QSAR calculations on fatty acid amide derivatives as anti-anxiety drugs

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In this work quantitative structure activity relationship (QSAR) study has been done on fatty acid amide derivatives for the treatment of anti-anxiety. Genetic algorithm (GA), Imperialist Competitive Algorithm (ICA). artificial neural network (ANN), multiple linear regressions (stepwise-MLR) were used to create the nonlinear and linear QSAR models. For this purpose, ab initio geometry optimization performed at B3LYP level with a known basis set (6–31G). Hyperchem, chemoffice and gaussian 09W softwares were used for geometry optimization of the molecules and calculation of the quantum chemical descriptors. Finally, unscrambler program was used for analysis of data. The results obtained this work indicate that ANN and MLR model is the most favorable method toward the other statistical methods and exhibit reasonable prediction capabilities. The best compounds to make the drugs are 7, 21, 24, 25, 27, 29. also the best descriptors are: G2s و F06[CN] و Mor15e و Mor22p و TPSA(NO) و Mor24p و Mor22m .[N-C]B08و MECC و Mor21 و

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