PHARMSCI DEPARTMENT NEWSLETTER
MAY 2025

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The purpose of the newsletter is to announce the achievements of faculty in their research, teaching, and service in a timely and succinct manner. The newsletter is meant to be a simple listing of your achievements and newsworthy events, so detailed elaborations are not necessary.

The Department newsletter is designed to be complementary to the School of Pharmacy's Event Notification. Please continue submitting your newsworthy events through the School of Pharmacy's Event Notification via the School of Pharmacy website:
View the faculty Resources.

PUBLICATIONS

1. **Wu Q**, Song D, Zhao Y, Verdegaal AA, Turocy T, Duncan-Lowey B, Goodman AL, Palm NW, Crawford JM. Activity of GPCR-targeted drugs influenced by human gut microbiota metabolism. *Nat Chem.* 2025. Epub 20250403. doi: 10.1038/s41557-025-01789-w. PubMed PMID: 40181149.

2. Huang, H., Mu, Y., Huang, Y., Ji, B., Wang, Y., Chen, C.Y., Chen, Y., Luo, Z., Li, S., Ziqian Zhang, Z., Wang, L., Conway, J.F., **Yang, D**., ***Wang, J**., *Sun, J., and ***Li, S**. Rational development of gemcitabine-based nanoplatform for targeting SERPINB9/Granzyme B axis to overcome chemo-immune-resistance. *Nature Communications* (in press).

3. Lu, X., Chen, D., Wang, M., Song, X., Ermine, K., Hao, S., Jha, A., Huang, Y., Lenz, H.J., **Li, S.,** Jin, Z., Yu, J., and Zhang, L. Depleting oxysterol-binding proteins by OSW-1 triggers

RIP1/RIP3-independent necroptosis and potentiates cancer immunotherapy. *Cell Death and Differentiation* (in press).

4. He X.; Man V.; Yang, W.; Lee, T.-S.; **Wang, Junmei**. ABCG2: A Milestone Charge Model for Accurate Solvation Free Energy Calculation. *J. Chem. Theory Comput*. 2025, 21, 3032−3043.

5. Wang, L.; Ji, B.; Zhai, J.; **Wang, Junmei**. Advancing Promiscuous Aggregating Inhibitor Analysis with Intelligent Machine Learning Classification. *Brief. Bioinform*. Accepted.

6. Zhai, J.; Qi, X.; Cai, L.; Liu, Y.; Tang, H.; Xie, L.; **Wang, Junmei**. NNKcat: Deep neural network to predict catalytic constants (Kcat) by integrating protein sequence and substrate structure with enhanced data imbalance handling. *Brief. Bioinform*. Accepted.

7. "GraphDeep-hERG: Graph Neural Network PharmacoAnalytics for Assessing hERG-Related Cardiotoxicity." Jing YK, Zhang YY, Zhao GY, McGuire T, Zhao J, Gibbs Ben, Hou GQ, **Feng ZW**, Xue Y and **Xie X-Q**. *Pharm Res*. 2025 Mar 26. Online ahead of print. DOI: 10.1007/s11095-025-03848-w

8. "Structural insight into CD20/CD3-bispecific antibodies by molecular modeling. Sun, Z. Y., Liang, T., Zhang, Y., Hou, G., Chu, X., Hou, J. Z., Li, W., **Xie, X.-Q**., & **Feng, Z**. *Computers in Biology and Medicine*." (2024). 185, 109497.https://doi.org/10.1016/j. compbiomed.2024.109497.

9. "AI-based IsAb2.0 for antibody design." Liang, T. #, Sun, Z. Y. #, Hines, M. G. #, Penrose, K. J., Hao, Y., Chu, X., Mellors, J. W., Dimitrov, D. S., **Xie, X.-Q**., Li, W., & **Feng, Z**. (2024). . *Briefings in Bioinformatics*, 25(5), 2024, bbae445. https://doi.org/10.1093/bib/bbae445.

10. "Blood-Brain Barrier Permeability Assessment for Small Molecule Drug Discovery Using Computational Techniques" Jing YK and **Xie X-Q**, Chapter 45 in Book: Oral Bioavailability and Drug Delivery: From Basics to Advanced Concepts and Applications (Wiley in Drug Discovery and Development) 1st Edition (pp.857-870), 2024. DOI:10.1002/9781119660699.ch45. SN - 9781119660651 Wiley publisher.

11. (Springer Nature Book) "Artificial Intelligence Technologies for Clinical Data PharmacoAnalytics Case Studies on Alzheimer's Disease." Zhao G, Zhao S, and **Xie X-Q***. Book Chapter 32, 2023 in The Quintessence of Basic and Clinical Research (editors: Dr. G. Jagadeesh, et al), Springer Nature 2023, ISBN 978-981-99-1283-4 (Book); ISBN 978-981-99-1284-1 (eBook).

12. (Springer Nature Book) “Artificial intelligence generative chemistry design of target-specific scaffold-focused small molecule drug libraries.” Bian Y, Hou G, and **Xie X-Q***. Book Chapter 31, 2023 in The Quintessence of Basic and Clinical Research (editors: Dr. G. Jagadeesh, et al), Springer Nature, ISBN 978-981-99-1283-4 (Book); ISBN 978-981-99-1284-1 (eBook).

13. Ainslie KM, Bowers AA, Chichewicz RH, Collier LS, Doorn JA, Frei CR, Ghandehari H, Gibbs RB, Lawrence DS, Lee CR, Mager DE, Marker P, Schwendeman A, Suryanarayanan R, Williams III RO, Xi Y, **Xie W**, Xie XQ, Zhu G, Nguyen J. Pharmaceutical Sciences: Insights and Observations from Academic Chairs and Vice Chairs. *AAPS J* **27:** 41 (2025) PMID: 39904863. (Peer-reviewed review article)

AWARDS

Dr. Ramen Venkataramanan received a Wiley Top Cited Article Reward; Whose work has been recognized as a top citied article* in: Xenotransplantation “Assessment of glomerular filtration and tubular secretion in baboons with life-supporting pig kidney grafts”

Dr. Simone Brixius-Anderko received the AACP 2025 Bench Research Excellence Award

Dr. Simone Brixius-Anderko received an ASPET Editorial Fellowship for the Drug Metabolism and Disposition journal

Dr. Simone Brixius-Anderko received an Early Career Abstract Award of the ASPET Drug Metabolism and Disposition Division.

Dr. Xiaochao Ma was selected as the recipient of the ASPET Top Reviewer Award for Drug Metabolism and Disposition (2024). This award recognizes outstanding performance as a manuscript reviewer for ASPET.

GRANTS

Junmei Wang
UPMCE TS Alder, Jonathan (PI) 03/01/2025-02/28/2028
Title: A Safe Mechanism to Lengthen Telomeres and promote Tolerance of Immune Suppression
Role: co-I

SERVICE AND INVITED PRESENTATIONS

Dr. Simone Brixius-Anderko gave a talk at the IDEA Luncheon at the ASPET Annual Meeting in Portland titled " Sciencing on the Autism Spectrum: Nothing wrong with us"

Dr. Simone Brixius-Anderko co-chaired a session at the ASPET Annual Meeting in Portland

Dr. Simone Brixius-Anderko was elected as ASPET IDEA Fellow

Dr. Simone Brixius-Anderko was elected as ASPET Drug Metabolism and Disposition Communications Officer for a second term

Dr. Song Li was invited to speak; "Tumor-penetrating Nanocarriers for Improved Cancer Therapy", School of Pharmacy and Pharmaceutical Sciences, University at Buffalo, The State University of New York, April 24, 2025.

Dr. Junmei Wang presented: "Accurate binding affinity prediction and hotspot residue identification via ligand-receptor binding profile analysis using machine learning" at Eli Lilly & Company, on March 26, 2025.

Dr. Junmei Wang presented: "Accurate Binding Affinity Prediction And Hotspot Residue Identification Via Ligand-receptor Binding Profile Analysis Using Machine Learning" at the PITT-CMU joint Molecular Biophysics and Structural Biology (MBSB) program's seminar series, on April 16, 2025.

Dr. Xiang-Qun Xie is the Senior Editor of Springer Nature AAPS Book Series (2025 – present)

Dr. Xiang-Qun Xie is part of the Scientific Review Group: ZDA1 SUY-S J1 R, Developing Regulated Therapeutic and Diagnostic Solutions for Patients Affected by Opioid and/or Stimulants use Disorders

Dr. Wen Xie gave a podium presentation at the 34th Asia-Pacific Association for the Study of the Liver (APASL) Annual Meeting, Beijing, China. March 29, 2025. The title of his presentation is *"Inhibition of Heme-thiolate Monooxygenase CYP1B1 Prevents Hepatic Stellate Cell Activation and Liver Fibrosis by Accumulating Trehalose."*

Dr. Wen Xie gave a presentation at China Pharmaceutical University, Nanjing, China. March 25, 2025. The title os his presentation is *"Cellular and Metabolic Basis for the Role of CYP1B1 Enzyme in HSC Activation and Liver Fibrosis."*

STUDY SECTIONS AND OTHER GRANT REVIEW SERVICE

Song Li: Translational Cancer Research-1 (CTCR-1) panel, Academic Research Program of the Cancer Prevention and Research Institute of Texas (CPRIT) (March 21, 2025)

Song Li: Nucleic Acid Therapeutic Delivery (NATD) - ZRG1 BBBT (81) Study Section (April 14-15, 2025)

Dr. Simone Brixius-Anderko was an ad-hoc reviewer for the UPMC CMRF Award

Dr. Wen Xie was an ad-hoc reviewer for the University of Pittsburgh Health Sciences CMRF Award

Dr. Junmei Wang was an Ad hoc reviewer of the NSF study section for the Division of Chemistry in 2025

Dr. Junmei Wang was an Ad hoc reviewer of a NIH COBRE Phase 3 study section in March 2025

GRADUATE DISSERTATION DEFENSE

STUDENT AND POSTDOC ACHIEVEMENT