, Z., Babu, K., Ganguly, C., Zolekar, A., Newsom, S., Rajan, R., Wang, Y. C. & Liu, J., Apr 2022, In: CRISPR Journal. 5, 2, p. 329-340 12 p.

### **Novel Use of Hypoxia-Inducible Polymerizable Protein to Augment Chemotherapy for Pancreatic Cancer**

Gdowski, A., Hayatshahi, H., Fudala, R., Joshi, R., Liu, J., Vishwanatha, J. K., Jeyarajah, R., Guzik, P. & Ranjan, A. P., Jan 2022, In: Pharmaceutics. 14, 1, 128.

### **Coordinated Actions of Cas9 HNH and RuvC Nuclease Domains Are Regulated by the Bridge Helix and the Target DNA Sequence**

Babu, K., Kathiresan, V., Kumari, P., Newsom, S., Parameshwaran, H. P., Chen, X., Liu, J., Qin, P. Z. & Rajan, R., 14 Dec 2021, In: Biochemistry. 60, 49, p. 3783-3800 18 p.

### **Tribute to Ruth Nussinov**

Keskin, O., Miller, Y., Liu, J. & Lu, S., 1 Jul 2021, In: Journal of Physical Chemistry B. 125, 25, p. 6733-6734 2 p.

### **Factors Governing Selectivity of Dopamine Receptor Binding Compounds for D2R and D3R Subtypes**

Hayatshahi, H. S., Luedtke, R. R., Taylor, M., Chen, P. J., Blass, B. E. & Liu, J., 28 Jun 2021, In: Journal of Chemical Information and Modeling. 61, 6, p. 2829-2843 15 p.

### **A Quick Route to Multiple Highly Potent SARS-CoV-2 Main Protease Inhibitors\*\***

Yang, K. S., Ma, X. R., Ma, Y., Alugubelli, Y. R., Scott, D. A., Vatansever, E. C., Drelich, A. K., Sankaran, B., Geng, Z. Z., Blankenship, L. R., Ward, H. E., Sheng, Y. J., Hsu, J. C., Kratch, K. C., Zhao, B., Hayatshahi, H. S., Liu, J., Li, P., Fierke, C. A., Tseng, C. T. K., & 2 others Xu, S. & Liu, W. R., 18 Mar 2021, In: ChemMedChem. 16, 6, p. 942-948 7 p.

### **Allosteric Modulation of Small Molecule Drugs on ACE2 Conformational Change upon Binding to SARS-CoV-2 Spike Protein**

Wang, D. S., Hayatshahi, H. S., Jayasinghe-Arachchige, V. M. & Liu, J., 2021, *Proceedings - 2021 IEEE International Conference on Bioinformatics and Biomedicine, BIBM 2021*. Huang, Y., Kurgan, L., Luo, F., Hu, X. T., Chen, Y.,

Dougherty, E., Kloczkowski, A. & Li, Y. (eds.). Institute of Electrical and Electronics Engineers Inc., p. 2587-2594 8 p. (Proceedings - 2021 IEEE International Conference on Bioinformatics and Biomedicine, BIBM 2021).

**Filtering out low-affinity bitropic ligands for dopamine receptors based on ligand conformation**

Hayatshahi, H. S. & Liu, J., 2 Sep 2020, In: ACS Chemical Neuroscience. 11, 17, p. 2523-2527 5 p.

**Allosteric regulation of CRISPR-Cas9 for DNA-targeting and cleavage**

Zuo, Z. & Liu, J., Jun 2020, In: Current Opinion in Structural Biology. 62, p. 166-174 9 p.