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Prediction of aqueous solubility by treatment of COSMO-RS data with empirical solubility equations: the roles of global orbital cut-off and COSMO solvent radius

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ABSTRACT:

Aqueous solubility values of (E)-2-(ethyl(4-((4-nitrophenyl)diazenyl)phenol)amino)ethanol [B1], (E)-2,2′-((4-((4-nitrophenyl)diazenyl)phenyl)azanediyl)diethanol [B2], (E)-2,2′-((3-methyl-4-((4-nitrophenyl)diazenyl)phenyl)azanediyl)diethanol [B3] and (E)-2-((4-((2,4-dinitrophenyl)diazenyl)phenyl)(ethyl)amino)ethanol [B4] were predicted by the treatment of relevant COSMO-RS data with Cramer et al. solubility equation (CSE) and general solubility equation (GSE). DMol^3 computational code was employed for the study, where all calculations were carried out using VWN-BP level of theory with double numerical basis set containing polarization functions (DNP). Effects of global orbital cut-off and COSMO solvent radius (CSR) on the predicted results were examined. The results revealed that COSMO-RS data performed very well with both the CSE and GSE, but the latter exhibited a greater prediction strength on average. For nearly all the studied molecules, GSE calculated solubility (S_{GSE}) was found to increase with orbital cut-off and reached an optimum value at a cut-off of 5.5 Å. S_{GSE} values obtained at this and higher cut-off values studied are comparable to experimental solubility values, especially for B1, B3 and B4, while better results were obtained for B2 at lower cut-off values. CSE calculated solubility (S_{CSE}) showed no constant trend with cut-off variation, but at cut-off values ≥ 7.0 Å the S_{CSE} values compare well with the experimental values, especially in the cases of B2 and B3. For all the studied molecules, S_{GSE} decreased with the increase in CSR and the most reliable CSR value for GSE was found to be 1.3 Å. On the contrary, S_{CSE} increased with CSR and for B1 and B4, this increase was followed by a drop in predicted values at CSR > 1.3 Å. However, the best CSR value for CSE was found to be 0.5 Å for almost all the molecules. Our findings have shown that aqueous solubility (in

mol/L) of azo dyes can be accurately predicted using CSE or GSE with some COSMO-RS data and that global orbital cut and COSMO solvent radius are essential parameters for accurate prediction.