Title: **Research of the drug discovery and study of the human and simulated intestinal media. CMC evaluation by ITC (iothermal titration calorimetry)**

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Prior to the market release of drugs, the pharmaceutical industry carries out a process called drug discovery. This development includes drug discovery, preclinical research, clinical trials and approval by competent organisms such as the EMA in Europe.

During the discovery of new drugs, the study of certain physicochemical parameters such as ionization, lipophilicity and solubility and their relationship with ADME (absorption, distribution, metabolism and excretion) parameters will be important to select the most promising candidates.

Water and simple buffers media had initially been used to anticipate the behaviour of drugs in contact with gastrointestinal fluids. However, their simplicity prevented from obtaining accurate results. Satisfactorily, nowadays much more complex media with components more like those of biological fluids have been synthetized. Among them, the biorelevant media FaSSIF - V2 and FeSSIF - V2 have been proposed to reflect better the small intestine conditions in fasted and fed state, respectively. In this work, the similarities and differences between these simulated media and actual conditions ones have been identified.

One of the components present in the intestinal fluids and the corresponding simulated media are surfactants and liposomes that, depend on their concentration, can form micelles that enhance the drug solubilization. An ITC (isothermal titration calorimetry) method has been successfully applied to measure the CMC (critical micelle concentration) and the enthalpy of the demicellization process of the surfactants. In this work the method has been reproduced using SDS as a surfactant. In the next future, the methodology will be used to characterize the intestinal micelles.

Keywords: Drug, ADME, physicochemical parameters, FaSSIF, FeSSIF, ITC, CMC, SDS