ABSTRACT

Chrionic Obstructive Pulmonary disease (COPD) is associated with malfunction of lungs due to breakdown of extracelluler matrix by proteases. A large number of Pakistan's population are affected by COPD. In this disease, proteases such as Cathepsins (Cats) are secreted by Neutrophills and Macrophages. These Cats assist in recruiting Adenoviruses and Mycoplasma to lungs which further damage respiratory system. In order to stop entry of Adenoviruses and Mycoplasma, Cats are good target. In this study, virtual screening based on molecular docking was performed with Cats enzymes and ZINC database of small molecules. The complexes with lowest binding energy were screened for LigPlot analysis. Based on LigPlot results, complexes with maximum number of interactions were separated and subjected to Lipinski's rule of five. The molecules with best physico-chemical properties and drug likeliness score were selected. These lead molecules are proposed to act as potent inhibitors of Cats.