Quinazolinone Derivatives as Growth Hormone Secretagogue Receptor Inhibitors: 3D-QSAR study

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Abstract : The 3D-QSAR (CoMFA and CoMSIA) analyses has been performed on a series of Quinazolinone Derivatives in order to understand their Growth Hormone Secretagogue Receptor inhibitory activities. CoMFA and CoMSIA studies were also included in this study for the evaluation of 3D-QSAR model. In the present investigation, the CoMFA and CoMSIA methods were successfully employed for internal and external validation. Leave-one-out, no-validation, cross-validation and bootstrapping analysis were providing the most significant correlation between structural description and biological activity. Taking into account of 3D-QSAR and docking results, a series of new molecules with high predicted activities were designed.

Keywords: Quinazolinone Derivatives, 3D-QSAR, CoMFA, CoMSIA, Autodock.

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