Using QSAR Calculation of Benzoxazine in Colon cancer

ali bahmani rad*,

Abstract: Quantitative structure activity relationship (QSAR) is an universal method for chemometrics, which reveals the relationship between chemical structures and their biological activities. As a supportive method fordrug design and prediction of drug activity, molecular docking is also applied to understand the structural interaction between drug and receptor. In this work QSAR study has been done on benzoxazine derivatives for anti- cancer drugs . Genetic algorithm , artificial neural network , multiple linear regression were used to creat non- linear and linear QSAR models . For this purpose , ab initio geometry optimization performed at (DFT) B3LYP level with a known basis set (6-31G(D)). Hyperchem , Chemoffice, Dragon and Gaussian 03w softwares were used for geometry optimization of the molecules and calculation of the quantum chemical descriptors . Finally for general studies we used PCR, PLS , MLR and predicting methods with Unscrambler 9.5 software and Jack – knife method for calculation in different layers finding the best derivative of benzoxazine .

Keywords : key words : Clone Cancer, QSAR Model, Genetic Algorithm, Artificial Neural Network PCR, PCA