Jinn-Moon Yang

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Education and Current position:

1. 2020/2-now: Dean of College of Biological Science and Technology, NYCU.
2. 2007/8-2013/7: Director of Institute of Bioinformatics and Systems Biology, NCTU
3. 2007/8-now: Professor of Institute of Bioinformatics and Systems Biology, NCTU
4. 2004/8-2007/7: Associate Professor of Institute of Bioinformatics and Systems Biology, NCTU
5. 2001/8-2004/7: Assistant Professor of Institute of Bioinformatics and Systems Biology, NCTU
6. 1994/9—2001/1: Ph.D., Computer Science, National Taiwan University, Taiwan
7. 1992/9—1994/6: Master, Computer Science, National Central University, Taiwan

Research Overview:

I (Jinn-Moon Yang) am dean of College of Biological Science and Technology, NYCU. We are the first team to introduce molecular interaction family, including protein-protein, protein-DNA, and protein-compound interacting families which are similar to the concept of the protein or gene families. Our primary goal is to study drug-protein-pathway-disease relationships in a cell. The major research areas include computational drug discovery, structural bioinformatics, and computational systems biology. I published over 100 SCI papers on some journals, such as *Nature Communications*, *ACS Nano*, *Genome Biology*, *Nucleic Acids Research*, *Angewandte Chemie International Edition*, *Journal of Medicinal Chemistry*, and *PLOS Computational Biology*. My h-index is 35 and 26 as well as total numbers of citations are over 4,700 and 2,600 based on Google scholar and ISI Web of Knowledge, respectively. Our team has developed a molecular docking (GEMDOCK), which is one of world-wide mostly used docking program times cited is over 700, and site-moiety map (SiMMap) for molecular interaction (e.g., protein-ligand and protein-protein) mechanism analysis. We have collaborated with over 40 university laboratories, five teaching hospitals, and 15 national institutes for drug discovery and systems biology. In addition, we have successfully discovered 45 lead compounds (<10 μM) and got several U.S. patents. In summary, for investigating molecular interactions for cell behaviors and disease mechanisms, we extensively explored new models of both computational drug design (e.g., Homopharma and protein-ligand interaction) and computational systems biology (e.g., protein-protein interaction, CaMPNet, module organization principle, and network dynamics across well-known species (e.g., human, mouse, zebrafish, and yeast). We rigorously collaborated with biological researchers and clinical teams for the validations and applications of our new models to address unmet clinical requirements, such as diagnostic/prognostic biomarkers, drug resistance, multi-target drugs, and drug repurposing. I also joined the editorial boards of *Scientific Reports* and *PLoS ONE*. Some papers are listed as follows:

(*: corresponding author)

1. Pathak. N., Chen, Y.T., Hsu, Y.C., Hsu, N.Y. , Kuo, C.J., Tsai, H. P., Kang, J.J., Huang, C.H., Chang, S.Y., Chang, Y.H., Liang, P.H., Yang, J.M.* (2021) Uncovering Flexible Active Site Conformations of SARS-CoV-2 3CL Proteases through Protease Pharmacophore Clusters and COVID-19 Drug Repurposing, **ACS Nano**, DOI: 10.1021/acsnano.0c07383.
2. Lin, C. Y., Lee, C. H., Chuang, Y. H., Lee, J. Y., Chiu,Y. Y., Wu Lee, Y. H., Jong, Y. J., Hwang, J. K., Huang, S. H., Chen, L. C., Wu, C. H., Tu, S. H., Ho, Y. S.*, and Yang, J. M.* (2019), Membrane protein-regulated networks across human cancers, ***Nature Communications***, Vol: 10: 3131. (Main Text: 17 pages and Supplementary Information: 145 pages)
3. Hsu, K. C., HuangFu, W. C., Lin, T. E., Chao, M. W., Sung, T. Y., Chen, Y. Y., Pan, S. L., Lee, J. C., Tzou, S. C., Sun, C. M. and Yang, J. M.* (2020) A site-moiety map and virtual screening approach for discovery of novel 5-LOX inhibitors, Scientific reports, 10(1), 1-12.
4. Chuang, Y. H., Lee, C. H., Lin, C. Y., Liu, C. L., Huang, S. H., Lee, J. Y., Chiu, Y. Y., Lee, J. C., Yang, J. M.* (2020) An Integrated Genomic Strategy to Identify CHRNB4 as a Diagnostic/Prognostic Biomarker for Targeted Therapy in Head and Neck Cancer, Cancers, 12(5), 1324.
5. Yang, W. Y., Rao, P. S., Luo, Y. C., Lin, H. K., Huang, S. H., Yang, J. M.*, Yuh, C. H.* (2019) Omics-based Investigation of Diet-induced Obesity Synergized with HBx, Src, and p53 Mutation Accelerating Hepatocarcinogenesis in Zebrafish Model, Cancers, 11(12), 1899.
6. Huang, S. H., Lo, Y. S., Luo, Y. C., Tseng, Y. Y., Yang, J. M.* (2018) A homologous mapping method for three-dimensional reconstruction of protein networks reveals disease-associated mutations, BMC Systems Biology, 12(2):13.
7. Pathak, N., Lai, M. L., Chen, W. Y., Hsieh, B. W., Yu, G. Y., Yang, J. M* (2017) Pharmacophore anchor models of flaviviral NS3 proteases lead to drug repurposing for DENV infection, BMC Bioinformatics, 18(16):548.
8. Hsu, K. C., Sung, T. Y., Lin, C. T., Chiu, Y. Y., Hsu, J. T., Hung, H. C., Sun, C. M., Barve, I., Chen, W. L., Huang, W. C., Huang, C. T., Chen, C. H., and Yang, J. M.* (2015) Anchor-based classification and type-C inhibitors for tyrosine kinases, Scientific Reports, 5:10938.
9. Chu, C. H., Wang, L. Y., Hsu, K. C., Chen, C. C., Cheng, H. H., Wang, S. M., Wu, C. M., Chen, T. J., Li, L. T., Liu, R. Hung, C. L., Yang, J. M.*, Kung, H. J.*, and Wang, W. C.* (2014) KDM4B as a target for prostate cancer: structural analysis and selective inhibition by a novel inhibitor, Journal of Medicinal Chemistry, 57(14):5975-85.
10. Chiu, Y. Y., Tseng, J. H., Liu, K. H., Lin, C. T., Hsu, K. C. and Yang, J. M.* (2014) Homopharma: A new concept for exploring the molecular binding mechanisms and drug repurposing, *BMC Genomics*, 15 Suppl 9:S8. (**Best paper award in The 13th International Conference on Bioinformatics**)
11. Chiu, Y. Y., Lin, C. T., Huang, J. W., Hsu, K. C., Tseng, J. H., You, S. R., and Yang, J.M.* (2013) KIDFamMap: a database of kinase-inhibitor-disease family maps for kinase inhibitor selectivity and binding mechanisms, *Nucleic Acids Research*, D430-440.
12. Hsu, K. C., Cheng, W. C., Chen, Y. F., Wang, W. C., and Yang, J. M.* (2013) Pathway-based screening strategy for multitarget inhibitors of diverse proteins in metabolic pathways, *PLOS Computational Biology*, 9(7):e1003127.
13. Hsu, K. C., Chen, Y. F., Lin, S. R., and Yang, J. M.* (2011) iGEMDOCK: a graphical environment of enhancing GEMDOCK using pharmacological interactions and post-screening analysis, BMC Bioinformatics, 12 Suppl 1:S33.
14. Chen, Y. F., Hsu, K. C., Lin, S. R., Wang, W. C., Huang, Y. C., and Yang, J. M.* (2010) SiMMap: a web server for inferring site-moiety map to recognize interaction preferences between protein pockets and compound moieties, Nucleic Acids Research, 38:W424-30.

15. Tung, C. H., Huang, J. W., and Yang, J. M.* (2007) Kappa-alpha plot derived structural alphabet and BLOSUM-like substitution matrix for rapid search of protein structure database, Genome Biology, 8(3):R31.
16. Yang, J. M.*, and Chen, C. C. (2004) GEMDOCK: A generic evolutionary method for molecular docking, Proteins-Structure Function and Bioinformatics, 55(2):288-304.