



UNIVERSITY of MARYLAND
SCHOOL OF PHARMACY

From the Chair's Desk

News from Paul Shapiro, PhD
Chair, Department of Pharmaceutical Sciences

In This Issue

Summer 2019

[SOP Launches
Nation's First
Master's in Medical
Cannabis Science
and Therapeutics](#)

[M-CERSI Conference
Spotlights Regulatory
Applications for
Dissolution Testing](#)

[Faculty Member
Testifies Before U.S
Senate HELP
Committee on Opioid
Crisis](#)

[PSC Researcher
Receives Biophysical
Society's Junior
Faculty Award](#)

[Student Competition
Spotlights Innovation
in Regulatory Science](#)

[Kudos!](#)

[Grants and
Fellowships](#)

Dear alumni and colleagues,

As chair of the Department of Pharmaceutical Sciences (PSC), I was thrilled to see PSC faculty sharing their ideas and projects at the recent annual meeting of the American Association of Colleges of Pharmacy. From posters and presentations to interacting with visitors at the University of Maryland School of Pharmacy's booth in the exhibit hall, our faculty were everywhere. I was also pleased to meet so many of our alumni and colleagues from other schools of pharmacy. It's always exciting to reconnect.

A highlight of the meeting for the department and the School was the session we hosted on Disruptive Innovation in Pharmacy - [Pharmapreneurship](#), at which Dean Eddington, special guests, and a faculty panel discussed the disruptive innovation needed in American pharmacy education related to entrepreneurship, innovation, and groundbreaking research and partnerships. [Click here](#) to view a video on our pharmapreneurship initiative.

The department achievements below highlight our faculty's expertise, influence, and impact. But most importantly, they highlight our commitment to advancing pharmacy education, scientific discovery, patient care, and community engagement across the state of Maryland and beyond.

Sincerely,

[Paul Shapiro, PhD](#)
Professor and Chair
Department of Pharmaceutical Sciences



**SOP Launches Nation's First Master's in Medical
Cannabis Science and Therapeutics**

MS in Medical Cannabis Science and Therapeutics



The School of Pharmacy has launched a new [Master of Science \(MS\) in Medical Cannabis Science and Therapeutics](#) to provide students with the knowledge and skills needed to support patients and the medical cannabis industry, add to existing research in the field, and develop well-informed medical cannabis policy. Based at the Universities at Shady Grove (USG) in Rockville, Md., the two-year program blends online learning with face-to-face experiences, and is designed for any individual who has completed his or her undergraduate degree and is interested in pursuing a career in the medical cannabis industry. The MS in Medical Cannabis Science and Therapeutics is the first graduate program in the country dedicated to the study of medical cannabis. It aims to meet the needs of all individuals interested in advancing their knowledge about medical cannabis, including health care professionals such as physicians, nurses, and pharmacists; scientists and regulators; growers and dispensary owners; and policy and industry professionals. [Read more here...](#)

M-CERSI Conference Spotlights Regulatory Applications for Dissolution Testing



The School of Pharmacy welcomed nearly 170 researchers from across academia, government, and industry to Pharmacy Hall on May 21 and 22, for "In Vitro Dissolution Profiles Similarity Assessment in Support of Drug Product Quality: What, How, and When." The conference sponsored by the [University of Maryland Center of Excellence in](#)

[Regulatory Science and Innovation \(M-CERSI\)](#) featured numerous presentations and breakout sessions that aimed to help participants better understand the reliability and predictive ability of the most commonly used mathematical approaches to assess dissolution profiles' similarity, identify best practices for the assessment of similarity in dissolution profiles, and recognize the role of similarity testing considering safe space and clinically relevant dissolution specifications. [Read more here...](#)

Faculty Member Testifies Before U.S Senate HELP Committee on Opioid Crisis



On Feb. 12, 2019, [Andrew Coop, PhD](#), professor in PSC and associate dean for academic affairs at the School of Pharmacy, testified before the U.S. Senate Committee on Health, Education, Labor, and Pensions (HELP) as part of a hearing titled "Managing Pain During the Opioid Crisis." Dr. Coop provided written and oral testimony during the hearing, and participated with other panelists in a lengthy question and answer session. Dr. Coop's remarks focused on his research to develop UMB 425 - an opioid painkiller with the potential for no abuse liability - and the role that pharmacists can play in helping to alleviate the opioid crisis. [Read more here...](#)

PSC Researcher Receives Biophysical Society's Junior Faculty Award



[Lisa Jones, PhD](#), assistant professor in PSC, received the Biophysical Society's 2019 Junior Faculty Award. Presented by the organization's Biopolymers In Vivo Subgroup, the Junior Faculty Award aims to boost the visibility of a beginning faculty member whose research and recent achievements focus on cutting-edge investigations of biomolecular processes in living organisms. Dr. Jones' research focuses on the use of protein footprinting methods, coupled with mass spectrometry, to study protein interactions in biological processes. One protein footprinting method in which Jones specializes is fast photochemical oxidation of proteins (FPOP). She and her research team use this emerging technique to identify protein interactions and conformational change of various protein systems. [Read more here...](#)

Student Competition Spotlights Innovation in Regulatory Science



A team of third-year students in the Doctor of Pharmacy program at the School of Pharmacy set out to develop new guidelines that could be used by the FDA to help draft official guidances and recommendations that establish ownership rights for data collected by wearable and implantable health care devices, as well as give patients broad control over how that data is shared and used by others. Team members Thomas Adriaens, Kira Aldrich, Uyen Nguyen, Khang Nong, and Mary Zhang presented their proposal to a panel of three judges from the School of Pharmacy at this year's "America's Got Regulatory Science Talent" Competition on Feb. 6, who awarded them first place for their innovation and creativity. Four teams competed in this year's talent competition. Second place was awarded to [PhD in PSC](#) graduate students Ana Coutinho, Angela Lee, Bryan Eng, Dongyue Yue, Sharmila Das, and Yuwei Lu for their proposal to define a standard puff for first generation e-cigarettes, which could better equip the FDA to evaluate the safety of all first generation e-cigarettes against a common standard. [Read more here...](#)

Kudos!

Our department's faculty and students are regularly recognized at the local and national level for their expertise. Here is a short list of recent accomplishments.

- **Amy Defnet** and **Dante Johnson**, graduate students, received Best Poster Awards at the University of Maryland, Baltimore's 41st Annual Graduate Research Conference.
- **Chad Johnson**, graduate student, received an American Association of Colleges of Pharmacy's Walmart Scholars Award.

- **Fang-Yu Lin**, graduate student, received the American Chemical Society's Chemical Computing Group's Excellence Award for Graduate Students for the project "Optimization of the Drude Polarizable Protein Force Field."
- **Alexander MacKerell, PhD**, the Grollman-Glick Professor and director of the Computer-Aided Drug Design Center, has been designated a World Class Researcher by Clarivate Analytics for his "exceptional research performance, demonstrated by production of multiple highly cited papers that rank in the top 1% by citations for field and year in Web of Science."
- **Marc Taraban, PhD**, research assistant professor, received a Best Poster Award at the Practical Applications of NMR in Industry Conference 2019.
- **Fengtian Xue, PhD**, associate professor, received a United States Patent for "Compounds for Treating Parasitic Infections."

Grants and Fellowships

- **Stephen Hoag, PhD**, professor, received a two-year \$56,335 contract from Battelle Memorial Institute for "The Effects of E-liquid Nicotine Concentration on the Abuse Liability of ENDS in Current Users."
- **Yuwei Lu**, graduate student, received a two-year \$69,500 grant from the United States Pharmacopeial Convention for "Development of In Vitro Gut Fermentation Model to Investigate the In Vivo Performance of Enteric-coated ABAB Antibody Producing *Saccharomyces Boulardi* Oral Dosage Form for the Treatment of *Clostridium*."
- **Alexander MacKerell, PhD**, the Grollman-Glick Professor of Pharmaceutical Sciences and director of the Computer-aided Drug Design Center, received a \$3.5 million grant from the National Institute of General Medical Sciences, for "Macromolecular Conformational Heterogeneity" and received a \$74,250 contract from SilcsBio, LLC for "Computational Methods for Accelerating Biologics Formulation."
- **Ryan Pearson, PhD**, assistant professor, received a one-year \$10,000 New Investigator Award from the American Association of Colleges of Pharmacy for "Programming Immune Cell Sensitivity towards Toll-like Receptor Agonists."
- **Jordan Pritts** and **Stephanie Shiffka**, graduates students, received pre-doctoral fellowships from the American Foundation for Pharmaceutical Education.
- **Bruce Yu, PhD**, professor and director of the Bio- and Nanotechnology Center, received a one-year \$123,196 contract from Pfizer for "Water NMR to Determine Aggregation."

Publications

- A Bejarano, CH Nadungodage, F Wang, AC Catlin, **SW Hoag**. Decision Support for Excipient Risk Assessment in Pharmaceutical Manufacturing. *AAPS PharmSciTech* 20 (6), 223
- **A Ibrahim**, BH Kothari, R Fahmy, **SW Hoag**. Prediction of Dissolution of Sustained Release Coated Ciprofloxacin Beads Using Near-infrared Spectroscopy and Process Parameters: a Data Fusion Approach. *AAPS PharmSciTech* 20 (6), 222
- B Jiang, A Jain, Y Lu, **SW Hoag**. Probing Thermal Stability of Proteins with Temperature Scanning Viscometer. *Molecular Pharmaceutics*
- T Wang, AR Potts, **SW Hoag**. Elucidating the Variability of Magnesium Stearate and the Correlations With Its Spectroscopic Features. *Journal of Pharmaceutical Sciences* 108 (4), 1569-1580
- Deepak V, Sahu MB, Yu J, **Jones JW**, **Kane MA**, Taylor RN, Badell ML, Sidell N, Rajakumar A. Retinoic Acid Is a Negative Regulator of sFLT1 Expression in Decidual Stromal Cells, and Its

Levels Are Reduced in Preeclamptic Decidua. *Hypertension*. 2019 Mar 18;HYPERTENSIONAHA11812564. doi: 10.1161/HYPERTENSIONAHA.118.12564. PMID: 30879360.

- **Jones JW**, Sarkar C, Lipinski MM, **Kane MA**. Detection and Structural Characterization of Ether Glycerophosphoethanolamine from Cortical Lysosomes Following Traumatic Brain Injury Using UPLC-HDMSE. *Proteomics*. 2019 Feb 20:e1800297. doi: 10.1002/pmic.201800297. PMID: 30790445.
- **Jones JW**, Alloush J, Sellamuthu R, Chua HL, MacVittie TJ, Orschell CM, **Kane MA**. Effect of Sex on Biomarker Response in a Mouse Model of the Hematopoietic Acute Radiation Syndrome. *Health Physics*. 2019 Apr;116(4):484-502. doi: 10.1097/HP.0000000000000961. PMID: 30681425.
- Carter CL, Hankey KG, Booth C, Tudor GL, Parker GA, **Jones JW**, Farese AM, MacVittie TJ, **Kane MA**. Characterizing the Natural History of Acute Radiation Syndrome of the Gastrointestinal Tract: Combining High Mass and Spatial Resolution Using MALDI-FTICR-MSI. *Health Physics*. 2019 Apr;116(4):454-472. doi: 10.1097/HP.0000000000000948. PMID: 30681424.
- Huang W, Yu J, **Jones JW**, Carter CL, Jackson IL, Vujaskovic Z, MacVittie TJ, **Kane MA**. Acute Proteomic Changes in the Lung After WTLI in a Mouse Model: Identification of Potential Initiating Events for Delayed Effects of Acute Radiation Exposure. *Health Physics*. 2019 Apr;116(4):503-515. doi: 10.1097/HP.0000000000000956. PMID: 30652977.
- Huang W, Yu J, **Jones JW**, Carter CL, Pierzchalski K, Tudor G, Booth C, MacVittie TJ, **Kane MA**. Proteomic Evaluation of the Acute Radiation Syndrome of the Gastrointestinal Tract in a Murine Total-body Irradiation Model. *Health Physics*. 2019 Apr;116(4):516-528. doi: 10.1097/HP.0000000000000951. PMID: 30624357.
- **Jones JW**, Clifford Z, Li F, Tudor GL, Farese AM, Booth C, MacVittie TJ, **Kane MA**. Targeted Metabolomics Reveals Metabolomic Signatures Correlating Gastrointestinal Tissue to Plasma in a Mouse Total-body Irradiation Model. *Health Physics*. 2019 Apr;116(4):473-483. doi: 10.1097/HP.0000000000000955. PMID: 30624349.
- Cohen EP, Hankey KG, Farese AM, Parker GA, **Jones JW**, **Kane MA**, Bennett A, MacVittie TJ. Radiation Nephropathy in a Nonhuman Primate Model of Partial-body Irradiation with Minimal Bone Marrow Sparing-Part 1: Acute and Chronic Kidney Injury and the Influence of Neupogen. *Health Physics*. 2019Mar;116(3):401-408. doi: 10.1097/HP.0000000000000960. PMID: 30608245.
- Bakhireva LN, **Kane MA**, Bearer CF, Bautista A, **Jones JW**, Garrison L, Begay MG, Ozechowski T, Lewis J. Prenatal Alcohol Exposure Prevalence as Measured by Direct Ethanol Metabolites in Meconium in a Native American Tribe of the Southwest. *Birth Defects Research*. 2019 Jan 15;111(2):53-61. doi: 10.1002/bdr2.1427. Epub 2018 Dec 14. PMID: 30549447.
- Ramalingam S, Ramamurthy VP, Gediya LK, Murigi FN, Purushottamachar P, Huang W, Choi EY, Zhang Y, Vasaitis TS, **Kane MA**, Lapidus RG, Njar VCO. The Novel Mnk1/2 Degradar and Apoptosis Inducer VNLG-152 Potently Inhibits TNBC Tumor Growth and Metastasis. *Cancers (Basel)*. 2019 Mar 3;11(3). pii: E299. doi: 10.3390/cancers11030299. PMID:30832411
- MacVittie TJ, Farese AM, **Kane MA**. ARS, DEARE, and Multiple-organ Injury: A Strategic and Tactical Approach to Link Radiation Effects, Animal Models, Medical Countermeasures, and Biomarker Development to Predict Clinical Outcome. *Health Physics*. 2019 Apr;116(4):453. doi: 10.1097/HP.0000000000001050. No abstract available. PMID:30789495
- Saha Ray A, Ghann WE, Tsoi PS, Szychowski B, Dockery LT, Pak YJ, Li W, **Kane MA**, **Swaan P**, Daniel MC. Set of Highly Stable Amine- and Carboxylate-Terminated Dendronized Au Nanoparticles with Dense Coating and Nontoxic Mixed-

Dendronized Form. *Langmuir*. 2019 Mar 5;35(9):3391-3403. doi: 10.1021/acs.langmuir.8b03196. Epub 2019 Feb 18. PMID:30712354

- Neu HM, Alexishin SA, **Brandis JEP**, Williams AMC, Li W, Sun D, Zheng N, Jiang W, Zimrin A, Fink JC, **Polli JE, Kane MA, Michel SLJ**. Snapshots of Iron Speciation: Tracking the Fate of Iron Nanoparticle Drugs via a Liquid Chromatography-Inductively Coupled Plasma-Mass Spectrometric Approach. *Molecular Pharmaceutics*. 2019 Mar 4;16(3):1272-1281. doi: 10.1021/acs.molpharmaceut.8b01215. Epub 2019 Feb 14. PMID:30676753
- MacVittie TJ, Farese AM, **Kane MA**. ARS, DEARE, and Multiple-organ Injury: A Strategic and Tactical Approach to Link Radiation Effects, Animal Models, Medical Countermeasures, and Biomarker Development to Predict Clinical Outcome. *Health Physics*. 2019 Mar;116(3):297-304. doi: 10.1097/HP.0000000000001045. PMID:30608246
- Teletin M, Vernet N, Yu J, Klopfenstein M, **Jones JW**, Féret B, **Kane MA**, Ghyselincq NB, Mark M. Two Functionally Redundant Sources of Retinoic Acid Secure Spermatogonia Differentiation in the Seminiferous Epithelium. *Development*. 2019 Jan 4;146(1). pii: dev170225. doi: 10.1242/dev.170225. PMID:30487180
- Swaroop, A., Oyer, J., Will, C., Huang, X., Yu, W., Troche, C., Bulic, M., Durham, B., Wen, Q., Crispino, J., **MackKerell, A.D., Jr.**, Bennett, R., Kelleher, N., and Licht, J., An Activating Mutation of the NSD2 Histone Methyltransferase Drives Oncogenic Reprogramming in Acute Lymphocytic Leukemia. *Oncogene*, 38: 671-686, 2019, PMC6358490, [DOI]
- Lin, F.-Y. and **MackKerell Jr., A.D.**, Improved Modeling of Halogenated Ligand-Protein Interactions using the Drude Polarizable and CHARMM Additive Empirical Force Fields. *Journal of Chemical Information and Modeling*, 59: 215-218, 2019, PMC6349471, [DOI]
- Khan, H.M., **MackKerell, A.D., Jr.**, and Reuter, N. Cation-π interactions between methylated ammonium groups and tryptophan in the CHARMM36 additive force field. *Journal of Chemical Theory and Computation*, In Press, 2018, [DOI]
- Brocke, S.A., Degen, A., **MackKerell, A.D., Jr.**, Dutagaci, B., and Michael Feig, M., "Prediction of Membrane Permeation of Drug Molecules by Combining an Implicit Membrane Model with Machine Learning," *Journal of Chemical Information and Modeling*, In Press, 2018, [DOI]
- Yu, W., Sunhwan Jo, S., Lakkaraju, S.K., Weber, D.J., and **MackKerell, A.D., Jr.**, Exploring Protein-protein Interactions using the Site-Identification by Ligand Competitive Saturation (SILCS) Methodology. *Proteins: Structure, Function and Bioinformatics*, In Press, 2019, [DOI]
- Aytenfisu, A.H., Simon, R., and **MackKerell, Jr., A.D.** Impact of Branching on the Conformational Heterogeneity of the Lipopolysaccharide from *Klebsiella pneumoniae*: Implications for Vaccine Design. *Carbohydrate Research*, In Press, 2019, [DOI]
- Lange M., Ok K., Shimberg G. D., Bursac B., Markó L., Ivanović-Burmazović I., **Michel S. L. J.**, Filipovic M. R., Direct Zinc Finger Protein Persulfidation by H₂S is Facilitated by Zn. *Angewandte Chemie*, 2019 Jun 11;58(24):7997-8001. *equally contributed
- Williams C. L., Neu H. M., **Michel S. L. J.**, Merrell D. S. Measuring Intracellular Metal Concentration via ICP-MS Following Copper Exposure. *Methods Molecular Biology*, 2019;1946:195-205.
- Neu H. M., Alexishin S. A., Brandis J. E. P., Williams A. M. C., Sun D., Zheng N., Jiang W., Zimrin A., Fink J. C., Polli J. E., Kane M. A., & **Michel S. L. J.** Snapshots of Iron Speciation: Tracking the Fate of Iron Nanoparticle Drugs via a Liquid Chromatography-Inductively Coupled Plasma-Mass Spectrometric Approach. *Molecular Pharmaceutics*, 2019, 16 (3), pp 1272-1281
- Nelson CE, Huang W, Brewer LK, Nguyen AT, **Kane MA, Wilks A, Oglesby-Sherrouse AG**. (2019) Proteomic Analysis of the *Pseudomonas aeruginosa* Iron Starvation Response Reveals PrF

- sRNA-dependent Regulation of Twitching Motility, Amino Acid Metabolism, and Zinc Homeostasis Proteins. *Journal of Bacteriology*. 201(12):e00754-18.
- Zygiel EM, Nelson CE, Brewer LK, **Oglesby-Sherrouse AG**, Nolan EM. (2019) The Human Innate Immune Protein Calprotectin Induces Iron Starvation Responses in *Pseudomonas aeruginosa*. *Journal of Biological Chemistry*. 294 (10):3549-3562.
 - Casey, L.M., Kakade, S., Decker, J.T., Rose, J., Deans, K., Shea, L.D., **Pearson, Ryan M.** Cargo-less Nanoparticles Program Innate Immune Cell Responses to Toll-like Receptor Activation. *Biomaterials* 2019. in press.
 - Saito, E., Kuo, R., **Pearson, Ryan M.**, Gohel, N., Cheung, B., King, N.J., Miller, S.D., Shea, L.D. Designing Drug-free Biodegradable Nanoparticles to Modulate Inflammatory Monocytes and Neutrophils for Ameliorating Inflammation. *Journal of Controlled Release* 300, (2019), 185-196.
 - Skoumal, M., Woodward, K.B., Zhao, H., Wang, F., Yolcu, E.S, **Pearson, R.M.**, Hughes, K.R., Garcia, A.J., Shea, L.D., Shirwin, H. Localized Immune Tolerance from FasL-functionalized PLG Scaffolds. *Biomaterials* 192, (2019), 271-281.
 - **Defnet AE**, Huang W, Polischak S, Yadav SK, **Kane MA**, **Shapiro P**, Deshpande DA. Effects of ATP-competitive and Function-selective ERK Inhibitors on Airway Smooth Muscle Cell Proliferation. *The FASEB Journal*. 2019 Jul 26:fj201900680R. doi: 10.1096/fj.201900680R. [Epub ahead of print] PMID:31266368
 - **Deredge D**, **Wintrode PL**, Tulapurkar ME, Nagarsekar A, Zhang Y, Weber DJ, **Shapiro P**, Hasday JD. A Temperature-dependent Conformational Shift in p38 α MAP Kinase Substrate Binding Region Associated with Changes in Substrate Phosphorylation Profile. *Journal of Biological Chemistry*. 2019 Jun 18. pii: jbc.RA119.007525. doi: 10.1074/jbc.RA119.007525. [Epub ahead of print] PMID:31213525
 - **Shapiro P**. A Promiscuous Kinase Inhibitor Reveals Secrets to Cancer Cell Survival. *Journal of Biological Chemistry*. 2019 May 24;294(21):8674-8675. doi: 10.1074/jbc.H119.009103.
 - Chothe PP, Czuba LC, Ayewoh EN, **Swaan PW**. Tyrosine Phosphorylation Regulates Plasma Membrane Expression and Stability of the Human Bile Acid Transporter ASBT (SLC10 A2). *Molecular Pharmaceutics*. 2019 Jul 8. doi: 10.1021/acs.molpharmaceut.9b00426. [Epub ahead of print] PMID:31194565
 - Saha Ray A, Ghann WE, Tsoi PS, Szychowski B, Dockery LT, Pak YJ, Li W, Kane MA, **Swaan P**, Daniel MC. Set of Highly Stable Amine- and Carboxylate-Terminated Dendronized Au Nanoparticles with Dense Coating and Nontoxic Mixed-Dendronized Form. *Langmuir*. 2019 Mar 5;35(9):3391-3403. doi: 10.1021/acs.langmuir.8b03196. Epub 2019 Feb 18. PMID:30712354
 - Liang, D.; Li, L.; Lynch, C.; Xia, M.; Wang, H.; **Xue, F.** 2019. DL5050: A Selective Agonist for the Human Constitutive Androstane Receptor. *ACS Medicinal Chemistry Letters*. in press.
 - Liang D, Li L, Lynch C, **Mackowiak B**, **Hedrich WD**, Ai Y, Yin Y, Heyward S, Xia M, Wang H, Xue F. 2019. Human Constitutive Androstane Receptor Agonist DL5016: A Novel Sensitizer for Cyclophosphamide-based Chemotherapies. *European Journal of Medicinal Chemistry*. 179:84-99.
 - Diethelm-Varela, B.; Ai, Y.; Liang, D.; **Xue, F.** 2019. Nitrogen Mustards as Anticancer Chemotherapies: Historic Perspective, Current Developments, and Future Trends. *Current Topics in Medicinal Chemistry* 19(9): 691-712.
 - Zhao, J.; Liang, D.; Robinson, E.; **Xue, F.** 2019. The Effects of Novel Heme Oxygenase Inhibitors on the Growth of *Pseudomonas aeruginosa*. *Microbial Pathogenesis* 129:64-67. PMID: 30716393.
 - Obianom ON, Ai Y, Li Y, Yang W, Guo D, Yang H, Sakamuru S, Xia M, **Xue F**, **Shu Y**. 2019. Triazole-Based Inhibitors of the Wnt/ β -Catenin Signaling Pathway Improves Glucose and Lipid Metabolism in Diet-Induced Obese Mice. *Journal of Medicinal*

- Ai, Y.; Obianom, O. N.; Kuser, M.; Li, Y.; **Shu, Y.; Xue, F.** 2019. Enhanced Tumor-Selectivity of 5-Fluorouracil using a Reactive Oxygen Species-Activated Prodrug Approach. *ACS Medicinal Chemistry Letters*. 10:127-131. PMID: 30655959.
- Cai, Y.; Abdel-Mohsen, M.; Tomescu, C.; **Xue, F.**; Wu, G.; Howell, B. J.; Ai, Y.; Sun, J.; Azzoni, L.; Coz, C. L.; Romberg, N.; Montaner, L. J. 2019. BCL6 Inhibitor-mediated Downregulation of pSAMHD1 and T Cell Activation Are Negatively Associated with HIV Infection and Reactivation. *Journal of Virology*. 93:e01073-18. PMID: 30355686.
- **Taraban, M.B.**, DePaz, R.A., Lobo, B., **Yu, Y.B.** (2019) Use of Water Proton NMR to Characterize Protein Aggregates: Gauging the Response and Sensitivity. *Analytical Chemistry*. 91, 4107-4115.
- J. L. Wilkerson, J. S. Felix, L. F. Restrepo, **M. I. Ansari, A. Coop**, L. R. McMahon. The Effects of Morphine, Baclofen, and Bupirone Alone and in Combination on Schedule-Controlled Responding and Hot Plate Antinociception in Rats. *Journal of Pharmacology and Experimental Therapeutics* (2019, in press) <https://doi.org/10.1124/jpet.118.255844>
- **Coop, A.**: Chapter 1 Concepts in Drug Discovery in Foye's *Principles of Medicinal Chemistry*, Wolters Kluwer Health (in press).
- **Richard N. Dalby**, Joanne Peart, Julie D. Suman, Paul M. Young and Daniela Traini, Editors. Respiratory Drug Delivery Europe 2019 (ISBN Book 1, 978-1-942911-34-0; Book 2, 978-1-942911-35-7), Davis Healthcare International Publishing, River Grove, Illinois (May 2019).
- Kazi A, Xiang S, Yang H, Chen L, Kennedy P, Ayaz M, **Fletcher S**, Cummings C, Lawrence HR, Beato F, Kang Y, Kim MP, Delitto A, Underwood PW, Fleming JB, Trevino JG, Hamilton AD, Sebti SM. Dual Farnesyl and Geranylgeranyl Transferase Inhibitor Thwarts Mutant KRAS-driven Patient-derived Pancreatic Tumors. *Clinical Cancer Research*. 2019 Jun 21. pii: clincanres.3399.2018. PMID: 31227505
- Chauhan J, Kwasny SM, **Fletcher S**, Opperman TJ, de Leeuw EPH. Optimization of a Small-molecule Lipid II Binder. *Bioorganic & Medicinal Chemistry Letters*. 2019 Jul 15;29(14):1849-1853.
- Conlon IL, Konsein K, Morel Y, Chan A, **Fletcher S**; Construction of 1H-indazoles from Ortho-aminobenzoximes by the Mitsunobu Reaction. *Tetrahedron Letters* 2019, in press
- Espino JA, **Jones LM**. Illuminating Biological Interactions with in Vivo Protein Footprinting. *Analytical Chemistry*. 2019 May 21;91(10):6577-6584. doi: 10.1021/acs.analchem.9b00244. Epub 2019 May 7. PubMed PMID: 31025855; PubMed Central PMCID: PMC6533598.
- Kaur U, Johnson DT, Chea EE, Deredge DJ, Espino JA, **Jones LM**. Evolution of Structural Biology through the Lens of Mass Spectrometry. *Analytical Chemistry*. 2019 Jan 2;91(1):142-155. doi: 10.1021/acs.analchem.8b05014. Epub 2018 Dec 6. PubMed PMID: 30457831; PubMed Central PMCID: PMC6472977.
- Rajawat GS, Belubbi T, Nagarsenker MS, Abrahamsson B, Cristofolletti R, Groot DW, Langguth P, Parr A, **Polli JE**, Mehta M, Shah VP, Tajiri T, Dressman J. Biowaiver Monograph for Immediate-Release Solid Oral Dosage Forms: Ondansetron. *Journal of Pharmaceutical Sciences*. 2019 Jun 8. pii: S0022-3549(19)30366-1. PMID:31181225
- Shemansky JM, McDaniel LP, Klimas C, Dertinger SD, Dobrovolsky VN, Kimoto T, Horibata K, **Polli JE**, Heflich RH. Pig-a gene Mutation Database. *Environmental and Molecular Mutagenesis*. 2019 May 15. PMID:31090953
- Das S, Pu X, Jiang X, Jiang W, Tung R, Ting TY, **Polli JE**. Exploring Generic Brittleness and the Demographic Factors for its Susceptibility in Patients with Epilepsy. *Epilepsy & Behavior*. 2019 Jan;90:197-203. PMID:30579779
- Raufman JP, Metry M, Felton J, Cheng K, Xu S, **Polli J.** A 19F Magnetic Resonance Imaging-based Diagnostic Test for Bile Acid

Diarrhea. *MAGMA*. 2019 Feb;32(1):163-171. Review.
PMID:30387017

- Liu R, Yue Z, Tsai CC, **Shen J**. Assessing Lysine and Cysteine Reactivities for Designing Targeted Covalent Kinase Inhibitors. *Journal of the American Chemical Society*. 2019 Apr 24;141(16):6553-6560. doi: 10.1021/jacs.8b13248. Epub 2019 Apr 16.
- Xiong Z, Cheng M, Zhu P, Huang S, Guo J, Zhang W, Zhou H, **Shu Y**, Li Q. Association of Blood Cell Counts with the Risk of Olanzapine- or Clozapine-induced Dyslipidemia in Chinese Schizophrenia Patients. *Human Psychopharmacology*. 2019 Jul 4:e2699. doi: 10.1002/hup.2699. [Epub ahead of print] PMID: 31273857
- Xu Y, Chen D, Lin XX, Zhao Q, Guo J, Chen LJ, Zhang W, Xiao J, Lian GH, Peng SF, Guo D, Yang H, Obianom O, **Shu Y**, Chen Y. The LRP6 Functional Mutation rs2302685 Contributes to Individual Susceptibility to Alcoholic Liver Injury Related to the Wnt/ β -catenin-TCF1-CYP2E1 Signaling Pathway. *Archives of Toxicology*. 2019 Apr 11. doi: 10.1007/s00204-019-02447-0. [Epub ahead of print]
- Zhou J, He F, Sun B, Liu R, Gao Y, Ren H, **Shu Y**, Chen X, Liu Z, Zhou H, Deng S, Xu H, Li J, Xu L, Zhang W. Polytropic Influence of TRIB3 rs2295490 Genetic Polymorphism on Response to Antihypertensive Agents in Patients with Essential Hypertension. *Frontiers in Pharmacology*. 2019 Mar 27; 10:236. doi: 10.3389/fphar.2019.00236. eCollection 2019.
- Ai Y, Obianom ON, Kuser M, Li Y, **Shu Y**, **Xue F**. Enhanced Tumor Selectivity of 5-Fluorouracil Using a Reactive Oxygen Species-Activated Prodrug Approach. *ACS Medicinal Chemistry Letters*. 2018 Dec 3; 10(1):127-131. doi: 10.1021/acsmchemlett.8b00539. eCollection 2019 Jan 10.
- Obianom ON, Ai Y, Li Y, Yang W, Guo D, Yang H, Sakamuru S, Xia M, Xue F, **Shu Y**. Triazole-Based Inhibitors of the Wnt/ β -Catenin Signaling Pathway Improve Glucose and Lipid Metabolisms in Diet-Induced Obese Mice. *Journal of Medicinal Chemistry*. 2019 Jan 24;62(2):727-741. doi: 10.1021/acs.jmedchem.8b01408. Epub 2019 Jan 10. PMID: 30605343
- Huang S, Zhu P, Sun B, Guo J, Zhou H, **Shu Y**, Li Q. Modulation of YrdC Promotes Hepatocellular Carcinoma Progression via MEK/ERK Signaling Pathway. *Biomedicine & Pharmacotherapy*. 2019 Apr 9;114:108859. doi: 10.1016/j.biopha.2019.108859. [Epub ahead of print] PMID: 30978526
- Wang S, Xia Y, Ma T, Weir MD, Ren K, Reynolds MA, **Shu Y**, Cheng L, Schneider A, Xu HHK. Novel Metformin-containing Resin Promotes Odontogenic Differentiation and Mineral Synthesis of Dental Pulp Stem Cells. *Drug Delivery and Translational Research*. 2019 Feb; 9(1):85-96. doi: 10.1007/s13346-018-00600-3. [Epub ahead of print] PMID: 30465181
- Lynch C, Mackowiak B, Huang R, Li L, Heyward S, Sakamuru S, **Wang H**, Xia M. Identification of Modulators That Activate the Constitutive Androstane Receptor From the Tox21 10K Compound Library. *Toxicological Sciences*. 2019; 167(1):282-292. PMID:30247703
- Dent, A. T., Mouriño, S., Huang, W., **Wilks, A.** (2019) Post-transcriptional Regulation of the *Pseudomonas aeruginosa* Heme Assimilation System (Has) Fine-tunes Extracellular Heme Sensing. *Journal of Biological Chemistry*. 294, 2771-2785.