Assignment:
Visit the following webpage: http://www2.epa.gov/expobox

Under the "Media" Column, click "Aquatic Biota" and then select the "Fate & Transport" Tab.

Click on the link for "Physicochemical/Environmental Factors" and look over the physicochemical properties in addition to the *Kow* or *log*P that can determine the solubility and transport of chemicals.

Many of these properties that help predict and determine the fate and transport a chemical has in the environment are also used in determining the biological activity (ADME - Adsorption, Distribution, Metabolism, Excretion) of chemicals in living organisms including us. In addition to *Kow* are factors such as the half-life which can be an index of persistence, Henry's law constant (K_H) which is an index of air/water partitioning. Consideration of all physicochemical properties is important, however the *Kow* of a chemical is very useful for environmental assessments. If the *Kow* of a compound is known, it can serve as a reliable predictor to estimate the *Kow* value for other chemicals within that class of compounds.

Consider the following data provided by the EPA investigating “Basic Concepts of Contaminant Sorption at Hazardous Waste Sites” (see References):

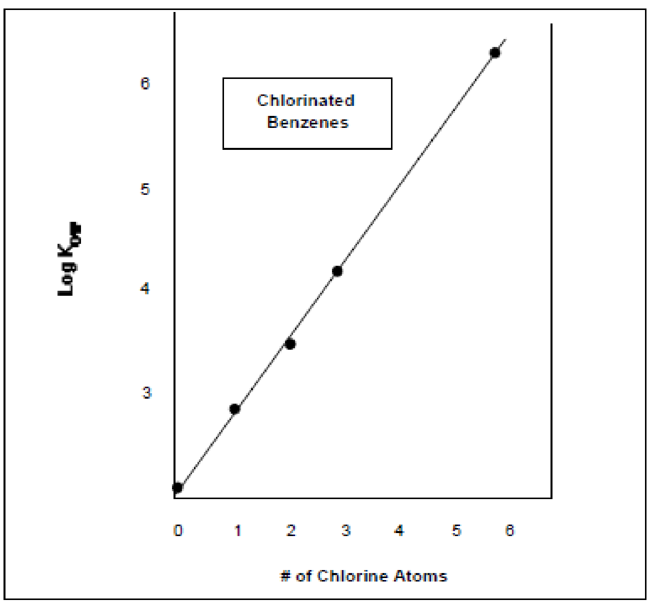


Figure A. Relationship of Molecular Structure to Hydrophobicity

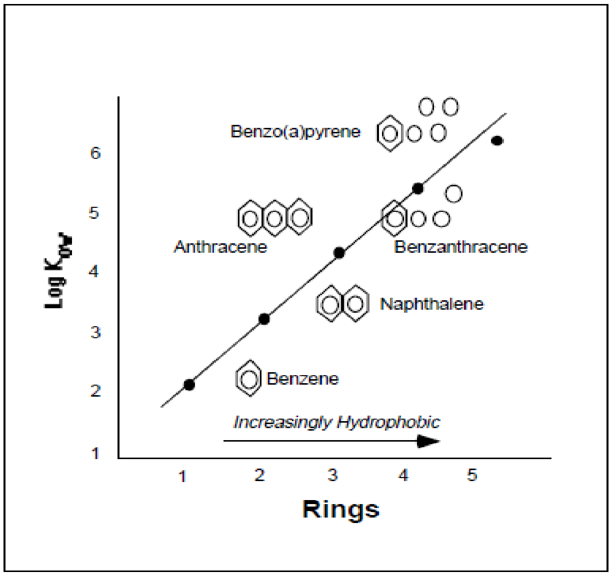
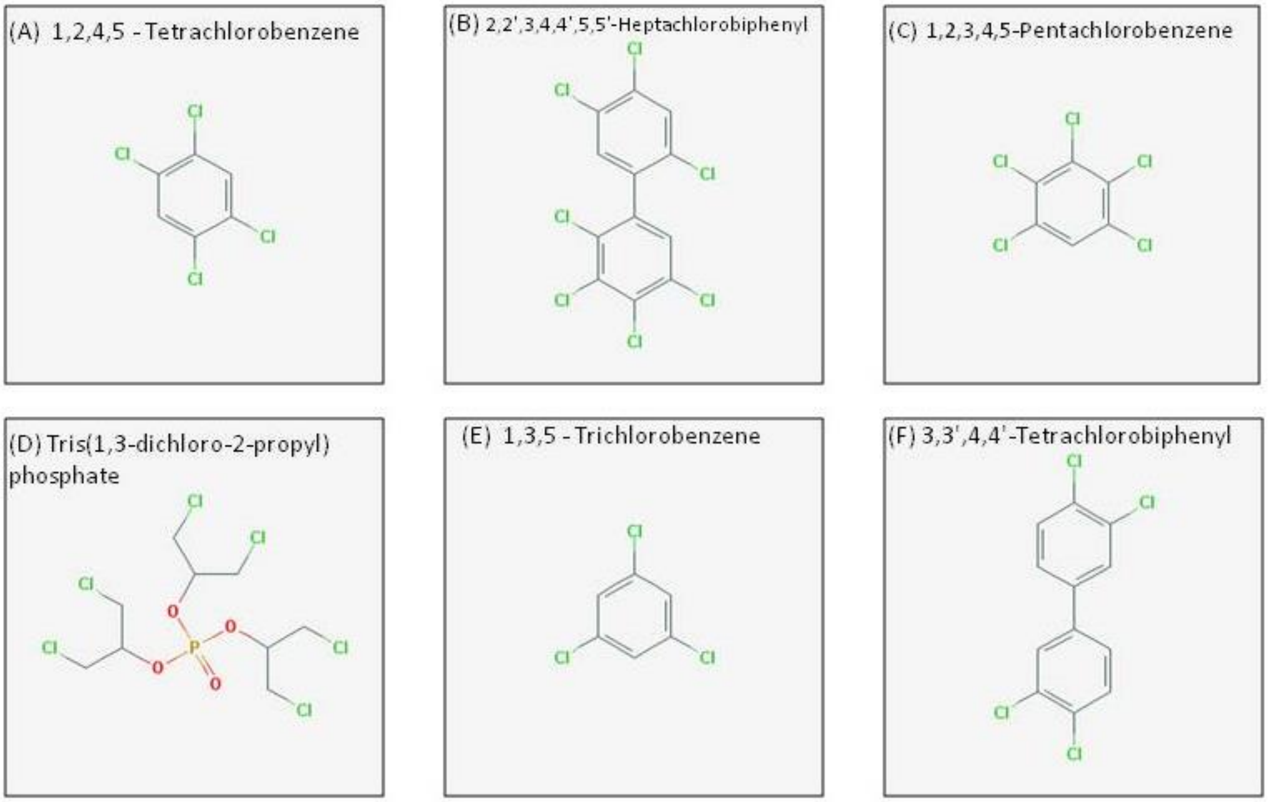


Figure B. Relationship of Molecular Structure to *Kow*

In these two examples, the *Kow* can be reliably predicted from the molecular structures. In the first graph it is correlated with the number of chlorine atoms, while in the second it is correlated with the number aromatic rings associated with the chemical. Now let us consider these concepts looking at some examples of a chemical class called Polychlorinated biphenyl's (PCB's) that were manufactured and used mainly as flame-retardant lubricants in the U.S. until they were banned by Congress in 1979.

Visit https://pubchem.ncbi.nlm.nih.gov/search/ and perform a search on each of the six chemicals to determine their respective K*ow*. How would you rank these chemicals from lowest to highest *Kow*?



Assignment Answer:

From lowest to highest K*ow*: E-3, D-3.65, A-4.7, C-5, E-6.72, B-7.5)

In consistency with the data presented in figures A & B above, the trend for *Kow* value increases with both the number of aromatic rings and the number of chlorines. Did compound D seem out of place? That is a chemical flame retardant from a different class of compounds identified as phosphate esters; specifically Tris(1,3-dichloro-2-propyl) phosphate (TDCP) with a *Kow* value of 3.65. It contains six chlorine and 9 carbon atoms, close in elemental composition to the PCB's. However, it also has a phosphate group at its core (PO_4^-). Despite having elements that are similar to PCB's the phosphate adds a constituent that makes the compound less hydrophobic.

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