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ABSTRACT BOOK

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PREDICTION OF STABILITY CONSTANTS OF THE METAL ION – ORGANIC LIGAND COMPLEXATION BY CONSENSUS QSPR MODELING

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Here we reports predictive QSPR models for the stability constants log*K* of the 1:1 (M:L) complexes of metal ions (M) with different classes of organic ligands (L) in aqueous solution at 298 K and an ionic strength 0.1 M. The complexation was studied for 42 metal ions: Li^{+}, Be^{2+}, Na^{+}, Mg^{2+}, Al^{3+}, K^{+}, Ca^{2+}, VO^{2+}, Mn^{2+}, Fe^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Ga^{3+}, Sr^{2+}, Y^{3+}, Ag^{+}, Cd^{2+}, In^{3+}, Ba^{2+}, La^{3+}, Hg^{2+}, Pb^{2+}, Ce^{3+}, Pr^{3+}, Nd^{3+}, Sm^{3+}, Eu^{3+}, Gd^{3+}, Tb^{3+}, Dy^{3+}, Ho^{3+}, Er^{3+}, Tm^{3+}, Yb^{3+}, Lu^{3+}, Th^{4+}, UO_2^{2+}, NpO_2^{+}, and Am^{3+}. Studied ligands are molecules of various organic classes. As a rule, acyclic or cyclic organic ligand has several functional groups, such as carboxylic, amine, phosphoryl, carboxy, sulfonic, ether, amide, phenolic groups in different combinations. The QSPR models have been built using ensemble multiple linear regression analysis and Substructural Molecular Fragment descriptors on data sets including from 883 (Cu^{2+}) to 28 (Am^{3+}) organic ligands. The models have reasonable prediction performance: root-mean squared error varies from 0.49 (Li^{+}) to 2.30 (In^{3+}) (the log*K* units) which is close to observed experimental systematic errors. The log*K* values were predicted by consensus models as arithmetic means of several hundreds of individual models taking into account their combined applicability domains. The Substructural Molecular Fragments enable detection of ligand moieties with important contributions into stability constants and they can be used as building blocks of new ligands. Developed models were applied for screening of selective ligands to every metal ion among some groups of metals using the 2962 organic ligands from the IUPAC Stability Constants Database. For technique aims, the obtained models allow one to assess the ligand selectivity of one metal with respect to another metal measured by the logarithm of a ratio of their stability constants.

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