QSPR Modelling of new electrolytes

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We report the building, validation and release of QSPR (Quantitative Structure Property Relationship) models aiming at facilitating the design of new electrolytes for the next generation of Li/Polymer batteries. The dataset is based on data collected from publications and new sets of experimental measures produced by our partner at Chimie Paristech. It includes properties values of about one hundred electrolytes on oxidation potential (Eox), conductivity (Λ_m), boiling point (Tb), melting point (Tm), viscosity (η) and dielectric constant (ε). The resulting models are consensus of SVM models build using from 9 to 19 sets of relevant ISIDA molecular descriptors (figure 1) [1].

The ISIDA/Predictor software [2] is used to release the models on demand. This tool applies the models individually and returns the consensus estimate taking into account the Fragment Control applicability domain [3] of each of them.

Recently, a virtual chemical library of 9965 esters and sulfones ware enumerated and screened using the QSPR models. The 20 most promising compounds were prioritized using a Pareto front strategy based on their estimated properties. Beside, the selected compounds should match the following criteria: Eox > 4V, Tb > 50°C and Tm < 20°C. These compounds are currently being synthesized and tested.

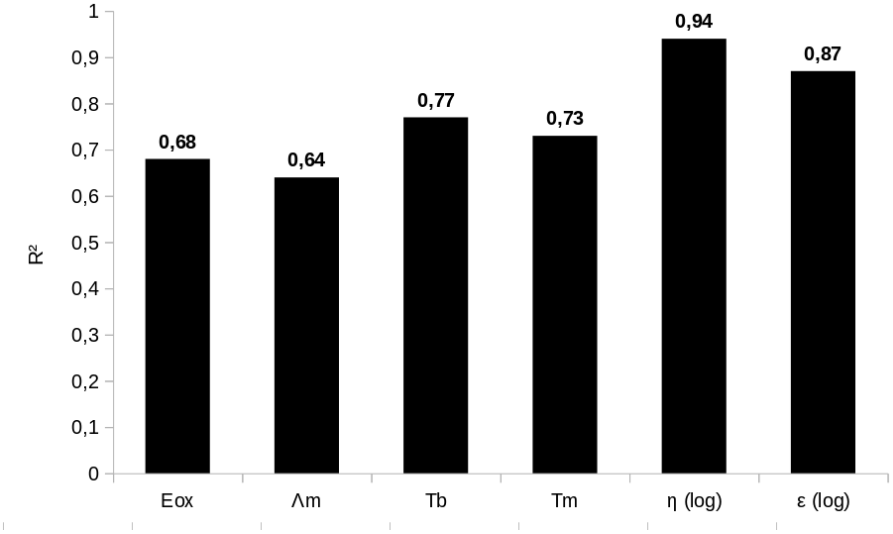

Figure 1: Determination coefficient of the 6 QSPR consensus models. The 6 proprieties are the oxidation potential (Eox), the conductivity (Λ_m), the boiling point (Tb), the melting point (Tm), the viscosity in log value (η (log)) and the dielectric constant in log value (ε (log)).

Bibliography:

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