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Editorial OMICS International

A Gastrointestinal Study on Linear and Non-Linear Quantitative Structure (Chromatographic) Retention Relationships (QSRR) Models for Analysis 5-Aminosalicylates Nano Particles as Digestive System Nano Drugs under Synchrotron Radiations

A Heidari*

Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA

***Corresponding author:** A Heidari, Faculty of Chemistry, California South University (CSU), 14731 Comet St. Irvine, CA 92604, USA, Tel: +1–775–410–4974; E-mail: mailto:Scholar.Researcher.Scientist@gmail.com

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Editorial

The analysis of 5-aminosalicylates nano particles as gastrointestinal and digestive system nano drugs under synchrotron radiations is mainly carried out by Gas Chromatography (GC), making use of their specific Retention Times (RT) which is related to their medicinal, pharmaceutical, physiochemical and topological properties [1-28]. Predicting chromatographic retention is an interesting subject. Quantitative Structure (Chromatographic) Retention Relationships (QSRR) has been demonstrated to be a powerful tool in chromatography. Linear and non-linear methods, such as Multiple Linear Regression (MLR) or Partial Least Squares Regression (PLSR) and Neural Network (NN) or Multiple Non-Linear Regression (MNLR), have been widely applied in the QSAR/QSRR area based on an assumption of linearity or non–linearity between the descriptors and an investigated experimental property [29-59]. Neural Network (NN) or Multiple Non–Linear Regression (MNLR), as non–linear regression methods, have been widely used as efficient regression methods and successfully applied to diverse medicinal, pharmaceutical, physiochemical and topological chemistry problems. The aim of this editorial is to research for an efficient method to build an accurate quantitative relationship between the chemical and molecular structure and the Retention Times (RT) of the some medicinal and pharmaceutical nano compounds by stepwise Multiple Linear Regression (MLR), Multiple Non–Linear Regression (MNLR) and Artificial Neural Networks (ANN) methods under synchrotron radiations.

One important step in Quantitative Structure (Chromatographic) Retention Relationships (QSRR) investigation is the computational representation of the chemical and molecular structure which often called molecular descriptor. The built model performance and accuracy of the results are strongly dependent on the way that descriptor was performed. The chemical and molecular structure of the 5-aminosalicylates studied molecules by performing HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6-31G*, 6-31+G*, 6-31G(3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09. To optimize the geometry of these 5-aminosalicylates molecules, the HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD (T), LDA, BVWN, BLYP and B3LYP geometrical optimizations was applied. Furthermore, the Gaussian 09 was used to calculate the descriptors in this editorial and a total of 5-aminosalicylates molecular descriptors were calculated for each 5-aminosalicylates molecule. The calculated descriptors were first analyzed for the existence of the constant or near-constant variables, and those detected were removed. In addition, to decrease the redundancy existing in the descriptor data matrix, the descriptors correlation with each other and with the Retention Times (RT) of the 5-aminosalicylates molecules was examined and the collinear descriptors were detected. Among the collinear descriptors, the one presenting the highest correlation with the property was retained and the others were removed from the data matrix.

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