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QSAR Study and Haptotropic Rearrangement in Estradiol Derivatives

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Abstract : In this work, we have developed QSAR model for Relative Binding Affinity (RBA) of a large diverse set of estradiol among these derivatives, the organometallic derivatives. By dividing the dataset into a training set of 24 compounds and a test set of 6 compounds. The DFT method was used to calculate quantum chemical descriptors and physicochemical descriptors (MR and MLOGP) were performed using E-Dragon. All the validations indicated that the QSAR model built was robust and satisfactory (R2 = 90.12, Q2LOO = 86.61, RMSE = 0.272, F = 60.6473, Q2ext =86.07). We have therefore apply this model to predict the RBA, for two isomers β and α wherein Mn(CO)3 complex with the aromatic ring of estradiol, and the two isomers show little appreciation for the estrogenic receptor (RBAβ = 1.812 and RBAα = 1.741).

Keywords : DFT, estradiol, haptotropic rearrangement, QSAR, relative binding affinity
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