PULSUS
WWW.PULSUSCONFERENCE.COM
39 YEARS IN ASSESSING THE IMPACT OF HEALTHCARE RESEARCH

12th WORLD NURSING FORUM

April 17, 2023 | Webinar

Received date: 08-06-2022 | Accepted date: 10-06-2022 | Published date: 27-04-2023

An integrative ligand-based pharmacophore modeling, virtual screening, and molecular docking simulation approaches identified natural lead compounds against lung cancer by targeting acetylcholinesterase

Golap Hossain
King Abdulaziz University, Saudi Arabia

Lung cancer is the most common cancer-related disease worldwide take millions of lives each year. Despite enormous efforts in lung cancer research, the incidence and mortality rates of lung cancer have not decreased substantially. Acetylcholinesterase (AChE) plays a key role in catalytic hydrolysis of cholinergic neurotransmitters and causes cholinergic overstimulation. The overstimulation caused by AChE enzymes is responsible for enhancing the cell proliferation in lung cancer and inhibition of the enzyme can block the activity cell proliferation responsible for lung cancer. As inhibition of the protein can hinder the activity of the lung cancer, therefore the study aimed to identify potential natural inhibitor against the protein through ligand-based pharmacophore modeling (LBPM) and virtual screening approaches. Initially, 26 active compounds of the protein were retrieved from the ChEMBL database and a LBPM was generated followed pharmacophore model validation, virtual screening, molecular docking and ADME (absorption, distribution, metabolism, and excretion) and toxicity properties analysis. The best pharmacophore model was validated and used to screen 172324 natural compounds from ZINC natural product database. The pharmacophore model based virtual screening process identified of 155 hits, which was further screened through molecular docking. Based on the molecular docking simulation four compounds ZINC03848771, ZINC04293271, ZINC12893621 and ZINC04152233 were chosen, which has binding scores of -11.7, -10.8, -10.8, and -10.4 kcal/mol, respectively. Additionally, analysis of the ADME and toxicity properties demonstrated the efficacy and nontoxic properties of the selected compound. The integrated ligand-based drug design approaches identified four potential natural lead compounds that can inhibit the activity of the desire protein subsequently block the activity of lung cancer. However, in-vitro and in-vivo assay are suggested to confirm their activity against the targeted protein.

golap.apon@gmail.com