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Modelling dissociation constants of organic acids by local molecular parameters

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The dissociation constant pKa defines the ionization degree of organic compounds. It is an important parameter that affects their toxicity and environmental behavior and fate. Among the present approaches to predict pKa values of organic chemicals, increment methods show a good performance but are limited by missing values of special groups. The purpose of this study is to develop models for predicting the pKa of organic acids directly from their molecular structures.

A quantum chemical method was introduced by employing local molecular parameters. Experimental pKa values of more than 1000 organic acids, including phenols, aromatic carboxylic acids, aliphatic carboxylic acids and alcohols were selected, and all molecules were optimized using the semi-empirical AM1 Hamiltonian. Simple models with several descriptors for different subsets were calibrated by multilinear regression (MLR). Substituent positions on aromatic rings were also taken into account.

The obtained models yield good predictive squared correlation coefficients q2 and superior performance compared with other quantum chemical models. The prediction capability is further evaluated using cross validation. The models unravel that the potential of oxygen atom conjoint to ionizable hydrogen atom to accept extra electronic charge is the single most important contribution to the dissociation of hydrogen atom.

Non-linear statistical analysis methods were also applied because of the non-linear character of the employed descriptors.

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