Comment on "QSPR study on the bioconcentration factors of nonionic organic compounds in fish by characteristic root index and semiempirical molecular descriptors"

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In their article, Sacan et al. [1] conduct a "QSPR [quantitative structure-property relationship] study on the bioconcentration factors of nonionic organic compounds in fish." In constrast, a number of the compounds examined by Sacan et al. [1] are not "nonionic" as claimed. The following compounds investigated by these authors and listed in their "Table 2. Bioconcentation Factors and Molecular Structure Descriptors for 122 Nonionic Organic Chemicals" have associated pK_a values that would render the molecules significantly, and - in some cases - effectively entirely, ionized under conditions relevant for bioconcentration in freshwater and/or marine aquatic systems: 2,4-dichlorophenol, 7.90 [2]; pentachlorophenol, 4.74 [2]; 2,4,6-trichlorophenol, 6.10 [2]; 2-chlorophenol, 8.56 [3]; 3-chlorophenol, 9.12 [3]; 4-bromophenol, 9.37 [3]; aniline, 4.87 [3]; 2-nitrophenol, 7.23 [3]; 2-methyl-4,6-dinitrophenol, 4.46 [4]; 3-nitrophenol, 8.36 [3]; and 2,4,6-tribromophenol [5].

References

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