Green Solvents from Biomass: Lactate Family

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The work we present now forms part of a broader project regarding to the physicochemical characterization of the green solvents from biomass and their ecotoxicological characterization through several bioassays. Finally, this information is studied and analysed and the goodness of these kinds of solvents is assessed from the point of view of Green Chemistry.

This work is focused on the lactate family compounds; generally considered as green solvents are widely used as paints, gums, dyes, oils, detergents, food additives, cosmetics, in pharmaceuticals, etc.[1] The consideration as green solvents is due to their origin from carbohydrate feedstock. The case of ethyl lactate is particularly attractive for industry due to its physicochemical properties such as high boiling point, low surface tension and low vapour pressure. Moreover, ethyl lactate has replaced solvents such as toluene, acetone and xylene, in several chemical processes resulting in a much safer workplace.[2] This means that there is an alternative way through the use of the lactate family solvents for a wide range of industrial and consumer uses, replacing environment-damaging solvents including several volatile organic compounds and ozone depleting fluids.[3] Furthermore, it is important to note that alkyl lactates are important compounds in pharmaceutical industry, for instance, they are used as a penetration enhancer for some drugs in transdermal administration.[4]

Despite of the great interest on these compounds from lactate family, a rigorous study confirming the greenness of them has not been carried out yet. Although all the origin of the studied lactates can be from renewable resources, we think that is needed to depth on their physicochemical properties[5-7] and to develop environmentally friendly chemical processes[8]. A comprehensive thermophysical study in this sense has be performed.

In order to achieve the latter, we have carried out a study regarding on the suitability of lactate family compounds from the Green Chemistry point of view based on the following: thermophysical properties and ecotoxicology.

Therefore, the combination of the information obtained in ecotoxicity bioassays and several physicochemical properties such as critical aggregation concentration or solubility that give information about aggregation behaviour provide useful information about bioavailability and biocompatibility.

New data about properties such as vapour pressure (Fig. 1), solubility[9] or ALOGP, have been used to get information about the greener character. Vapour pressure is an important property that needs to be studied because it determines the volatile organic compounds, VOC, nature. Lactates present low vapour pressures compared with VOC compounds. The obtained results, indicate that the vapour pressures of the green chemicals studied here are much lower than some traditional solvents; therefore, they are thought to have lower VOC character. [10]

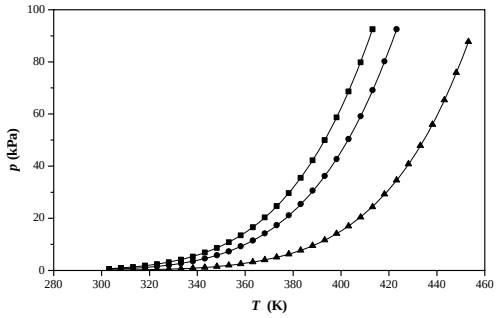

Fig. 1- Vapour pressure, *p*, as a function of temperature for the studied solvents: ■ *methyl lactate,* ● *ethyl lactate,* ▲ *butyl lactate.*

Finally, new data about acute ecotoxicity of lactates in water have been obtained (Fig 2.). A relationship between the structure of lactates and their toxicity can be seen by examining physicochemical characterizations of the compound.

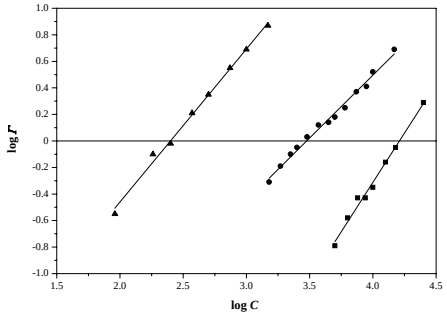

Fig. 2- Doses-response in *Vibrio fischeri* for the studied solvents: ■ *methyl lactate,* ● *ethyl lactate,* ▲ *butyl lactate.*

Furthermore, the relationship of toxicity with hydrophobicity[11] has been investigated; the log EC_{50} values of chemicals studied were plotted against their log *P* values as shown in Fig. 3.

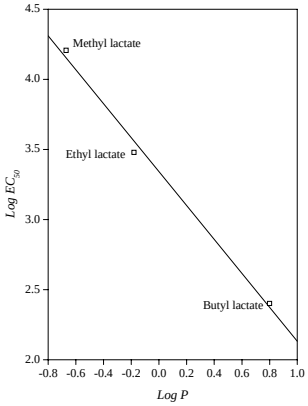

Fig. 3- Plots of acute toxicity, log EC50 versus the logarithm of the octanol-water partition coefficients: ■ *methyl lactate,* ● *ethyl lactate,* ▲ *butyl lactate.*

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