Qualitative understanding of partition preferences

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Case IIb

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.

compound	/	solvent	K solvent / air	
ethanol	/	decane	38	
ethanol	/	cyclohexane	45	Bipolar compounds
ethanol	/	benzene	229	in monopolar phases
ethanol		isopropylether	470	or monopolar compounds
ethanol	/	heptanedioxane	1920	in monopolar phases of opposite polarity
dioxane	/	CCI ₄	4326	=> H-bonds occur between the compound <i>i</i> and the bulk phase
dioxane	/	cyclohexane	1106	but not in the cavity energy.
dioxane	/	ethyl ether	2436	Partitioning increases
dioxane	/	chloroform	27366	with strength of H-bonds
dioxane	1	CH ₂ Cl ₂	18712	-

For all remaining cases, i.e. partitioning of mono- and bipolar solutes into mono and bipolar phases we cannot derive any simple rule because here H-bonds occur both in the cavity energy and in the interaction energy between solute and phase so that they partially cancel. It is not always a simple task to predict which ones dominate.

For an extreme case, however, we can still set up an additional, valuable rule (although this cannot be derived here):

6) Almost all organic compounds prefer all organic phases over water due to the strong cavity effect in water. (Exceptions are small polar molecules and ionic organic molecules)

