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Facilitated proton transfer across liquid|liquid interfaces under forced hydrodynamic conditions. Determination of partition coefficients of neutral weak bases.

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Abstract:

A novel quantitative methodology to determine the partition coefficients of neutral weak bases is developed. This new electrochemical approach is based on the measurement of the total transferred charge across the oil|water interface under forced hydrodynamic conditions. The complete procedure has been validated by computational simulations and experimental results (Tylosin A). In addition, flow pattern caused inside the electrochemical cell were simulated with computational fluid dynamics using finite element methods and correlated with experimental results obtained by magnetic resonance imaging.

Keywords: Finite element method, partition coefficient, facilitated proton transfer, liquid|liquid interface, forced hydrodynamic conditions, Magnetic Resonance Imaging.

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