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(57) Abstract :
A method (300) for identifying a binding site of a Cabergoline drug, the method comprising: developing pharmacophore models to extract features from the Cabergoline drug; validating the developed pharmacophore models by comparing with pre-defined models of existing coronavirus drugs; performing a virtual screening of a database of drugs with the validated pharmacophore models; performing a structure-based virtual screening of the validated pharmacophore models by structural docking of a target protein into the validated pharmacophore models; assigning a score to each pharmacophore model of the Cabergoline drug in order to identify the validated pharmacophore models with a high binding affinity and efficiency; and comparing the score obtained from the virtual screening and the structure based virtual screening for classifying the scored pharmacophore models based on the target protein binding affinity and efficiency for the coronaviridae family of virus.

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