**Acute toxicity of nitrophenols to freshwater algae *Chlorella vulgaris***

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Green algae are the most important components in the aquatic ecosystem by providing oxygen and nutrient to higher organisms and purifying water. Disruption of algal communities by pollutants can cause malfunctioning of the aquatic ecosystem. Primarily caused by production and degradation of pesticides, nitrophenols also emanate from the usage of dyes, solvents, plastics and explosives. Due to their ecological significance, REACH requires ecotoxicity data obtained from algal growth inhibition tests for compounds manufactured in or imported into the European Union greater than 1 ton/annum. However, despite the ecological significance of algae and in contrast to the regulatory needs for data obtained from algal growth inhibition tests, ecotoxicity data on algae are scarce.

In this study, the toxicity of ten nitro phenols including mono nitrophenols, dinitrophenols and methyl substituted nitrophenols to *Chlorella vulgaris* was determined in 96-hour static algal growth inhibition assay. Following range finding assays, the definitive tests were conducted in three parallels using five test concentrations and a control. The toxicity (*p*T) is defined by the concentration that inhibits algal growth by 50% (i.e., *IC*50) at the end of test period. The analytical concentrations of tested chemicals were verified by gas chromatography.

The data set is diverse with respect to MOA: A polar narcosis, four respiratory uncouplers and four soft-electrophilic compounds. All respiratory uncoupler compounds have lower acidity constants (*p*Ka) than experiment’s *p*H value. There is no correlation between hydrophobicity and 96h-toxicity for this data set. All of the compounds showed excess toxicity as expected. Toxicity of the compounds of the data set ranged between 39.4 ppm to 2.9 ppm. Of the mono-nitrophenols *p*-nitrophenol was found to be the most toxic to *C. vulgaris.* This is reasonable because nitro group offers an additional resonance form for *p*-nitrophenol that is not possible for *m*-nitrophenol. Among the nitrophenols tested, four of them were classified as toxic and six of them were harmful according to the toxicity scheme provided by the European Union.

It is of our interest to find a relationship between the structure of nitrophenols and their toxicity to algae. Within this scope, structural features of the compounds were calculated using SPARTAN 10 (Wavefunction, 2010) and DRAGON (version 6.0.38; Talete, 2014) software packages. All Subsets tool in QSARINS (version 2.2.1; Gramatica et. al., 2013; 2014) program was used to search a representative descriptor among 2369 descriptors calculated from DRAGON 6. A three-dimensional MoRSE (Molecule Representation of Structures based on Electron diffraction) class descriptor, Mor02s, was found to have a high correlation (*R*2=0.744) with the toxicity of this small data set. The MoRSE descriptors have been shown to have good relationships for different biological and physicochemical properties. Mor02s descriptor revealed that ionization state of the compound is important in explaining toxicity of nitrophenols. This is reasonable regarding the *p*Ka values of nitrophenols used in this study.

In this study, toxicity of most of the chemicals were assessed in a 96h bioassay for the first time to this freshwater algae. Since freshwater algal toxicity data was determined with up-to-date procedures in the same laboratory, by the same researchers, this study will contribute to the literature regarding the requirements for quality data.

**References:**

Gramatica, P., Chirico, N., Papa, E., Cassani, S., Kovarich, S., J. Comp. Chem., 34 (2013), 2121-2132.

Gramatica, P., Cassani, S., Chirico, N., J. Comp. Chem. 35 (2014) 1036–1044. <http://www.qsar.it>

Talete srl. (2014), DRAGON for Windows 6.0.38, Milan, http://www.talete.mi.it/

Wavefunction, Inc. (2010), SPARTAN 10, Irvine, USA, http://wavefun.com

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