

Qualitative understanding of partition preferences

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Rules for partitioning of various compounds (4/5)

Partitioning between an organic phase and water: Combining the statements from Rule 7, 8 and 9 we get:

Rule 10:

Logarithmic organic phase/water partition constants, $\log K_{i,org./water}$, increase linearly with molecular size for compounds that otherwise possess identical functional groups. For bipolar organic phases this increase becomes smaller (i.e., shallower slope) with increasing cohesive energy.

This rule is illustrated in Figure 6 .

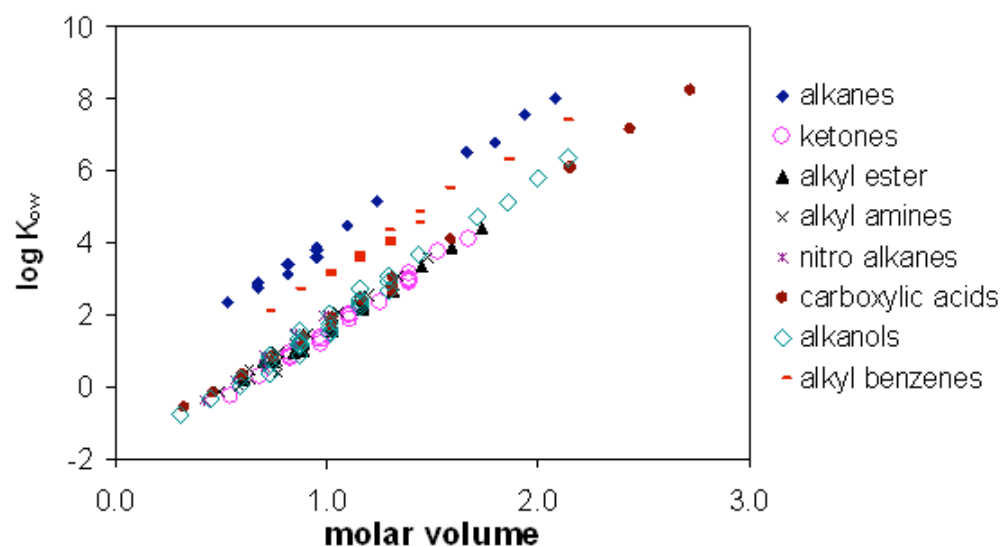


Figure 6: Increasing molar volume shifts the octanol/water partitioning towards the organic phase.

