PIT-SLOPE, EACN AND COSMO-RS AS USEFUL EXPERIMENTAL AND THEORETICAL TOOLS TO PREDICT PROPERTIES AND RATIONALIZE SURFACTANT/OIL/WATER SYSTEMS

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Formulated systems are complex matrices with many ingredients, often incompatible, and likely to interact. To avoid a long and tedious traditional trial and error approach, it seems appropriate to have robust experimental and theoretical tools which will help in predicting, understanding and rationalizing the behavior of some components in order to be able, *in fine,* to establish relationships between chemical structures, physicochemical properties and functional properties. The CÏSCO research group of the University of Lille has been developing and using new experimental methods and conceptual tools for several years. We will illustrate, through concrete examples, the method that we named "PIT-slope" which is particularly robust for surfactants and additives to quantify their amphiphilicity (Fig.1A), the EACN (Equivalent Alkane Carbon Number) which provides a useful classification of perfumes and complex oils (Fig. 1B), and how it can be related to their solubilization in water, and finally, the COSMO-RS method which can predict some physicochemical properties of biosourced emollients in order to substitute silicones (Fig.1C).
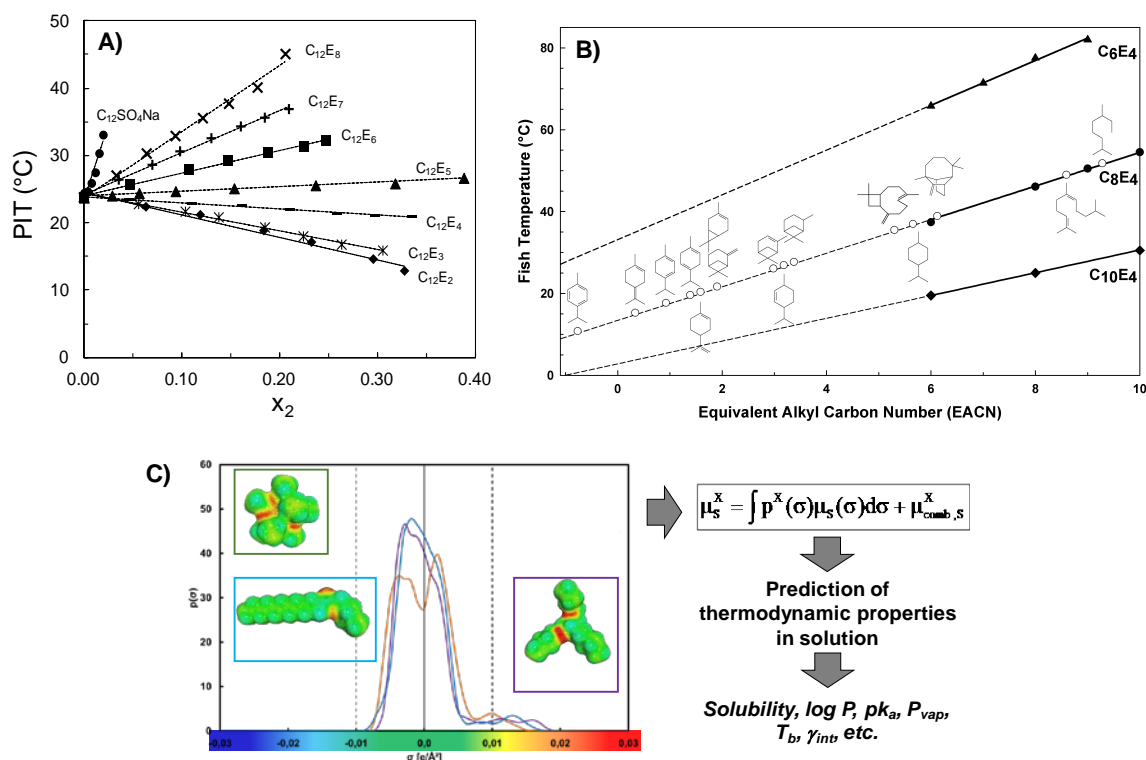

Figure 1. A) PIT-SLOPE method ofr the *classification of surfactants*. B) EACN scale for the *classification of terpenes*. C) COSMO-RS modelling for the *prediction of oils and surfactants properties.*

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