Experiment proposal for
Comprehensive Organic Chemistry Experiments for the Laboratory Classroom

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Experiment title:	Determining partition coefficients of sulfonamides by reversed-phase chromatography		
Section of the table of contents in which this experiment should be included:			**20**

Abstract:

The physicochemical properties of an organic substance, such as lipophilicity, are among its most important traits. This property is implicated in both pharmacokinetic and pharmacodynamic events of drugs and is characterized early in drug discovery process. Reversed-phase chromatography has become an important method for determining lipophilicity expressed as the logarithm of the partition coefficient (log P).

The objective of the practical experiment described here is to determine the logarithm of the log P of three sulfonamides, sulfanilamide, sulfathiazole and sulfamethazine, antibacterial drugs with a significant historical value, by two different chromatographic methods. By reversed–phase high resolution liquid chromatography (RP-HPLC), the retention factors (expressed as log K) are used to estimate the log P of the three sulfonamides since there is a correlation between these two parameters. The chromatographic analyses are performed using octadecylsilica as stationary phase and 0.1% aqueous acetic acid /methanol: 85/15 (v/v) as mobile phase. By reversed-phase thin layer chromatography (RP-TLC), log P values are correlated with the chromatoghaphic parameter Rm. The Rm for each sulfonamide is calculated directly from the Rf value which is determined by TLC using a silica gel plate impregnated with 1-octanol and an aqueous buffer at pH 7.4 as mobile phase. The experimental logP values of this lab section are compared with predicted log P values calculated in ChemBioDraw®.

This experimental work takes a lab section with a low hazard level and targets advanced master students. This experiment offers an opportunity to show multidisciplinary applications with two important chromatographic techniques, HPLC and TLC, involving concepts of physicochemical properties and *in silico* calculations.

Graphical abstract