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QUANTUM CHEMICAL STUDY OF THE RELATIONSHIPS BETWEEN ELECTRONIC STRUCTURE AND ANTIVIRAL ACTIVITIES AGAINST INFLUENZA A H1N1, ENTEROVIRUS 71 AND COXSACKIE B3 VIRUSES OF SOME PYRAZINE-1,3-THIAZINE HYBRID ANALOGUES

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ABSTRACT

We have studied the relationships between the electronic structure and the antiviral activity againat H1N1, enterovirus 71 and Coxsackie B3 pathogens. The local atomic reactivity indices were obtained at the B3LYP/6-31G (d,p) level. For two of them (coxsackievirus B3 and H1N1) we obtained statistically significant equations that led to the correponding pharmacophores displaying atomic sites that can be sustituted to obtain molecules endowed with higher inhibitory activity. The results for enterovirus 71 strongly suggest that the molecules seem to have more than one mechanism of action.

KEYWORDS: H1N1, Enterovirus, Coxsackievirus, QSAR, DFT, Influenza