Qualitative understanding of partition preferences

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Rules for partitioning of various compounds (2/5)

For compound classes with an identical functional group:

Rule 7:

Logarithmic partition coefficients between air and any kind of organic phase (apolar or polar) increase linearly with molecular size within compound classes (i.e. compounds with identical functional groups).

With increasing cohesive energy of a sorbing phase (i.e. increasing number and/or strength of H-bonds) an increase in the size of a molecule results in less net energy gain because more cavity energy is required:

Rule 8:

The increase in partition constants with increasing size of the solute becomes smaller (i.e., the slope becomes shallower) with increasing cohesive energy of the sorbing phase.

Examples for rule 8 are shown in Figure 3-5 for solvents with increasing cohesive energy (hexadecane, octanol, methanol, water). Within this selection of sorbents the average slope of the linear relationships between log K and molar volume decreases from 0.036 (hexadecane) to -0.0008 (water).

