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Biomimetic HPLC property measurements to estimate human in vivo distribution and tissue binding of drug discovery compounds

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Biomimetic HPLC stationary phases such as Immobilized Artificial Membrane (Regis IAM. PC.DD2), Human Serum Albumin (Chiral-HSA) and α-1-glycoprotein (Chiral-AgP) can mimic the in vivo interactions of the drug molecules to lipids and proteins. The calibrated retention times obtained on the biomimetic HPLC stationary phases can be used to build models for in vivo tissue-plasma partition, unbound volume of distribution, drug efficiency, and cellular concentration without using animal experiments. The measurements can be fully automated and large number of compounds can be ranked for further studies for the fraction of the cost of in vivo experiments. The methodology can be applied for new modalities in drug discovery such as peptides that would be difficult to characterize by traditional methods such as equilibrium dialysis to estimate their tissue binding and volume of distribution. Comparison of IAM partition and membrane disruption of antibiotic peptides has been investigated in order to predict their interactions with lipids. The chromatographic retention of potential drug molecules on biomimetic stationary phases can mimic in vivo binding to lipids and proteins that was validated using human clinical data of over 150 known drug molecules.

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