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In Silico Screening Inhibitors Histamine H_2 Chemical Compounds In Licorice Plants (*Glycyrrhiza glabra* L.) Using Autodock Vina

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ABSTRACT

The inquiry about on in silico screening of chemical compounds of Histamine H_2 of Liquorice *(Glycyrrhiza glabra* L.), aimed to get the potential bioactive compounds found in plants The Liquorice (*Glycyrrhiza glabra* L.) as a potential inhibitor Histamine H_2 with a screening *in silico* by Autodock Vina Docking process is carried out on enzyme Histamine H_2 as receptors and 105 chemical compounds in plants Liquorice (*Glycyrrhiza glabra* L.) as ligands using Autodock Vina program. ΔG_{bind} value and lowest RMSD of each compound that has been in the docking taken the value of the free energy change (ΔG) as a result of docking. Docking results showed that of the 105 chemical compounds of plant Liquorice (*Glycyrrhiza glabra* L.) are all potential as inhibitors Histamine H_2 with free energy change (ΔG) most low at Glabrene amounted to -9.6 kcal/mol, and the highest Isotachioside amounted to -4, 5 kcal/ mol.

Keywords: Histamine H_2, *Glycyrrhiza glabra* L., *in silico*, Autodock Vina