

**Theoretical Approach for physicochemical factors
affecting human toxicity of dioxins**

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Dioxins refer to a family of chemicals comprising 75 polychlorinated dibenzo-p-dioxin (PCDD) and 135 polychlorinated dibenzo-p-furan (PCDF) congeners, which may cause skin disorder, human immune system disruption, birth defects, severe hormonal imbalance, and cancer.

The effects of exposure of dioxin-like compounds such as PCBs are mediated by binding to the aryl hydrocarbon receptor (AHR), which is a ligand-activated transcription factor. To grasp physicochemical factors affecting human toxicity of dioxins, six geometrical and topological indices, eleven thermodynamic variables, and quantum mechanical descriptors including

ESP (electrostatic potential) were analyzed using QSAR and semi-empirical AM1 method. Planar dioxins with high lipophilicity and large surface tension show the probability that negative electrostatic potential in the lateral oxygen may make hydrogen bonding with DNA bases to be a carcinogen..

Keywords : dioxin, Ah receptor, molecular descriptors, PCDD, QSAR, ESP

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