



Qualitative understanding of partition preferences

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Rules for partitioning ...

...of a given compound into various phases 	Partitioning into bulk phases where only vdW–interactions occur	Case Ia apolar molecules in apolar or monopolar phases	Rule 1(a–c) Partitioning into different bulk phases differs by less than a factor of three.
		Case Ib monopolar molecules in monopolar phases of the same polarity and in apolar phases	
		Case Ic bipolar molecules in apolar phases	
	Partitioning into bulk phases where also H–bond interactions occur	Case IIa apolar molecule in bipolar phases	Rule 2 The partitioning of an apolar molecule into various bipolar phases will decrease with the number– density and strength of H–bonds in these phases.
Case IIb various chemicals in monopolar phases		Rule 3 Partitioning of a compound to a monopolar phase will increase with the strength and number of H–bonds that it can form with this phase.	
Other cases IIc		Rule 4 Almost all organic compounds prefer all organic phases over water due to the strong cavity effect in water.	
... of various compounds in a given two–phase system 	Rule 5 There is a linear trend between the logarithmic partition constants between air and apolar phases, $\ln K_{i\text{ air/apolar phase}}$ and molecular size for any organic compound.		
	Rule 6 Organic molecules prefer to stay in any organic phase as compared to the gas phase because they always gain more energy in this phase (even if they only interact by van der Waals forces) than they will loose due to the cavity effect; i.e. $K_{i\text{ org.phase/air}}$ values are generally larger than 1.		
	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).		
	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.		
	Rule 9 Logarithmic water/air partition constants, $\log K_{i\text{ water/air}}$, show a slight linear <i>decrease</i> with molecular size for compounds that possess identical functional groups.		
Rule 10 Logarithmic organic phase/water partition constants, $\log K_{i\text{ org./water}}$, 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.			

