

INFLUENCE OF HEAD GROUP NATURE IN OXIME-FUNCTIONALIZED SURFACTANTS ON OCTANOL/WATER PARTITION COEFFICIENT

*Burakov N. I.*¹, Serdyuk A. A.¹, Shumeiko A. E.^{1,2}, Kapitanov I. V.¹

¹L. M. Litvinenko Institute of Physical Organic and Coal Chemistry NASU, Kiev, Ukraine

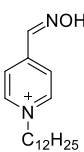
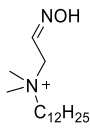
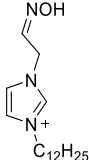
²Institute of Organic Chemistry NASU, Kiev, Ukraine

ashumeiko@ukr.net

One of the most important and fundamental property of chemical compounds is octanol/water partition coefficient (K_{ow}), which is usually used in logarithmic form ($\log P$). This parameter characterizes the compounds hydrophobicity and very often controls the biological effects as well as aggregation ability.

Values of $\log P$ were evaluated for series of oxime-functionalized surfactants with different nature of charged center in the head group (pyridinium /ammonium /imidazolium) and similar hydrophobic alkyl chain (*n*-dodecyl) with the two open access tools (<http://www.vcclab.org/lab/alogps/> and <http://www.molinspiration.com/services/logp.html>) using SMILES (Simplified Molecular Input Line Entry System) notation.

Table 1. Octanol/water partition coefficient ($\log P$) for series of oxyme-functionalized surfactants

Parameter	Compounds		
			
$\log P$ (www.vcclab.org)	1.27	1.27	1.41
$\log P$ (www.molinspiration.com)	1.38	1.39	1.55

Obtained results (see Table 1) are demonstrated that nature of charged center in the head group of oxime-functionalized surfactants has not significant influence on hydrophobic properties of the surfactant molecule.

The expected bioactivity profile for these molecules evaluated with open access tools <http://www.molinspiration.com/services/logp.html> included ion channel modulator and enzyme inhibitor activities.