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Title: Estimation of the aqueous solubility ($-lgS_w$) of all polychlorinated dibenzo-furans (PCDF) and polychlorinated dibenzo-p-dioxins (PCDD) congeners by density functional theory.

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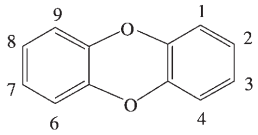
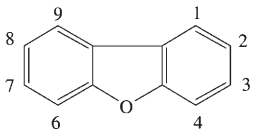
Compounds: 76 Polychlorinated dibenzo-p-dioxins (PCDDs) of type I and 135 polychlorinated dibenzo-furans (PCDFs) of type II.



I



II

Data taken from the literature:

S_w [aqueous solubility (dimension not given)].

Computational methods:

Molecular modeling (all 76 PCDD and 136 PCDF congeners were calculated at the B3LYP/6-31G* level in the GAUSSIAN98 program yielding the structural parameters used for modeling);

TLSER [Theoretical Linear Solvation Energy Relationships had the following general form: $XYZ = XYZ_0 + a \cdot \alpha + b \cdot E_{LUMO} + c \cdot q^- + d \cdot E_{LUMO} + e \cdot qH^+ + f \cdot \mu$;

MLR (stepwise Multivariate Linear Regression analysis);

LOO (Leave-One-Out cross-validation).

Data calculated:

TSLER descriptors [the following TSLER descriptors were calculated using ab initio optimized compounds: mean molecular polarizability, α ($10^{-30} \cdot$esu); dipole moment of the molecules, μ (Debye); energy of the highest occupied molecular orbital, E_{HOMO}, (eV); energy of the lowest unoccupied molecular orbital, E_{LUMO} (eV); the most negative atomic partial charge in molecule q^- (e); the most positive partial charge on a hydrogen atom, qH^+ (e); molecular volume, V_m ($Å^3$)];

q^2 (cross-validated correlation coefficient).

Results: The aqueous solubility of all PCDF and PCDD congeners has been modeled using density functional theory (DFT). The calculated TSLER parameters were taken as ab initio derived theoretical descriptors to establish a novel QSPR model for predicting aqueous solubility (pS_w) of PCDFs and PCDDs. The regression model developed contains two descriptors (Eq. 1).

$$pS_w = -0.1367\mu + 0.0601\,\alpha \quad (1)$$

$n = 211$ $r = 0.965$ $s = 0.489$ F not given $q^2 = 0.9153$

The results of cross-validation showed that the model is reliable and shows better predictive power than the AM1 derived model published previously. The study demonstrated that the DFT method could be an effective tool for the QSPR study of environmental contaminants.

(B. B.)

