Molecular Docking of secondry metabolite in agrimonia as Acetylcholinesterase Inhibitors in Alzheimer's disease Treatment

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Abstract: Today the use of medicinal plant Agrimonia eupatoria is commonly known as Agrimony. The Agrimonia species have been reported to possess several activities, including antiviral, antitumor, diuretic and antidiabetic properties[1]. Alzheimer's disease (AD) is a progressive neurodegenerative disease that impairs memory and cognitive judgment and is often accompanied by mood swings disorientation[2]. Acetylcholinesterase is an enzyme that catalyzes the breakdown of acetylcholine and of some other choline esters that function as neurotransmitters. Acetylcholinesterase inhibitors increase the level and duration of the neurotransmitter. Acetylcholinesterase inhibitors can be applied in neurodegenerative disease treatment like Alzheimer's disease. The basic aim of this study is to evaluate the anti-Alzheimer's disease activities of Agrimonia's secondary metabolites that contain the best results in antibacterial studies and include Agrimonin from Tannans' category, Triterpens and Kampfol from Flavonoids' category and Katechin from Fenavenols' category[3]. Molecular docking simulation studies were performed with Auto dock 4.2.6 software. Binding energy, Number of hydrogen bonds, Hydrogen bond interacting residues, and Van der Waals bond interacting residues were calculated. Significant Acetylcholinesterase inhibitory activities was observed. These inhibitory observations have shown some interesting results suggesting that this plant, in addition to its antibacterial properties, can be used for inhibiting the Acetylcholinesterase. The findings of the present study suggest the potential of secondary metabolite of Agrimonia, including Agrimonin, Triterpens, Kampfrol and, Katechin for use in the development of therapeutic or preventive agents for Alzheimer's disease, especially through inhibition of Acetylcholinesterase.

Keywords : Agrimonia; secondry metabolite; Molecular Docking; Alzheimer's disease; Acetylcholinesterase

References

[1] D. H. Kwon, H. Y. Kwon, Inhibition of Hepatitis B Virus by an Aqueous Extract of *Agrimonia eupatoria* L. Phytotraphy Research, 19(2005) 355-358

[2] E.Scarpini, P.Scheltens, H.Feldman, "Treatment ofAlzheimer's disease: current status and new perspectives" LancetNeurol, 2(2003) 539–547. [3] م. مسجدی، م. کیهانفر، م. بهبهانی، بررسي تأثير عصاره متانولي 4 بخش مختلف گیاه غافث، فصل نامه گیاهان دارویی، (1396) 167-168.