221st National Meeting, San Diego, CA
April 1-5, 2001

TUESDAY AFTERNOON

Advances in 3D Searching and Pharmacophores: Novel Approaches
Hyatt Regency, Regency D

O. F. Güner, *Organizer*

2:30 — 51. Modeling of ion complexation and extraction using substructural molecular fragments method. **A. Varnek**, G. Wipff, V. Soloviev

2:30 — Modeling of ion complexation and extraction using substructural molecular fragments method. Alexandre Varnek[1], Georges Wipff[1], and Vitaly Soloviev[2]. (1) Department of Chemistry, Louis Pasteur University, 4, rue B. Pascal, Strasbourg 67000, France, Fax: +33-3-88416104, varnek@chimie.u-strasbg.fr, (2) Institute of Physiologically Active Compounds, Russian Academy of Sciences

A Substructural Molecular Fragment (SMF) method has been developed to model the relationships between the structure of organic molecules and their thermodynamical parameters of complexation or extraction. The method is based on the splitting of a molecule into fragments, and on calculations of their contributions to a given property. It uses two types of fragments: atom/bond sequences, and "augmented atoms" (atoms with their nearest neighbours). The SMF approach is tested on physical properties of C2 – C9 alkanes (boiling point, molar volume, molar refraction, heat of vaporisation, surface tension, melting point, critical temperature, and critical pressures) and on octanol/water partition coefficients. Then, it is applied to the assessment of (i) complexation stability constants of alkali cations with crown-ethers and phosphoryl-containing podands, and of betha-cyclodextrins with mono- and 1,4-disubstituted benzenes, (ii) solvent extraction constants for the complexes of uranyl cation by phosphoryl-containing ligands, and, (iii) distribution coefficients of Hg, In and Pt extracted by 26 phosphoryl-containing monopodands, and of uranium extracted by 32 mono- and tripodands or by 22 monoamides.