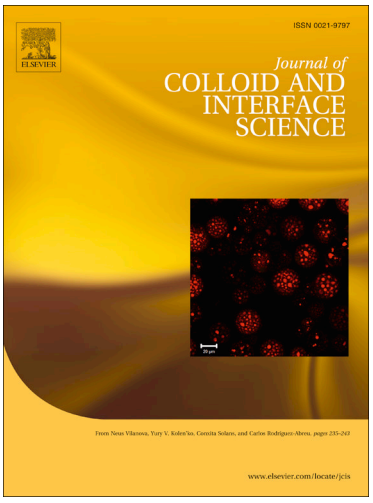

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Investigating the impact of sugar-based surfactants structure on surface tension at critical micelle concentration with structure-property relationships

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Abstract

Hypothesis. Surface tension of aqueous solutions of surfactants at their critical micelle concentrations (γ_{CMC}), may be quantitatively linked to the surfactant structure using Quantitative Structure Property Relationships (QSPR), all other factors held equal (temperature, presence of additive or salts). Thus, QSPR models can allow improved understanding and quantification of structure-γ_{CMC} trends, direct γ_{CMC} predictions, and finally help to design renewable substitutes for petroleum-based surfactants.

Experiments and methods. A dataset of 70 γ_{CMC} of single surfactants at ambient temperature has been gathered from several research papers. Then, descriptors of the whole structure, of polar heads and of alkyl chains of the 70 surfactants were calculated and introduced in multilinear regressions to evidence the most predictive and physically meaningful structure property relationships.

Findings. The best model, based on quantum chemical descriptors, achieved a standard error of 2.4 mN/m on an external validation. Simpler models were also achieved based solely on the count of H atoms of the polar head but with prediction error of 2.9 mN/m. Among all identified factors affecting γ_{CMC} of sugar-based surfactants (polar head size, alkyl chain length and branching), polar head size was found to exhibit the only effect clearly taken into account by all the models.