Structure-property modeling of thermodynamic properties of supramolecular systems involving metals or hydrogen bonds

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This presentation concerns the structure – property modeling of the thermodynamic properties of supramolecular systems involving metals or hydrogen bonds. The structure - property studies of existing systems and computer-aided design of new compounds have been performed using the "**I**n **S**ilico" **D**esign and data **A**nalysis (**ISIDA**) system which consists of QSPR, clustering and combinatorial modules as well as some supplementary tools. The **ISIDA** system operates with two types of fragment descriptors: (*i*) the atom/bond sequences containing from 2 to 15 atoms and (*ii*) atoms with their nearest environment ("augmented" atoms). Optionally, the fragment descriptors can be mixed with any other "external" descriptors.

The **ISIDA** tools has been successfully tested in modeling of various properties: octanol/water partition coefficients and aqueous solubility of organic molecules, thermodynamic parameters of complexation of metal and neutral guests in solution and in biphasic liquid-liquid systems, biological activities [1-8]. The ensemble of **ISIDA**'s modules has been used for computer-aided design of new binders of some lanthanides and actinides; experimental tests confirms the robustness of predictions. Recently, the assessment of free energy and enthalpy for

the 1:1 hydrogen bond complexation of organic acids with organic bases has been performed using an original "labeled atoms" technique. In principle, fragments' contributions to free energy for H-bonding or metal cation – ligand interactions allow one to design new building blocks of supramolecular assemblies possessing desirable binding efficiency.

References

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