

BII – Structure-based Ligand Discovery and Design

**** (Publications sorted: Newest – Oldest)**

1.	Zhang X, Wang Y, Supekar S, Cao X, Zhou J, Dang J, Chen S, Jenkins L, Marsango S, Li X, Liu G, Milligan G*, Feng M*, Fan H*, Gong W*, Zhang C* . Pro-phagocytic function and structural basis of GPR84 signaling . Nature Communications. 2023, 14(1):5706.
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3.	Go MK, Zhu T, Lim KJH, Hartono YD, Xue B, Fan H, Yew WS . Cannabinoid biosynthesis using noncanonical cannabinoid synthases . Int. J. Mol. Sci. 2023, 24, 2, 1259.
4.	Goh JJN, Behn J, Chong CS, Zhong G, Maurer-Stroh S, Fan H*, Loo LH* . Structure-based virtual screening of CYP1A1 inhibitors: towards rapid tier-one assessment of potential developmental toxicants . Archives of Toxicology. 2021, 95:3031–3048.
5.	Liu H, Deepak RNVK, Shiriaeva A, Gati C, Batyuk A, Hu H, Weierstall U, Liu W, Wang L, Cherezov V*, Fan H*, Zhang C* . Molecular basis for lipid recognition by the prostaglandin D2 receptor CRTH2 . PNAS August 10, 2021 118 (32) e2102813118; https://doi.org/10.1073/pnas.2102813118
6.	Tang LWT, Teng JW, Koh SK, Zhou L, Go ML, Chan ECY, Verma RK, Fan H . Infigratinib is a Reversible Inhibitor and Mechanism-based Inactivator of Cytochrome P450 3A4 . Drug Metab Dispos. 2021 Jul 29:DMD-AR-2021-000508. doi: 10.1124/dmd.121.000508. Online ahead of print.
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8.	Goh JJN, Behn J, Chong CS, Zhong G, Maurer-Stroh S, Fan H*, Loo LH* . Structure-based virtual screening of CYP1A1 inhibitors: towards rapid tier-one assessment of potential developmental toxicants . Arch Toxicol 2021.
9.	Yap J, Deepak RNVK, Tian Z, Ng WH, Goh KC, Foo A, Tee ZH, Mohanam MP, Sim YR, Degirmenci U, Lam P, Chen ZZ, Fan H*, Hu J* . The Stability of R-spine Defines RAF Inhibitor Resistance: A Comprehensive Analysis of Oncogenic BRAF Mutants with In-frame Insertion of αC-β4 loop . Science Advances 2021 In press
10.	Leow JWH, Verma RK, Lim ABH, Fan H, Chan ECY . Atypical kinetics of cytochrome P450 2J2: Epoxidation of arachidonic acid and reversible inhibition by xenobiotic inhibitors . Eur J Pharm Sci. 2021 May 24;164:105889. doi: 10.1016/j.ejps.2021.105889.
11.	Kuang W, Zhang J, Lan Z, Deepak RNVK, Liu C, Ma Z, Cheng L, Zhao X, Meng X, Wang W, Wang X, Xu L, Jiao Y, Luo Q, Meng Z, Kee K, Liu X, Deng H, Li W, Fan H, Chen L . SLC22A14 is a mitochondrial riboflavin transporter required for sperm oxidative phosphorylation and male fertility . Cell Rep. 2021 Apr 20;35(3):109025. doi: 10.1016/j.celrep.2021.109025.

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