PHARMSCI DEPARTMENT NEWSLETTER
NOVEMBER 2024

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Our department newsletter will be distributed to departmental faculty every two months. 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 Intranet: https://intranet.pharmacy.pitt.edu.

PUBLICATIONS

1. Luo, Z., Huang, Y., Chen, S., Zhang, B., Huang, H., Dabiri, S., Chen, Y., Zhang, A., Alexis R. Andreas, A.R., and **Li, S**. Delivery of PARP inhibitors through 2HG-incorporated liposomes for synergistically targeting DNA repair in cancer. *Cancer Letters* 2024; 604: 217268.

2. Huang, H., Ji, B., Huang, Y., Li, S., Luo, Z., Chen, S., Li, S., Chen, Y., Bain, D.J., Sun, J., Yang, D., Burns, T.F.,Wang, J., and **Li, S**. Advanced hierarchical computational modeling-based rational development of platinum (II) nanocomplex to improve lung cancer therapy. *Advanced Functional Materials* (in press).

3. Chaudhari, K.; Zhang, K.; Yam, P.T.; Zang, Y.'; Kramer, D. A.; Gagnon, S.; Jean-Francois Michaud, J. F.; Collins, M.; **Wang, Junmei;** Srour, M.; Chen, B.; Charron, F.; Bashaw. G. J. A human DCC variant causing mirror movement disorder reveals that the WAVE regulatory complex mediates axon guidance by netrin-1–DCC. *Science Signaling* 2024, 17 (856), eadk2345.

4. Wang, L.; He, X.; Ji, B.; Han, F.; Niu, T.; Cai, L.; Zhai, J.; Hao, H.; **Wang, Junmei**. Geometry Optimization Algorithms in Conjunction with the Machine Learning Potential ANI-2x Facilitate the Structure-Based Virtual Screening and Binding Mode Prediction. *Biomolecules* 2024, 14 (6), 648.

5. Niu T.; Wang, N. X.; **Wang, Junmei**. Machine learning and deep learning-based scoring functions in deciphering ligand-receptor binding: An application in drug design for GPCRs. *Annual Reports in Computational Chemistry* 2024, 20, 51.

6. Duan, Y.; Niu, T.; **Wang, Junmei**, Cieplak, P.; Luo, R. PCMRESP: A Method for Polarizable Force Field Parameter Development and Transferability of the Polarizable Gaussian Multipole Models Across Multiple Solvents. *J. Chemical Theory & Computation*, 2024, 20(7), 2820-2829.

7. Zhang J, Huang Y, Li H, Xu P, Liu Q, Sun Y, Zhang Z, Wu T, Tang Q, Jia Q, Xia Y, Xu Y, Jing X, Li J, Mo L, **Xie W**, Qu A, He J, Li Y. B3galt5 functions as a PXR target gene and regulates obesity and insulin resistance by maintaining intestinal integrity. *Nat Commun.* 15: 5919 (2024)

8. Tung HC, Kim JW, Zhu J, Li S, Yan J, Liu Q, Koo I, Koshkin SA, Hao F, Zhong G, Xu M, Wang Z, Wang J, Huang Y, Xi Y, Cai X, Xu P, Ren S, Higashiyama T, Gonzalez FJ, Li S, Isoherranen N, Yang D, Ma X, Patterson AD, **Xie W**. Inhibition of heme-thiolate monooxygenase CYP1B1 prevents hepatic stellate cell activation and liver fibrosis by accumulating trehalose. *Sci Transl Med.* 16: eadk8446 (2024).

9. Kim JW, Tung HC, Ke M, Xu P, Cai X, Xi Y, Xu M, Ren S, Huang Y, Bhowmik A, Carroll KS, Bae YS, Li S, **Xie W**. The de-sulfinylation enzyme sulfiredoxin-1 attenuates hepatic stellate cell activation and liver fibrosis by modulating the PTPN12-NLRP3 axis. *Hepatology* 2024 Oct 24. Epub ahead of print. PMID: 39446334.

AWARDS

Velvet Journigan has been awarded the American Chemical Society (ACS) Pittsburgh Women Chemists Committee Award for Excellence in the Chemical Sciences. This award recognizes the achievements of female chemists and chemical engineers in the greater Pittsburgh area who have a record of accomplishment in their field. There will be a ceremony at the ACS Awards Dinner held at the Central Regional Meeting (CERM) 2024 in November of 2024 where the award will be presented.

GRANTS

Simone Brixius-Anderko
Project number: R35GM155319-01
Funding Period: 07/01/2024-06/30/2029
Title: Studies on fatty acid metabolizing cytochrome P450 enzymes
Funding Agency: National Institute of Health (NIH) $1.88M

Simone Brixius-Anderko
Funding Period: 07/01/2024 – 06/30/2026
Title: Elucidating structural and functional differences between cytochrome P450 fatty acid hydroxylases
Funding Agency: UPMC Competitive Medical Research Fund (CMRF) FY2024 $30,000

Song Li
Project number: 1R41CA278033-01A1
Funding Period: 08/15/24-08/14/25
Title: Stroma-Penetrating Nanomedicine to Improve Treatment for Pancreatic Cancer
Funding Agency: National Institute of Health (NIH)

SERVICE AND INVITED PRESENTATIONS

Simone Brixius-Anderko was invited to give a talk at the 81st Pittsburgh Diffraction Conference at Cornell University (2024)

Simone Brixius-Anderko was invited to give a talk at the P450 Biodiversity and Biotechnology conference in Turin, Italy (2024)

Simone Brixius-Anderko was invited to give a talk at the 2024 Leading Edge Symposium, Janelia Research Campus Ashburn, VA

Simone Brixius-Anderko was invited to give a seminar talk at Emory University at the Department of Pharmacology and Chemical Biology (2024)

Simone Brixius-Anderko was invited to give a virtual Talk at the International Gender Summit 2024 (2024)

Simone Brixius-Anderko was a Session chair at the 81st Pittsburgh Diffraction Conference at Cornell University

Simone Brixius-Anderko was a Session chair 2024 Leading Edge Symposium, Janelia Research Campus Ashburn, VA

Simone Brixius-Anderko was a Panelist for "Navigating your faculty position" at the 2024 Leading Edge Symposium, Janelia Research Campus Ashburn, VA

Song Li presented "*Tumor-penetrating Nanocarriers for Improved Cancer Therapy*", Department of Molecular Microbiology and Immunology, Keck School of Medicine, University of Southern California, June 12, 2024. (Zoom seminar)

Xiang-Qun (Sean) Xie presented his lab AI data science driven research work, "PharmacoAnalytics Journey from '*Cell*' to '*Cells*': Advancing Cannabinoid Therapeutics via 3D Cryo-EM Cannabinoid CB2 Signaling Complex and Generative AI Modeling, The Protein Society Annual Symposium 2024. July 26, 2024

Dr. McGuire was invited to be a guest speaker at the Pitt School of Pharmacy Student Society of Cannabis Pharmacists (SSCP) (a PharmD student organization) and presented a talk entitled, "Leveraging Cannabinoid Receptor 2 Biology to Advance Therapies". October 22, 2024

SERVICE

Xiang-Qun (Sean) Xie attended the Editorial Board Member Meeting of the American Association of Pharmaceutical Scientists (AAPS) October 21, 2024

Xiang-Qun (Sean) Xie serves as a Charter Member and attended the US FDA Science Board Meeting. October 7, 2024

Xiang-Qun (Sean) Xie attended the University of Pittsburgh RDS@Pitt Data Science Steering Committee meeting, October 14, 2024

Song Li reviewed for NIH Cancer Diagnostics and Treatments (CDT) SEP (ZRG1 CDPT-V (13)) (July 17-18, 2024)

Song Li reviewed for NCI Program Project (P01) Review SEP-A (2025/01 ZCA1 RPRB-J (J1) P) (September 26-27)

Song Li reviewed for Translational Cancer Research-1 (CTCR-1) panel, Academic Research Program of the Cancer Prevention and Research Institute of Texas (CPRIT) (October 25, 2024)

Junmei Wang served as a judge for the 2024 ACS "Chemical Computing Group Excellence Award for Graduate Students"

Junmei Wang served as an ad hoc reviewer for NIH DMPB study-section, June 27-28, 2024

Junmei Wang served as an ad hoc reviewer for NIH BDMA study section, October 17-18, 2024

Wen Xie was appointed Vice Chair, AACP Research and Graduate Affairs Committee

Wen Xie was elected Member, Microsomes and Drug Oxidations (MDO) International Scientific Advisory Committee (ISAC) (2024-2028)

Wen Xie was an *ad hoc* Reviewer, 2024 Department of Defense (DOD) Rare Cancers Research Program on the Concept - Neurological Cancers - 2 (CON-NC-2) peer review panel. September-October, 2024

Wen Xie *was an ad hoc* Reviewer, Pitt Momentum Funds, Office of Sponsored Programs & Research Development, University of Pittsburgh (November 2024)