# Successful "In Silico" Design of $UO_2^{2+}$ extractants using the ISIDA software suite

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New methods and original software tools for computer-aided molecular design have been used to develop "in silico" new monoamides which efficiently extract $UO_2^{2+}$. A set of available experimental values of the uranyl partition coefficient (logD) in water/toluene system for 22 monoamides[1] have been used by the ISIDA program in order to establish quantitative relationships between structure of the molecules and their extraction properties. Then, developed structure – property models have been applied to screen a virtual combinatorial library containing more than 20000 molecules. Selected hits (21 new molecules) have been synthesised and studied experimentally as extractants using the same protocol as for the molecules from the initial data set. Comparison between predicted and experimentally obtained logD values for new extractants is discussed. Good quantitative correspondence between predicted and experimental logD values demonstrates the reliability of suggested theoretical approach.

REFERENCES

1. C. Rabbe, C. Sella, C. Madic, A. Godard, *Solvent Extr. and Ion Exch*, 17(1), 87-112 (1999)