Comment on "QSPR model for bioconcentration factors of nonpolar organic compounds using molecular electronegativity distance vector descriptors"

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In their article, Qin et al. [1] construct a "QSPR model for bioconcentration factors of nonpolar organic compounds using molecular electronegativity distance vector descriptors." A number of the compounds examined by Qin et al. [1] are not "nonpolar" as claimed. The following compounds investigated by these authors and listed in their "Table 1. Six MEDV descriptors, and the experimental and calculated log BCF of 172 compounds" are not only polar, but they 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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