Functional Group Distributions, Partition Coefficients, and Resistance Factors in Lipid Bilayers Using Site Identification by Ligand Competitive Saturation.
Functional Group Distributions, Partition Coefficients, and Resistance Factors in Lipid Bilayers Using Site Identification by Ligand Competitive Saturation.

Small molecules such as metabolites and drugs must pass through the membrane of the cell, a barrier primarily comprising phospholipid bilayers. Our work demonstrates the importance of accurate site identification in predicting both property distributions and absolute free-energy profiles.