A Study of Drug-Receptor Interaction through DFT Based Local Descriptors

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ABSTRACT

Recently we have successfully predicted QSAR model for the series of oxazoline derivatives invoking DFT based global descriptors. Our proposed model has nicely correlated the experimental ovicidal activity of oxazoline derivatives with computed theoretical global descriptors. As we are aware that drug activity is not a global property, but rather a local property. In this venture we have tried to explore the drug-receptor interaction in terms of local DFT based descriptors. The local DFT based descriptors viz. fukui functions, local softness and local philicity indices are very important tools to predict drug activity.In this venture we have nicely explained the mechanistic bio-activity of oxazoline derivatives invoking DFT based local descriptors. The effect of substitution on parent moiety of oxazoline has also been successfully predicted.