QSAR Study of 1-aminobenzyl -1H – indazole- 3- carboxamide analogus for the treatment of hepatitis C

Hadi Hendiani*,

Abstract: Hepatitis C is one of the most common causes of chronic infection in humans is known, the design of new drugs with better performance is needed. In this study, using quantitative structure activity relationship (QSAR) on derivatives, 1-Aminobenzyl-1H-indazole-3-carboxamide, as anti-hepatitis drugs have been studied. Genetic Algorithm (GA), Imperialist Competitive algorithm (ICA), artificial neural network (ANN) and multiple linear regression (MLR) for linear and non-linear models (QSAR) is created and used. For this purpose, a program was written by MATLAB software and a set of descriptors were defined by the Dragon. Using DFT (B3LYP) and the basic set 6- 31G (d) the optimal structure of the compounds was obtained. The SPSS statistical software was used to get the best model. Software Hyperchem, Chemoffice Gaussian 03 W and Dragon to optimize the quantum chemistry of molecules and calculate descriptors are used. The Unscrambler were used to analyze the data the application. Overall, the survey methods GA-PCR, GA-PLS and Jackknife method in different layers and different experimental purposes, compounds 5 and 10 with minimum deviation as the best combination for making drugs are predicted. The best descriptors include: X4A, RDF120m, Mor20m, GGI2, Mor19v, Mor20v, Methyl 4-((3-((3-carbamoyl-1H-indazol-1-yl) methyl) phenyl) amino)-4-oxobutanoate No.5 1-(3-(3-methylbenzamido) benzyl)-1H-indazole-3-carboxamide No.10

Keywords : Keywords: Hepatitis C, Quantitative structure activity relationship (QSAR), Genetic algorithm (GA), Artificial Neural Network (ANN), multiple linear regressions (MLR)