Predictive Model for the Molar Mass of Humic Substances

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Size exclusion chromatography (SEC) is known to be the most powerful tool for determination of the molecular weight and polydispersity of humic substances (HS). However, specific interactions of the charged humic macromolecules with the gel-matrix render application of SEC subject to artefacts. To avoid the erroneous results, the studies directed toward quantifying the deviation of experimental SEC parameters of HS from theory are in need. In this paper, the general problems of SEC application to molecular weight determination of HS will be discussed. An original approach for quantification of the deviation of experimental SEC parameters (K_d exp) of HS from theory (K_d^0), expressed as ΔK_d, will be described. The constraints of the predictive QSPR - model ΔK_d = f(structural descriptors) developed by the authors with a use of model ionogenic compounds will be considered. The undertaken adjustment of the predictive model to the specific features of HS, such as polyelectrolytic character and irregularity of the structure, will be described. A special attention will be given to explanation of the principles of generation of the proper structural descriptors of HS. Different experimental approaches to the structural characterisation of HS will be discussed. The results of application of the obtained structure - ΔK_d relationship to the results of SEC-fractionation of an extensive set of HS of different origin will be discussed. On the basis of the comparison of the calculated values of the molecular weight of HS with the results of the standard techniques will be concluded about the perspectives of the proposed predictive model.