

Jin Liu, PhD
UNT System College of Pharmacy
Pharmaceutical Sciences
Institute for Healthy Aging
Email: Jin.Liu@unthsc.edu



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

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.

Editorial overview: Allosteric assemblies

Liu, J. & Lai, L., Jun 2020, In: Current Opinion in Structural Biology. 62, p. vi-vii

Probing Protein Allostery as a Residue-Specific Concept via Residue Response Maps

Hayatshahi, H. S., Ahuactzin, E., Tao, P., Wang, S. & Liu, J., 25 Nov 2019, In: Journal of Chemical Information and Modeling. 59, 11, p. 4691-4705 15 p.

A Genetically Encoded, Phage-Displayed Cyclic-Peptide Library

Wang, X. S., Chen, P. H. C., Hampton, J. T., Tharp, J. M., Reed, C. A., Das, S. K., Wang, D. S., Hayatshahi, H. S., Shen, Y., Liu, J. & Liu, W. R., 28 Oct 2019, In: Angewandte Chemie - International Edition. 58, 44, p. 15904-15909 6 p.

Design, synthesis, and evaluation of N-(4-(4-phenyl piperazin-1-yl)butyl)-4-(thiophen-3-yl)benzamides as selective dopamine D₃ receptor ligands

Chen, P. J., Taylor, M., Griffin, S. A., Amani, A., Hayatshahi, H., Korzekwa, K., Ye, M., Mach, R. H., Liu, J., Luedtke, R. R., Gordon, J. C. & Blass, B. E., 15 Sep 2019, In: Bioorganic and Medicinal Chemistry Letters. 29, 18, p. 2690-2694 5 p.

Structural and functional insights into the bona fide catalytic state of *Streptococcus pyogenes* Cas9 HNH nuclease domain

Zuo, Z., Zolekar, A., Babu, K., Lin, V. J. T., Hayatshahi, H. S., Rajan, R., Wang, Y. C. & Liu, J., Jul 2019, In: eLife. 8, e46500.

Assessing the Performance of the Nonbonded Mg²⁺ Models in a Two-Metal-Dependent Ribonuclease

Zuo, Z. & Liu, J., 28 Jan 2019, In: Journal of Chemical Information and Modeling. 59, 1, p. 399-408 10 p.

Analogues of Arylamide Phenylpiperazine Ligands to Investigate the Factors Influencing D₃ Dopamine Receptor Bitropic Binding and Receptor Subtype Selectivity

Hayatshahi, H. S., Xu, K., Griffin, S. A., Taylor, M., Mach, R. H., Liu, J. & Luedtke, R. R., 19 Dec 2018, In: ACS Chemical Neuroscience. 9, 12, p. 2972-2983 12 p.

Stress and interferon signalling-mediated apoptosis contributes to pleiotropic anticancer responses induced by targeting NGLY1

Zolekar, A., Lin, V. J. T., Mishra, N. M., Ho, Y. Y., Hayatshahi, H. S., Parab, A., Sampat, R., Liao, X., Hoffmann, P., Liu, J., Emmitte, K. A. & Wang, Y. C., 11 Dec 2018, In: *British Journal of Cancer*. 119, 12, p. 1538-1551 14 p.