Toxicity test

In a toxicity test for naphthalene, phenantrene and pyrene at 25°C the following, very different EC_{50}-values have been measured (the EC_{50}-value is the concentration in water at which the organisms show an effect when they are kept in this water for a defined time span). The tests had been conducted for each compound separately.

Naphthalene	1266 µg/L	$\log K_{lipid/water} = 3.30$ (L_{water}/L_{lipid})
Phenantrene	105 µg/L	$\log K_{lipid/water} = 4.46$ (L_{water}/L_{lipid})
Pyrene	22 µg/L	$\log K_{lipid/water} = 5.20$ (L_{water}/L_{lipid})

a) Estimate the respective equilibrium concentrations (in µmol/L) in the membrane-lipids of the organisms and comment on the result.

b) The EC_{50}-values from above apply to pure water. Which amount of pyrene would have to be added (per liter) in order to achieve the same toxic effect if the water contained 1 mg/L DOC (e.g. humic acid): $\log K_{DOC/water} = 4.18$ (L_{water}/kg_{DOC})? (Assume that the humic acid exhibits no direct influence on the tested organisms, and that the organisms do not significantly affect the dissolved concentration of pyrene by uptake or metabolism.)

Answer:

a) Assuming that the given lipid/water partition constants can be applied to the partitioning into membranes the following equilibrium membrane concentrations can be calculated:

Naphthalene	MW 128.2	$2.5 \cdot 10^6$ µg/L_{lipid}	=> $1.95 \cdot 10^4$ µmol/L_{lipid}
Phenantrene	MW 178.2	$3.0 \cdot 10^6$ µg/L_{lipid}	=> $1.68 \cdot 10^4$ µmol/L_{lipid}

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Pyrene MW 202.2 $3.5 \cdot 10^6$ µg/L_{lipid} => $1.72 \cdot 10^4$ µmol/L_{lipid}

The toxic concentrations in the membrane are very similar for all compounds. Note this characteristic membrane concentration has been found for many other compounds as well (not only PAHs) and therefore is regarded as a universal threshold for non-specific toxicity.

b) In order to achieve the same effect as before, the freely dissolved aqueous concentration of pyrene will have to be the same as in the experiment without DOC. Thus, more pyrene will have to be added to the water because part of the pyrene will be sorbed by the DOC.

Based on the $K_{oc/water}$ one can calculate that the equilibrium concentration of pyrene in DOC will be 333 µg/g_{DOC} or 0.333 µg/mg_{DOC} in equilibrium with a freely dissolved aqueous concentration of 22 µg/L.

Hence, per liter of water an additional 0.33 µg pyrene will have to be added in order to achieve the same toxic effect as before.