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Biological membranes are highly specialized interfaces in organisms that protect and organize cells. They play critical roles in biological processes via complex interplays between lipids and other molecules. A major challenge in drug discovery is to design and synthesize drug molecules with good membrane permeability for efficient drug uptake through oral administration and for drug efficacy on intracellular targets. However, our understanding of the detailed mechanisms by which molecules interact and permeate through membranes is limited. Despite the prominent interest in peptide-based therapeutics, our ability to design permeable peptides is hampered by a lack of fundamental insight into how such molecules engage membranes. Similarly, signal transduction plays an essential role in biology and drug discovery. Much research has been done to understand the role that membrane-protein interactions play in cell signaling. However, detailed structural and dynamic information on membrane recruitment of peripheral proteins is still lacking. Therefore, we focus on two main research areas: investigating the structure-permeability-relationship at molecular and atomic levels; exploring the membrane recruitment through structures and dynamics of membrane-ligand-protein ternary complexes. Since solid state NMR can elucidate anisotropic properties

of the membrane structure and delineating molecular interactions in membranes, it will be one of our main tools. Other technologies such as solution NMR will also be employed for these studies. Gaining knowledge of interactions between membranes and other molecules (small molecules, peptides and proteins etc) at atomic level will not only benefit the fundamental understanding of biophysics and biochemistry, but also the design of better drugs.

Selected Publications

Interactions between γ -2-Adrenoceptor Ligands and Membrane: Atomic-Level Insights from Magic-Angle Spinning NMR. [2]

Yan S, Shaw DE, Yang L, Sandham DA, Healy MP, Reilly J, Wang B.
J Med Chem. 2017 Aug 24;60(16):6867-6879.

In-tube derivatization for determination of absolute configuration and enantiomeric purity of chiral compounds by NMR spectroscopy. [3]

Gao J, Rajan S, Wang B.
Magn Reson Chem. 2017 Apr;55(4):269-273.

Discovery of diamide compounds as diacylglycerol acyltransferase 1 (DGAT1) inhibitors. [4]

Nakajima K, April M, Brewer JT, Daniels T, Forster CJ, Gilmore TA, Jain M, Kanter A, Kwak Y, Li J, McQuire L, Serrano-Wu MH, Streeper R, Szklennik P, Thompson J, Wang B.
Bioorg Med Chem Lett. 2016 Feb 15;26(4):1245-8.

[Click here](#) [5] for additional publications.

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[2] <https://www.ncbi.nlm.nih.gov/pubmed/28703592>

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