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### MOLECULAR DOCKING STUDIES TO IDENTIFY SECONDARY METABOLITES PRESENT IN ASHWAGANDHARISHTA AND THEIR EFFECTIVENESS TOWARDS MEMORY RELATED DISORDERS

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#### ABSTRACT

Ashwagandharishta is a famous Ayurveda medicine (in Asian countries) that is used to treat psychiatric conditions, dullness, memory related diseases, anxiety, schizophrenia sluggishness, epilepsy, depression and etc. Memory defects are closely allied with imperfect cholinergic neurotransmission. Repairing mechanisms for these impaired processes afford promising treatment strategies for these kinds of disorders. Alpha-7 nicotinic acetylcholine receptor is a sub type of nicotinic acetylcholine receptor which has been recognized as one of the most useful drug target for the treatment of nervous system associated disorders. Molecular docking analyses have been carried out to detect any possible secondary metabolites present in Ashwagandharishta that could act as agonists of *alpha-7* nicotinic acetylcholine receptor. According these computational findings, it has been found that two phytochemicals; anaferine and anahygrine exhibit promising agonistic activity towards the receptor. Thus anaferine and anahygrine have high possibility to serve as alpha-7nAChR agonists which demonstrate potential drug action towards memory related disorders.

#### INTRODUCTION

Memory defects are thoroughly allied with imperfect cholinergic neurotransmission. Repairing mechanisms for these impaired processes provide potential treatment strategies for these kinds of disorders. Cholinergic neurotransmission comprises the release of the neurotransmitter, acetylcholine and its activation of the postsynaptic receptor. Chemicals that bind to activate receptors are called agonists. Acetylcholine serves as the endogenous agonist for cholinergic receptors. Alternative agonists of these receptors are mostly employed in repairing mechanisms for disorders such as Alzheimer's disease, schizophrenia and attention-deficit hyperactivity disorder [1-3].

Ashwagandharishta has been mentioned as a medicine in “BhaishajyaRatnavali” (an Ayurveda pharmacopoeia) could be used to treat conditions that includes nervous system related diseases, psychiatric conditions, dullness, loss of memory, epilepsy, depression, anxiety, sluggishness and schizophrenia<sup>2</sup>. Ashwagandharishta is manufactured using Ashwagandha (*Withaniasomnifera*) roots as the major ingredient. *Withaniasomnifera* has been recognized as a pharmacologically important plant due to the presence of a range of phytochemicals which possess medicinal properties including steroidal lactones, phytosterols, sitoindosides and alkaloids<sup>3</sup>. Efficacy of this plant for a wide range of memory related disorders reveals the presence of these phytochemicals could repair the defects of cholinergic neurotransmission. Scope of this research was to identify potent phytochemicals which linked to the drug action and to compute how their structural properties involved in drug action on cholinergic receptors. Molecular docking is an essential tool in drug designing process and it can be used to evaluate the ligand-receptor interactions. Phytochemicals which are responsible for drug likeness, human intestinal absorption and blood brain barrier penetration are listed in Table 1 [3]. Those which exhibited higher human intestinal absorption and blood brain barrier penetration have been selected for the molecular docking. Acetylcholine (ACh) is a neurotransmitter which involved in both central nervous system (CNS) and peripheral nervous system (PNS). Two types of acetylcholine receptors (AChRs) are associated in Ach mediated action [4].