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THEORETICAL INVESTIGATIONS FOR SOME N-SUBSTITUTE BENZENE SULPHONAMIDES FOR ACTING AS ANTIMICROBIAL AND ANTICANCER THERAPY

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Indeed, investigations using quantitative structure activity relationships (QSAR) are quite essential for modern chemistry and biochemistry. For qualified scientists such investigations having additional advantages as giving the background interpretations for the fine effect of each predicted descriptor. Among these of very important applications is that the exploiting of QSAR in drug design and discovery. Recently, Kumar and his co-workers have addressed 32 derivatives of 4-(1-aryl-2-oxo-1,2-dihydro-indol-3-ylideneamino)-N-substituted benzene sulphonamides [Arabian Journal of Chemistry (2014) 7, 396-408]. It seems interesting to investigate theoretically the main factors that influence the activity of these synthesised compounds for antimicrobial and anticancer therapy. This could lead to have an important hint that may be quite helpful for predicting and developing new molecules that could be more effective in those issues. The results showed that there is a good correlation between topological properties of molecules with their antimicrobial activity. For example, the Balaban index that depending on the number of edges for molecules plays a major role which gives an individual correlation coefficient of +0.714. In a similar manner, the cluster count and polar surface area as also belonging to topological properties give a good correlation. On the other hand, the results indicate that there is no any significant correlation between all properties with anticancer activity. In other words, there is no connection between the parameters that affecting antimicrobial activity with that of anticancer. Therefore, extensive efforts must be paid in order to find the suitable parameters that could help for predicting new anticancer compounds.

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