

## **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*. <a href="#">Pro-phagocytic function and structural basis of GPR84 signaling</a> . Nature Communications. 2023, 14(1):5706.
2.	Cheng L, Deepak RNVK, Wang G, Meng Z, Tao L, Xie M, Chi W, Zhang Y, Yang M, Liao Y, Chen R, Liang Y, Zhang J, Huang Y, Wang W, Guo Z, Wang Y, Lin J, Fan H*, Chen L*. <a href="#">Hepatic mitochondrial NAD+ transporter SLC25A47 activates AMPKα mediating lipid metabolism and tumorigenesis</a> . Hepatology. 2023, doi: 10.1097/HEP.0000000000000314.
3.	Go MK, Zhu T, Lim KJH, Hartono YD, Xue B, Fan H, Yew WS. <a href="#">Cannabinoid biosynthesis using noncanonical cannabinoid synthases</a> . Int. J. Mol. Sci. 2023, 24, 2, 1259.
4.	Wei S, Behn J, Poore CP, Low SW, Nilius B, Fan H & Liao P. <a href="#">Binding epitope for recognition of human TRPM4 channel by monoclonal antibody M4M</a> . Sci Rep 12, 19562 (2022). <a href="https://doi.org/10.1038/s41598-022-22077-4">https://doi.org/10.1038/s41598-022-22077-4</a> .
5.	Krishna Deepak RNV*, Verma RK, Hartono YD, Yew WS, Fan H*. Recent Advances in Structure, Function, and Pharmacology of Class A Lipid GPCRs: Opportunities and Challenges for Drug Discovery. Pharmaceuticals 2022, 15(1):12.
6.	Liu Y, Chi W, Tao L, Wang G, Deepak RNVK, Sheng L, Chen T, Feng Y, Cao X, Cheng L, Zhao X, Liu X, Deng H, Fan H, Jiang P, Chen L, <a href="#">Ablation of H+/glucose Exporter SLC45A2 Enhances Melanosomal Glycolysis to Inhibit Melanin Biosynthesis and Promote Melanoma Metastasis</a> , The Journal of Investigative Dermatology (2022), doi: <a href="https://doi.org/10.1016/j.jid.2022.04.008">https://doi.org/10.1016/j.jid.2022.04.008</a> .
7.	Lim KJH, Hartono YD, Xue B, Kho MB, Fan H*, Yew WS*. <a href="#">Structure-Guided Engineering of Prenyltransferase NphB for High-Yield and Regioselective Cannabinoid Production</a> . ACS Catal. 2022, 12, 4628–4639. April 5, 2022; <a href="https://doi.org/10.1021/acscatal.2c00786">https://doi.org/10.1021/acscatal.2c00786</a> .
8.	Tang LWT, Wei W, Verma RK, Koh SK, Zhou L, Fan H, Chan ECY. <a href="#">Direct and Sequential Bioactivation of Pemigatinib to Reactive Iminium Ion Intermediates Culminate in Mechanism-Based Inactivation of Cytochrome P450 3A</a> . Drug Metabolism and Disposition February 13, 2022, DMD-AR-2021-000804; <a href="https://doi.org/10.1124/dmd.121.000804">https://doi.org/10.1124/dmd.121.000804</a> .
9.	Krishna Deepak RNV, Verma RK, Hartono YD, Yew WS, Fan H. Recent Advances in Structure, Function, and Pharmacology of Class A Lipid GPCRs: Opportunities and Challenges for Drug Discovery. Pharmaceuticals. 2022; 15(1):12. <a href="https://doi.org/10.3390/ph15010012">https://doi.org/10.3390/ph15010012</a> .
10.	Goh JJN, Behn J, Chong CS, Zhong G, Maurer-Stroh S, Fan H*, Loo LH*. <a href="#">Structure-based virtual screening of CYP1A1 inhibitors: towards rapid tier-one assessment of potential developmental toxicants</a> . Archives of Toxicology. 2021, 95:3031–3048.
11.	Liu H, Deepak RNVK, Shiriaeva A, Gati C, Batyuk A, Hu H, Weierstall U, Liu W, Wang L, Cherezov V*, Fan H*, Zhang C*. <a href="#">Molecular basis for lipid recognition by the prostaglandin D2 receptor CRTH2</a> . PNAS August 10, 2021 118 (32) e2102813118; <a href="https://doi.org/10.1073/pnas.2102813118">https://doi.org/10.1073/pnas.2102813118</a>

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