

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

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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 Log ₁₀ (BCF)	1,579	1,208	1,553	1,786	2,242	2,076
Daphnia magna LC50 -Log ₁₀ (mol/L)	4,321	5,208	5,175	5,934	5,179	5,918
Fathead Minnow LC50 Log ₁₀ (mmol/L)	-2,355	-2,951	-2,843	-3,492	-3,034	-3,556
Tetrahymena pyriformis IGC50 -Log ₁₀ (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.