## **Sample preparation**

Sample preparation - context

Sample preparation - motivation

Purpose of sample preparation

Overview of preparation methods

- ↓ Liquid liquid extraction (LLE)
- ↓ Solid phase extraction (SPE)
- ↓ Solid phase microextraction (SPME)
- ↓ Purge and trap (PT)
- ↓ (Accelerated) Solvent extraction ((A)SE)
- ↓ Supercritical fluid extraction (SFE)
- ↓ Filter Techniques (FT)
- Box 10 Filtration
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- Problems
- ↓ <u>1) Adsorbents</u>
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## 3) Solvents for liquid extraction

## Problem:

In the following table you find some solvents that are typically used in liquid extraction, together with their saturated vapor pressures at 25°C.

Solvent	Molar volume (m <sup>3</sup> /mol)	Saturated vapor pressure at 25°C (Pa)		
Methylcyclohexane	9.86 10 <sup>-5</sup>	6180		
Methanol	4.05 10 <sup>-5</sup>	16800		
Diethyl ether	7.31 10 <sup>-5</sup>	71700		

**3a)** For each of the solvents, calculate the minimum volume of air that needs to be passed over a 20 ml-extract of this solvent in order to reduce its volume to 3 ml. Assume a temperature of 25°C.

**3b)** Estimate the percentage of analyte that will be lost to the air while the solvent is evaporated. Do the calculation for each of the following analytes: naphtalene, chlorobenzene, 1,2,4-trichlorobenzene, 2-chlorophenol.

You can calculate the required solvent/air partition constants using equation on the page ppLFERs with the system

descriptors at 25°C from Flanagan et al. (2005)<sup>1</sup> given in the Table below for K<sub>solvent/air</sub> in [L<sub>air</sub>/L<sub>solvent</sub>].

Do your estimation for a worst-case scenario.

Solvent/air partitioning	v <sub>sa</sub>	s <sub>sa</sub>	a <sub>sa</sub>	b <sub>sa</sub>	l sa	C <sub>sa</sub>
Methylcyclohexane	0.407	0	0	0	0.902	0.213

Methanol	0.175	1.031	3.885	1.634	0.703	-0.05
Diethyl ether	0.870	0.927	3.213	0	0.737	0.031

<sup>1</sup> Reference: Flanagan, K.B., W.E. Acree, and M.H. Abraham (2005) Comments regarding "predicting the equilibrium partitioning of organic compounds using just one linear energy relationship (LSER)". Fluid Phase Equilibria, 237: 224-226 Journal Link .

**3c)** Alternatively, try to solve this problem without using all the data given here but by predicting all required data with the <u>SPARC software</u>. You will have to use the "property" function in the menue. The CAS number that you need as compound input can easily be found with a search in the www (look for the compound name and CAS). Help: The saturated vapor pressure of a solvent is nothing else than its partitioning between its pure liquid phase and the gas phase. The respective partition coefficient for this partitioning can be calculated with SPARC. It is the "Henry constant" for the respective liquid. For convenience choose units of mol/L / mol/L for the Henry constant under "Options" before you do the calculation.

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proceed to next problem

