CHEM 331: Kow –HPLC Lab Notes

Theory Section

- Relevance of partitioning in fate and distribution
- Kow as predictor of BCF, K_{oc} etc
- Definition of Kow in terms of concentration ratio
- Solubility related to activity coefficients, solute-solvent intermolecular interactions
- HPLC retention times related to partitioning between mobile and stationary phases
- Similar intermolecular interactions
- Establish correlation for structurally related series of cmpds (mention cmpds used in this experiment). Show chemical structures.

Experimental Section

- HPLC operating parameters and conditions
- Solution preparations to make individual and combined suite solutions
- Division of duties and responsibilities for shared data including HPLC's of combined standards (reference data sources other than your own group)

Data

- Chromatograms attached as Figures with descriptive titles or captions
- Data table to summarize retention time assignments and dead volumes from individual and combined suites

Results

- Capacity factors from combined suites
- Table to summarize parameters used in correlation (log k' and log K_{ow})
- Figure showing plot of LFER with Eqn of best fit line and R^2 (label points)
- Table showing results for unknowns (estimates of uncertainties)

Discussion

- Summary of trendline for PAH training set (comparison of different group results)
- Summary of results based on this trendline and a comparison to 'accepted values'
- Reliance of HPLC method on having 'good' K_{ow} values for training set cmpds and appropriate choice of cmpds to be included in this training set
- Structural relatedness of unknowns to training set (halogenated nonpolar aliphatic vs substituted aromatic or PAH)
- Suggested improvements to methodology appropriate for dieldrin, bisphenol-A
- Explanation of necessity for consistency of HPLC operating parameters and why isocratic conditions are required and the advantages of running combined stds solutions
- Description of what others have reported in the literature using this or related methods and how well/why it works
- Discussion of why accurate K_{ow} values are important in environmental chemistry, the need for 'evaluated' values and the controversy created by disparate values in the literature

Student sourced references for Kow – HPLC lab

Goss et al; LFER used to evaluate equil partitioning of org cmpds, EST, 2001, 35, 1-9

Lei et al; HPLC based method for estimating the temperature dependence on n-octanol water partition coefficients, J Chem Eng Data, 2000, 45, 738-742

Opperhuizen; Relationships between Kow aqueous activity coefficients and reverse phase HPLC capacity factors of alkylbenzenes, chloronapthalenes and chlorobiphenyls, Toxicol Envirn Chem, 1987, 15, 249-264

Donovan et al; Method for measuring the log Kow by using short octadecyl-polyvinyl alcohol hplc columns, J Chromat A, 2002, 952, 47-61

Kaune et al; Predicting 1-octanol water partition coefficients by hplc gradient elution, Anal Bioanalytical Chem, 1995, 353, 303-312

Eadsforth et al; Applications of HPLC for the determination of partition coefficients, Pestic Sci, 1986, 17, 311-325

Yamagami et al; Hydrophobicity parameters determined by RPLC: Optimal conditions for prediction of log P by using RP-HPLC procedures, Chem Pharm Bull, 2002, 50, 1578-1583

Voice et al; Sorbent concentration effects in liquid/solid partitioning, EST, 1985, 19, 789-796

Mackay; Correlation of bioconcentration factors EST, 1982, 16, 274-278

Pontolillo et al; Water Resources Investigations Report 01-4201; USGS 2001

DeKock et al; A simple procedure for determining octanol water partition coefficients using reverse HPLC, Chemosphere, 1987, 16, 133-142

Wei et al; Partition properties of 18 polychlorinated cmpds correlation with molecular descriptors, J. Liq Chromato. Rel Technol., 2002, 25, 627-637

Log Kow data sets:

http://logkow.cisti.nrc.ca/logkow/