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SCREENING OF NOVEL ANTIASTHMATIC CONSTITUENT OF LOBELIA NICOTINAFOLIA BY DOCKING

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ABSTRACT

The docking of selected protein with ligand was performed by using Hex 8.0.0. Cuda1. Hex is an interactive molecular graphics program for calculating and displaying feasible docking mode pair of protein and of DNA molecule. The three-dimensional structure, of histamine receptor, INOS was obtained from protein data bank (PDB). This structure was determined using X ray diffraction missing atom and loop were corrected by Prepare protein module under Accelrys. Discovery Studio 4(DS4); residue of were protonated of histamine receptor in pH 7.4 condition. The phytoconstituents which was selected for study shown better results in terms of ADME properties as well as drug likeness model score of vasicoline. The docking energy of vasicolinon receptor occupancy was satisfied as compare to standard used lobelanine

Keywords*:* - Proteins, DNA, Antihistamine, Lobelia nicotinafolia

SHORT COMMUNICATION

The docking of selected protein with ligand was performed by using Hex 8.0.0.Cuda[1]. Hex is an interactive molecular graphics program for calculating and displaying feasible docking mode pair of protein and of DNA molecule. Hex can also calculate protein-ligand docking, assuming the ligand is rigid and it can be superpose pair of molecule using only knowledge of their 3D shape in hex "s docking calculation, each molecule is modelled using 3D expansion real orthogonal spherical polar basic function to encode both surface shape electrostatic charge and potential distribution[2-5].

Antihistamine H1 antagonists have been disappointing in asthma therapy, and this presumably reflects the fact that all of the actions of histamine are mimicked by other mediators. New and more potent antihistamines appear to have greater beneficial effects in asthma, so that histamine may have a more important role finding efficient mimicking agents of *Lobelia nicotinafolia*[6-11]. Scientist are further thinking to include the studies of some nutraceuticals like probiotics exhibiting antioxidant and anticancer activities for docking as future studies[12-29].

METHODOLOGY:

Target identification:

The three-dimensional structure, of histamine receptor, INOS was obtained from protein data bank (PDB). This structure was determined using X ray diffraction missing atom and loop were corrected by Prepare protein module under Accelrys. Discovery Studio 4(DS4); residue of were protonated of histamine receptor in pH 7.4 condition.

Ligand identification:

Lobelanine and vasicolinon (with pub chem ID) was retrieved form NCBI pub chem compound database 17,18, The 2D and 3D structure of the ligand retrieved. The structure was dowanloaded in SDF format and was then converted into PDB format using OPEN BABEL 2.2.199 and farther used for docking studies.

Docking FTO:-

The Graphical User Interface program "Auto-Dock Tools" "Hex 8.00 Cuda Software" was used to prepare, run, and analyses the docking simulation.

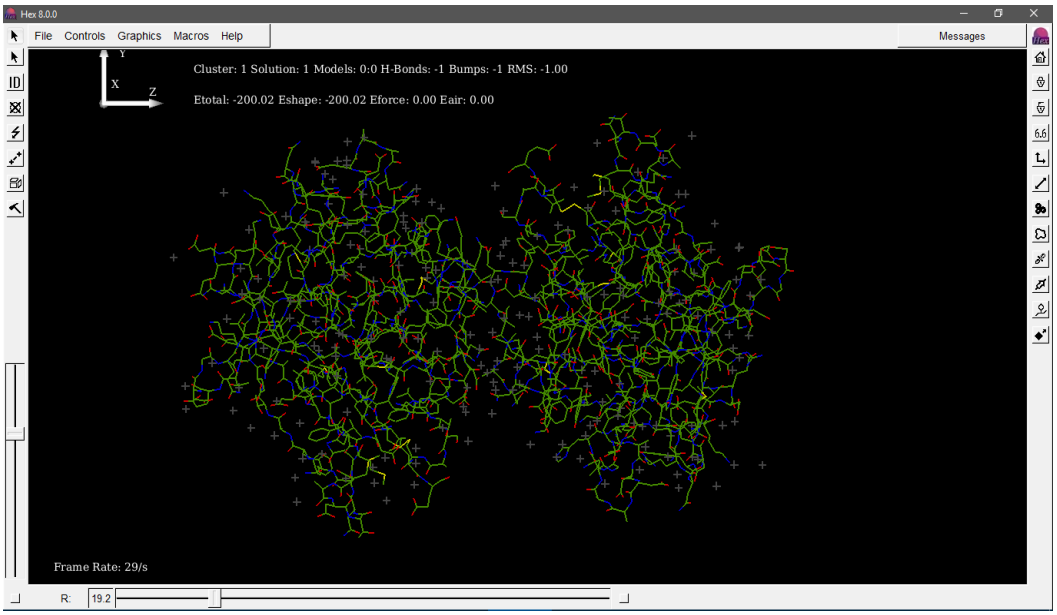

Fig.1. Docking of Histamine receptor &vasicolinon

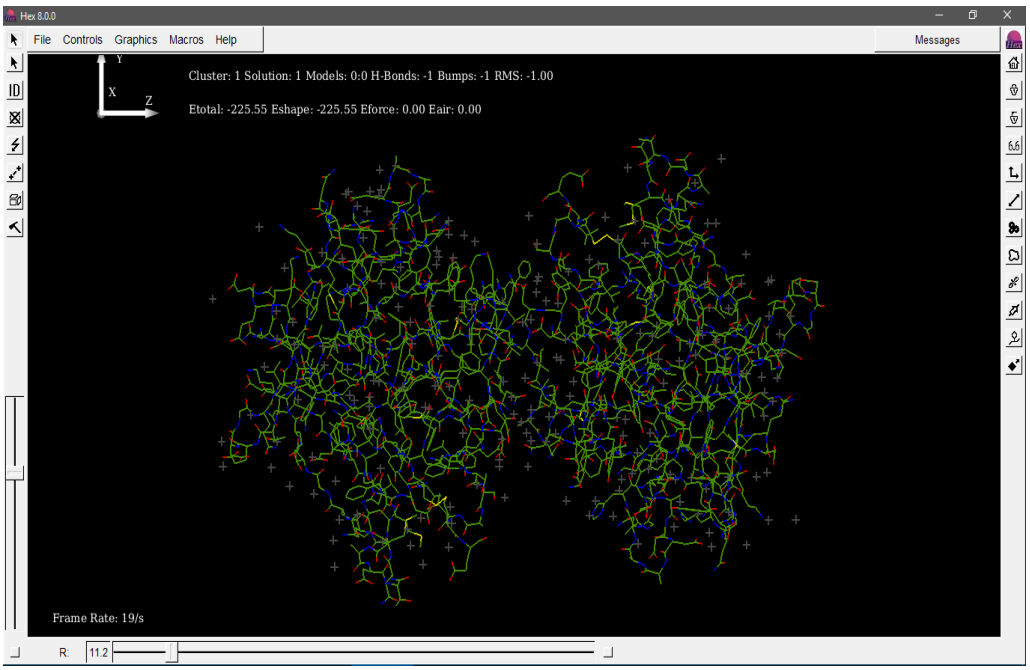

Fig.2. Docking of histamine receptor & lobelanine

CONCLUSION:

The phytoconstituents which was selected for study shown better results in terms of ADME properties as well as drug likeness model score of vasicoline. The docking energy of vasicolinon receptor occupancy was satisfied as compare to standard used lobelanine.

CONCLUSION

Citrullus colocynthis is reported as having anti-diabetic, antioxidant, anti-inflammatory, profibrinolytic, analgesic, anti-allergic, and anti-microbial properties in this overview article, although anti-diabetic activity is the most significant. It could also have an impact on the reproductive system and fertility. It appears that more study is needed to investigate the mechanism of this action.

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