

# PREDICTION OF ENVIRONMENTAL TOXICITY FOR SERIES OF AMPHIPHILIC OXIMES USING GUSAR SOFTWARE

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
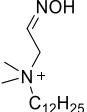
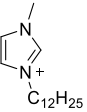
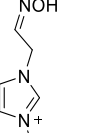
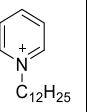
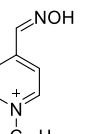
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Applications of amphiphilic compounds are very often connected with water systems and evaluation of possible environmental effects (e.g. *toxicity*) is important step on a way to eco-friendly compositions.

Using GUSAR software (<http://www.way2drug.com/gusar/environmental.html>) was performed analysis of potential environmental toxicity for series of amphiphilic oximes (Ib-IIIb) compared with non-functionalized analogs (Ia-IIIa) (see Tabl. 1). The used QSAR model was developed for the following endpoints: 96-hour fathead minnow 50 % lethal concentration, 48-hour daphnia magna 50 % lethal concentration, Tetrahymena pyriformis 50 % growth inhibition concentration and Bioconcentration Factor.

Table 1. Environmental toxicity for series of amphiphilic oximes (prediction by GUSAR)

Activity	Compounds					
						
	Ia	Ib	IIa	IIb	IIIa	IIIb
Bioaccumulation factor Log10(BCF)	1,579	1,208	1,553	1,786	2,242	2,076
Daphnia magna LC50 -Log10 (mol/L)	4,321	5,208	5,175	5,934	5,179	5,918
Fathead Minnow LC50 Log10 (mmol/L)	-2,355	-2,951	-2,843	-3,492	-3,034	-3,556
Tetrahymena pyriformis IGC50 -Log10 (mol/L)	1,686	2,033	2,350	2,729	2,374	2,695

In all cases introduction of oxime group demonstrate significant influence on environmental toxicity of compounds Ia-IIIa / Ib-IIIb. The nature of cationic center also determinate observed tendencies.