# COMET – Predictive Tool to Assess Stability of Metal Complexes in Solution.

***N.Kireeva[a, b], G. Marcou[a], V.P. Solov'ev[b], D.Fourches[a], O.Klimchuk[a] and A.Varnek[a]****

*[a]Laboratoire d'Infochimie, Université Louis Pasteur, 4, rue B.Pascal,Strasbourg,67000, France*
*[b]Institute of Physical Chemistry and Electrochemistry, RAS, Leninsky pr-t, 31, Moscow,119991 Russia*

Chemoinformatics technologies can be efficiently used to predict metal binding affinity of organic molecules. Several machine learning methods and fragment descriptors implemented in the ISIDA *(In Silico* Design and Data Analysis) software have been applied to build quantitative models linking structure of organic molecules with stability constants (log*K*) of their 1:1 complexes with metals in water. The obtained models have been validated by means of 5-fold external cross-validation procedure and used in the COMET (**CO**mplexation of **MET**als) program for theoretical estimations of log*K* and for *„in silico"* design of new selective metal binders. "Models aapplicability domain" approach is applied to estimate reliability of predictions.

The current version of „COMET Predictor" involves log*K* models for alkaline-earth ($Ca^{2+}$, $Sr^{2+}$ and $Ba^{2+}$), lanthanides ($Ce^{3+}$, $Pr^{3+}$, $Nd^{3+}$, $Sm^{3+}$, $Eu^{3+}$, $Gd^{3+}$, $Tb^{3+}$, $Dy^{3+}$, $Ho^{3+}$, $Er^{3+}$, $Tm^{3+}$, $Yb^{3+}$, $Lu^{3+}$) and transition metals ($Ag^{+}$ ) with organic ligands in aqueous solutions. The WEB-version of the predictor is available for the users at http://infochim.u-strasbg.fr/cgi-bin/predictor.cgi

***Acknowledgement:*** GDRE SupraChem, ARCUS « Alsace – Russia/Ukraine », CDE Strasbourg and the French Embassy in Russia are acknowledged for the support

**References.**