Contribution ID: **50** Type: **Short talk**

Octanol-Water Partition Coefficient: Fact or Fiction

Thursday, 18 June 2015 09:44 (20 minutes)

In pharmaceutical sciences, determining the partition coefficient P of a drug is a must, as this quantifies the drug solubility and distribution in the body. P is defined as the ratio of a drug concentration in a mixture of two immiscible phases, usually octanol and water. It implies that the two phases are structurally unaffected by the drug. SAXS reveals that octanol, as well as octanol in equilibrium with water, is structured, having polar groups that form a mesophase. Introducing drugs of different hydrophobicity changes the regularly packed water nanodroplets in the hydrated octanol mesophase. It is also possible for certain drugs to bring and keep more water into octanol by expanding the droplets into freely diffusing aqueous lacunae. We have proved that drugs do not partition into a homogeneous octanol, but mainly binds to a responsive octanol-water mesophase, which is heterogeneous. One should consequently reinterpret the P data in terms of octanol-water binding constants.

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Session Classification: Softmatter II

Track Classification: Soft matter