



**COLLEGE OF
PHARMACY**

UNIVERSITY OF MICHIGAN

PK Core Supported Publications

2024 Publications

1. Takyi-Williams J, Leino AD, Li R, Downes KJ, Zuppa AF, Bwint A, Wen B, Sun D, Scheetz MH, Pai MP. Bioanalysis of six antibiotics from volumetric microsamples: a new tool for precision dosing in critically ill children. *Bioanalysis*. 2024 Jan;16(1):19-31.
2. Koschmann C, Al-Holou WN, Alonso MM, Anastas J, Bandopadhayay P, Barron T, Becher O, Cartaxo R, Castro MG, Chung C, Clausen M, Dang D, Doherty R, Duchatel R, Dun M, Filbin M, Franson A, Galban S, Garcia Moure M, Garton H, Gowda P, Marques JG, Hawkins C, Heath A, Hulleman E, Ji S, Jones C, Kilburn L, Kline C, Koldobskiy MA, Lim D, Lowenstein PR, Lu QR, Lum J, Mack S, Magge S, Marini B, Martin D, Marupudi N, Messinger D, Mody R, Morgan M, Mota M, Muraszko K, Mueller S, Natarajan SK, Nazarian J, Niculcea M, Nuechterlein N, Okada H, Opiari V, Pai MP, Pal S, Peterson E, Phoenix T, Prensner JR, Pun M, Raju GP, Reitman ZJ, Resnick A, Rogawski D, Saratsis A, Sbergio SG, Souweidane M, Stafford JM, Tzaridis T, Venkataraman S, Vittorio O, Wadden J, Wahl D, Wechsler-Reya RJ, Yadav VN, Zhang X, Zhang Q, Venneti S. A road map for the treatment of pediatric diffuse midline glioma. *Cancer Cell*. 2024 Jan 8;42(1):1-5.
3. Zhou W, Zhao Z, Lin A, Yang JZ, Xu J, Wilder-Romans K, Yang A, Li J, Solanki S, Speth JM, Walker N, Scott AJ, Wang L, Wen B, Andren A, Zhang L, Kothari AU, Yao Y, Peterson ER, Korimerla N, Werner CK, Ullrich A, Liang J, Jacobson J, Palavalasa S, O'Brien AM, Elaimy AL, Ferris SP, Zhao SG, Sarkaria JN, Győrffy B, Zhang S, Al-Holou WN, Umemura Y, Morgan MA, Lawrence TS, Lyssiotis CA, Peters-Golden M, Shah YM, Wahl DR. GTP Signaling Links Metabolism, DNA Repair, and Responses to Genotoxic Stress. *Cancer Discov*. 2024 Jan 12;14(1):158-175.

2023 Publications

1. Bu Y, Traore MDM, Zhang L, Wang L, Liu Z, Hu H, Wang M, Li C, Sun D. A gastrointestinal locally activating Janus kinase inhibitor to treat ulcerative colitis. *J Biol Chem*. 2023 Dec;299(12):105467. doi: 10.1016/j.jbc.2023.105467. Epub 2023 Nov 17. PMID: 37979913; PMCID: PMC10755797.
2. Yuan X, Jiang H, Fu D, Rech JC, Robida A, Rajanayake K, Yuan H, He M, Wen B, Sun D, Liu C, Chinnaswamy K, Stuckey JA, Paczesny S, Yang CY. Prophylactic Mitigation of Acute Graft versus Host Disease by Novel 2-(Pyrrolidin-1-ylmethyl)pyrrole-Based Stimulation-2 (ST2) Inhibitors. *ACS Pharmacol Transl Sci*. 2023 Aug 16;6(9):1275-

3. Xiang W, Zhao L, Han X, Xu T, Kregel S, Wang M, Miao B, Qin C, Wang M, McEachern D, Lu J, Bai L, Yang CY, Kirchhoff PD, Takyi-Williams J, Wang L, Wen B, Sun D, Ator M, McKean R, Chinnaiyan AM, Wang S. Discovery of ARD-1676 as a Highly Potent and Orally Efficacious AR PROTAC Degrader with a Broad Activity against AR Mutants for the Treatment of AR + Human Prostate Cancer. *J Med Chem.* 2023 Sep 28;66(18):13280-13303.
4. Chen Z, Hu B, Rej RK, Wu D, Acharyya RK, Wang M, Xu T, Lu J, Metwally H, Wang Y, McEachern D, Bai L, Gersch CL, Wang M, Zhang W, Li Q, Wen B, Sun D, Rae JM, Wang S. Discovery of ERD-3111 as a Potent and Orally Efficacious Estrogen Receptor PROTAC Degrader with Strong Antitumor Activity. *J Med Chem.* 2023 Sep 14;66(17):12559-12585.
5. Yang L, Tu W, Huang L, Miao B, Kaneshige A, Jiang W, Leng L, Wang M, Wen B, Sun D, Wang S. Discovery of SMD-3040 as a Potent and Selective SMARCA2 PROTAC Degrader with Strong *in vivo* Antitumor Activity. *J Med Chem.* 2023 Aug 10;66(15):10761-10781.
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7. Han X, Zhao L, Xiang W, Miao B, Qin C, Wang M, Xu T, McEachern D, Lu J, Wang Y, Metwally H, Yang CY, Kirchhoff PD, Wang L, Matvekas A, Takyi-Williams J, Wen B, Sun D, Ator M, McKean R, Wang S. Discovery of ARD-2051 as a Potent and Orally Efficacious Proteolysis Targeting Chimera (PROTAC) Degrader of Androgen Receptor for the Treatment of Advanced Prostate Cancer. *J Med Chem.* 2023 Jul 13;66(13):8822-8843.
8. Thomas JE 2nd, Wang M, Jiang W, Wang M, Wang L, Wen B, Sun D, Wang S. Discovery of Exceptionally Potent, Selective, and Efficacious PROTAC Degraders of CBP and p300 Proteins. *J Med Chem.* 2023 Jun 22;66(12):8178-8199.
9. Bu Y, Gao R, Zhang B, Zhang L, Sun D. CoGT: Ensemble Machine Learning Method and Its Application on JAK Inhibitor Discovery. *ACS Omega.* 2023 Mar 27;8(14):13232-13242.
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11. Qu P, Rom O, Li K, Jia L, Gao X, Liu Z, Ding S, Zhao M, Wang H, Chen S, Xiong X, Zhao Y, Xue C, Zhao Y, Chu C, Wen B, Finney AC, Zheng Z, Cao W, Zhao J, Bai L, Zhao S, Sun D,

- Zeng R, Lin J, Liu W, Zheng L, Zhang J, Liu E, Chen YE. DT-109 ameliorates nonalcoholic steatohepatitis in nonhuman primates. *Cell Metab.* 2023 May 2;35(5):742-757.
12. Roy J, Kyani A, Hanafi M, Xu Y, Takyi-Williams J, Sun D, Osman EEA, Neamati N. Design and Synthesis of Orally Active Quinolyl Pyrazinamides as Sigma 2 Receptor Ligands for the Treatment of Pancreatic Cancer. *J Med Chem.* 2023 Jan 24.
13. Pasternak AL, Park JM, Pai MP. Predictive Capacity of Population Pharmacokinetic Models for the Tacrolimus Dose Requirements of Pediatric Solid Organ Transplant Recipients. *Ther Drug Monit.* 2023 Feb 1;45(1):95-101.
14. Kaneshige A, Bai L, Wang M, McEachern D, Meagher JL, Xu R, Wang Y, Jiang W, Metwally H, Kirchhoff PD, Zhao L, Jiang H, Wang M, Wen B, Sun D, Stuckey JA, Wang S. A selective small-molecule STAT5 PROTAC degrader capable of achieving tumor regression in vivo. *Nat Chem Biol.* 2023 Jun;19(6):703-711.
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17. Yun HG, Smith AJF, DeBacker KC, Pai MP. Estimated glomerular filtration rate with and without race for drug dosing: Cystatin C vs. serum creatinine. *Br J Clin Pharmacol.* 2023 Mar;89(3):1207-1210.
18. Pai MP, Sitaruno S, Abdehnabi M. Removing race and body surface area indexation for estimated kidney function based drug dosing: Aminoglycosides as justification of these principles. *Pharmacotherapy.* 2023 Jan;43(1):35-42.
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21. Leino AD, Takyi-Williams J, Pai MP. Volumetric Absorptive Microsampling to Enhance the Therapeutic Drug Monitoring of Tacrolimus and Mycophenolic Acid: A Systematic Review and Critical Assessment. *Ther Drug Monit.* 2023 Aug 1;45(4):463-478.

- 22.Jin G, Ho JW, Keeney-Bonthrone TP, Pai MP, Wen B, Ober RA, Dimonte D, Chtraklin K, Joaquin TA, Latif Z, Vercruyse C, Alam HB. Prolonging the therapeutic window for valproic acid treatment in a swine model of traumatic brain injury and hemorrhagic shock. *J Trauma Acute Care Surg.* 2023 Jun 14.
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- 24.Liu S, Matvekas A, Naimi T, Ghanem A, Li R, Rajanayake K, Derstine B, Ross B, Sullivan J, Yun HG, Regenbogen S, Byrn J, Su G, Wang S, Pai MP. Morphomics-informed population pharmacokinetic and physiologically-based pharmacokinetic modeling to optimize cefazolin surgical prophylaxis. *Pharmacotherapy.* 2023 Sep
- 25.Leino AD, Magee JC, Kershaw DB, Pai MP, Park JM. A comprehensive mixed-method approach to characterize the source of diurnal tacrolimus exposure variability in children: Systematic review, meta-analysis, and application to an existing dataset. *J Clin Pharmacol.* 2023 Sep 23.
- 26.Jennaro TS, Puskarich MA, Flott TL, McLellan LA, Jones AE, Pai MP, Stringer KA. Kidney Function as a Key Driver of the Pharmacokinetic Response to High-Dose L-Carnitine in Septic Shock. *Pharmacotherapy.* 2023 Sep 29
- 27.Hall RG 2nd, Liu S, Putnam WC, Kallem R, Gumbo T, Pai MP. Optimizing anidulafungin exposure across a wide adult body size range. *Antimicrob Agents Chemother.* 2023 Nov 15;67(11)
- 28.Mike JK, White Y, Hutchings RS, Vento C, Ha J, Manzoor H, Lee D, Losser C, Arellano K, Vanhatalo O, Seifert E, Gunewardena A, Wen B, Wang L, Wang A, Goudy BD, Vali P, Lakshminrusimha S, Gobburu JVS, Long-Boyle J, Wu YW, Fineman JR, Ferriero DM, Maltepe E. Perinatal Azithromycin Provides Limited Neuroprotection in an Ovine Model of Neonatal Hypoxic-Ischemic Encephalopathy. *Stroke.* 2023 Nov;54(11):2864-2874

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2. Begley LA, Opron K, Bian G, Kozik AJ, Liu C, Felton J, Wen B, Sun D, Huang YJ. Effects of Fluticasone Propionate on Klebsiella pneumoniae and Gram-Negative Bacteria

Associated with Chronic Airway Disease. *mSphere*. 2022 Dec 21;7(6):e0037722.

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10. Rom O, Liu Y, Finney AC, Ghrayeb A, Zhao Y, Shukha Y, Wang L, Rajanayake KK, Das S, Rashdan NA, Weissman N, Delgadillo L, Wen B, Garcia-Barrio MT, Aviram M, Kevil CG, Yurdagul A Jr, Pattillo CB, Zhang J, Sun D, Hayek T, Gottlieb E, Mori, Chen YE. Induction of glutathione biosynthesis by glycine-based treatment mitigates atherosclerosis. *Redox Biol*. 2022 Jun;52:102313.
11. Xue D, Xu Y, Kyani A, Roy J, Dai L, Sun D, Neamati N. Multiparameter Optimization of Oxidative Phosphorylation Inhibitors for the Treatment of Pancreatic Cancer. *J Med Chem*. 2022 Feb 24;65(4):3404-3419.
12. Xue D, Xu Y, Kyani A, Roy J, Dai L, Sun D, Neamati N. Discovery and Lead Optimization of Benzene-1,4-disulfonamides as Oxidative Phosphorylation Inhibitors. *J Med Chem*.

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13. Sitaruno S, Santimaleeworagun W, Pathharachayakul S, DeBacker KC, Vattanavanit V, Binyala W, Pai MP. Comparison of Race-Based and Non-Race-Based Equations for Kidney Function Estimation in Critically Ill Thai Patients for Vancomycin Dosing. *J Clin Pharmacol*. 2022 May 11.
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15. Liu S, Pai MP, Lester CA. Medication Use Among U.S. Adults After Bariatric Surgery: A Population-Based Analysis of NHANES 2015-2018. *Diabetes Care*. 2022 Jan 19:dc212285.
16. Yun HG, Smith AJF, DeBacker KC, Pai MP. Estimated glomerular filtration rate with and without race for drug dosing: Cystatin C vs. serum creatinine. *Br J Clin Pharmacol*. 2022 Nov 11.
17. Pai MP, Sitaruno S, Abdehnabi M. Removing race and body surface area indexation for estimated kidney function based drug dosing: Aminoglycosides as justification of these principles. *Pharmacotherapy*. 2022 Nov 19.
18. Pai MP, Cojutti PG, Gerussi V, Della Siega P, Tascini C, Pea F. Linezolid Population Pharmacokinetics to Improve Dosing in Cardiosurgical Patients: Factoring a New Drug-Drug Interaction Pathway. *Clin Infect Dis*. 2022 Nov 25

2021 Publications

1. Luo Y, Guo Y, Wang H, Yu M, Hong K, Li D, Li R, Wen B, Hu D, Chang L, Zhang J, Yang B, Sun D, Schwendeman AS, Eugene Chen Y. Phospholipid nanoparticles: Therapeutic potentials against atherosclerosis via reducing cholesterol crystals and inhibiting inflammation. *EBioMedicine*. 2021 Dec; 74:103725.
2. Pai MP, Crass RL. Translation of Pharmacodynamic Biomarkers of Antibiotic Efficacy in Specific Populations to Optimize Doses. *Antibiotics (Basel)*. 2021 Nov 9;10(11):1368.
3. Rej RK, Wang C, Lu J, Wang M, Petrunak E, Zawacki KP, McEachern D, Yang CY, Wang L, Li R, Chinnaswamy K, Wen B, Sun D, Stuckey JA, Zhou Y, Chen J, Tang G, Wang S. Discovery of EEDi-5273 as an Exceptionally Potent and Orally Efficacious EED Inhibitor Capable of Achieving Complete and Persistent Tumor Regression. *J Med Chem*. 2021 Oct 14;64(19):14540-14556.
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5. Xiang W, Zhao L, Han X, Qin C, Miao B, McEachern D, Wang Y, Metwally H, Kirchhoff PD, Wang L, Matvekas A, He M, Wen B, Sun D, Wang S. Discovery of ARD-2585 as an Exceptionally Potent and Orally Active PROTAC Degrader of Androgen Receptor for the Treatment of Advanced Prostate Cancer. *J Med Chem.* 2021 Sep 23;64(18):13487-13509.
6. Han X, Zhao L, Xiang W, Qin C, Miao B, McEachern D, Wang Y, Metwally H, Wang L, Matvekas A, Wen B, Sun D, Wang S. Strategies toward Discovery of Potent and Orally Bioavailable Proteolysis Targeting Chimera Degraders of Androgen Receptor for the Treatment of Prostate Cancer. *J Med Chem.* 2021 Sep 9;64(17):12831-12854.
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10. Wang Y, Xie Y, Niu Y, Song P, Liu Y, Burnett J, Yang Z, Sun D, Ran Y, Li Y, Sun L. Carboxypeptidase A4 negatively correlates with p53 expression and regulates the stemness of breast cancer cells. *Int J Med Sci.* 2021 Feb 18;18(8):1753-1759.
11. Wang H, Ong E, Kao JY, Sun D, He Y. Reverse Microbiomics: A New Reverse Dysbiosis Analysis Strategy and Its Usage in Prediction of Autoantigens and Virulent Factors in Dysbiotic Gut Microbiomes From Rheumatoid Arthritis Patients. *Front Microbiol.* 2021 Feb 25;12:633732.
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13. Pai MP. Antimicrobial Dosing in Specific Populations and Novel Clinical Methodologies: Obesity. *Clin Pharmacol Ther.* 2021 Apr;109(4):942-951. doi:10.1002/cpt.2181.

14. Ali RA, Gandhi AA, Dai L, Weiner J, Estes SK, Yalavarthi S, Gockman K, Sun D, Knight JS. Antineutrophil properties of natural gingerols in models of lupus. JCI Insight. 2021 Feb 8;6(3):138385.
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nanomedicine design criteria in three types of preclinical cancer models for better clinical translation. Biomaterials. 2021 Aug;275:120910.

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2020 Publications

1. Falcone M, Menichetti F, Cattaneo D, Tiseo G, Baldelli S, Galfo V, Leonildi A, Tagliaferri E, Di Paolo A, Pai MP. Pragmatic options for dose optimization of ceftazidime/avibactam

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