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In Silico Design of Sugar-based Surfactants

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PURPOSE OF THE ABSTRACT

Surfactants from the market are nowadays mostly produced from crude oil whose reserves may be depleted in this century. In this context, efforts have been engaged to replace such petroleum-based compounds by bio based alternatives within the framework of biorefineries, that aim the production of valuable materials from biomass. Among other products, such biomass contains sugars and fatty acid esters that can be used to produce sugar-based surfactants. These last represent good renewable alternatives to conventional petroleum-based surfactants in various applications like detergent and cosmetic formulation, enhanced oil or mineral recovery, etc. [1].

The structures of sugar-based surfactants can be very diverse and sometimes complex, consisting of polar heads with many alcohol moieties in particular configurations, pyranose cycles etc. [2]. To evidence the best candidates for target applications, large experimental screening should be performed. However, since such intensive experimental syntheses and characterizations are time and cost expensive, estimations of the relevant properties of possible candidates using predictive methods can be of particular interest to select the most promising ones for detailed experiment campaigns [3].

In this perspective, a series of new predictive models of the amphiphilic properties of sugar-based surfactants have been developed to better anticipate their performances in terms of detergency, dispersive power, emulsifying power, etc. These models allowed the estimation of the amphiphilic properties of sugar-based surfactants (describing surface and self-assembly activities) from relevant molecular descriptors, using quantum chemistry and quantitative structure-property relationships (QSPR) [4-6].

This contribution will demonstrate how these models can be used to design sugar-based surfactants with target properties in the perspective of substitution of petroleum-based surfactants. After the definition of target specifications in terms of critical micelle concentration (CMC), surface tension at CMC, adsorption efficiency (pC20) and Krafft point, a large virtual library of thousands of surfactant structures was built. QSPR models were then applied to screen this database of virtual surfactants to evidence those fitting at best with the defined specifications and to propose them for synthesis and experimental validation at University of Picardy Jules Verne in Amiens and at University of Technology of Compiègne. This In Silico design strategy revealed already powerful by proposing new possible candidates not already synthesized in open literature. Work in progress intends to improve it by looking at predictive approaches to estimate functional properties like foaming capabilities.

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FIGURES

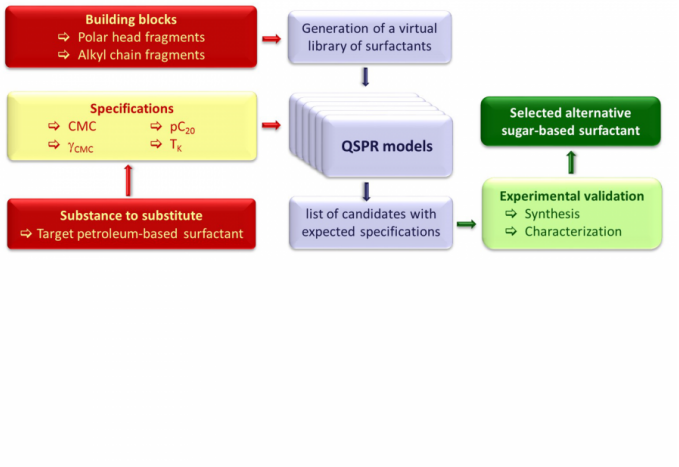

FIGURE 1

FIGURE 2

Figure 1

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KEYWORDS

Sugar-based surfactants | QSPR models | In Silico Design | Substitution

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