A NEW APPROACH TO DESCRIPTION OF STRUCTURE OF HUMIC SUBSTANCES AND ITS APPLICATION TO ESTIMATING A QUANTITATIVE STRUCTURE - PROPERTY RELATIONSHIP

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A new approach to description of structure of humic substances (HS) is proposed along with a demonstration of its applicability to estimation of quantitative relationship between structural and detoxification properties of HS in relation to heavy metals. The approach is developed on the basis of the widely accepted fact, that humic molecules regardless of HS origin are composed of a limited set of the following structural fragments: aromatic rings and aliphatic chains, randomly substituted by functional groups (predominantly - by carboxylic and hydroxylic ones). A sequence and relative amount of the fragments in the molecule are determined by the genesis of HS. Hence, a structure of a humic macromolecule could be described by a standard set of the respective parameters. Upon expressing the given parameters via proper experimental data, a system of equations, describing structural peculiarity of HS under study, can be obtained. Solution of such a system will allow to characterize individual structural features of HS sample via a calculated set of the structural parameters. The advantage of such a presentation of structural information is a feasibility of its usage in follow-up correlation analysis. The next structural parameters were chosen for the description of humic molecule: number of carbon atoms in aromatic and aliphatic fragments, quantity of COOH, alcoholic and phenolic OH groups. The parameters were expressed via data of elemental analysis, ^{1}H and ^{13}C NMR spectroscopy. An overdefined system of equations was constructed to achieve more reliable results. It was being solved by least-squares method under requirement of non-negative solutions. Given an unequal accuracy of the used experimental data, weight factors were introduced in the system. Upon solving the system, coefficients related to a degree of substitution of an aromatic ring and the distribution of COOH groups between aromatic and aliphatic fragments were varied to decrease a dependence of the obtaining parameters on inaccuracy of the used structural model. A distribution of the calculated structural parameters had one maximum, which was considered as respected to the most probable structural description of HS. The described approach was applied to HS samples isolated from peat, soil, riverine and marine water. The obtained results and previously determined values of detoxification ability of these HS in relation to Cu, Cd, and Pb were subjected to correlation analysis. The highest correlation with detoxification ability of HS showed the expressions O_{Ph}/O_{OH} and $([COOH]+[O_{OH}])*C_{Ar}$, both of which were proportional to an amount of "salicylate" units in HS molecule and had highest values for all the terrestrial HS. It was concluded that the highest detoxification potential in relation to heavy metals might be intrinsic to the enriched with salicylate units HS.