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Synthesis, Characterization, Theoretical prediction of activities and Evaluation of biological activities of Some Sulfacetamide based hydroxytriazenes

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Six new *N* [(4-aminophenyl)sulfonyl]acetamide based hydroxytriazenes have been synthesized and characterized using elemental analysis, IR, ^{1}H NMR, ^{13}C NMR and MASS spectral analysis. Further, their theoretical predictions for probable activities have been taken using PASS (Prediction of Activity Spectra for Substance). Although a number of activities have been predicted but specifically anti-inflammatory, anti-radical, anti-diabetic activities have been experimentally validated which proves that theoretical predictions agree with the experimental results. The object of the paper is to establish Computer Aided Drug Design (CADD) using our compounds.

Hydroxytriazenes have been extensively used as spectrophotometric reagents in our laboratory and elsewhere for determination of transition elements. Transition elements of first series extensively have been investigated using them as chelating agents. These reagents along with other spectrophotometric reagents have been reported by authors of our laboratory in form of reviews[1-2]. However, few hydroxytriazenes have been screened for their biological or pharmacological activities[3-8]. The earlier study[9-11] and theoretical prediction using PASS indicates that this series of compounds can be potential lead candidates for bioactivity if screened thoroughly. Based on this approach the present paper deals with CADD using known antibiotic sulfacetamide based hydroxytriazenes. Before planning experimental validation a theoretical prediction (PASS) was taken and out of many predicted activities only anti-inflammatory, anti-radical and anti-diabetic activities have been validated experimentally.

We have synthesized six hydroxytriazenes based on *N* [(4-aminophenyl)sulfonyl]acetamide [A.R. Grade purchased form Sigma (CAS No.: 144-80-9)] using method of Elkins and Hunter and further modified by Sogani and Bhattacharya[12-14]. The method involves reduction

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