

MOLECULAR DOCKING STUDIES OF COMPOUNDS FROM EDIBLE MUSHROOMS ON PROSTATE CANCER PROTEIN TARGETS

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Introduction:

Prostate cancer also known as carcinoma of the prostate, is the second most commonly occurring cancer in men and the fourth most commonly occurring cancer overall. Many cases are managed with active surveillance or watchful waiting. Which option is best depends on the stage of the disease, the Gleason score, and the PSA level [3]. Because most treatments can have significant side effects, such as erectile dysfunction and urinary incontinence, treatment discussions often focus on balancing the goals of therapy with the risks of lifestyle alterations.

For centuries, mushrooms have been used as human food as well as for medicinal purposes. Several bioactivities of mushrooms have been studied including Anti-oxidant, Anti-diabetic, Anti-cancer, Anti-allergic, Anti-microbial agents [6][1]. The aim of this research is to carry out a molecular docking studies on the effects of these identified anti-cancer compounds from the edible mushroom on prostate cancer protein targets; drug likeliness, pharmacokinetics and the toxicity of the compounds.

Materials and Methods:

Structures of compounds from edible mushrooms which are known to have anti-cancer properties were downloaded [4] and docked on the target proteins of prostate cancer [5] using PyRx docking tool. On this study, the molecular properties of the ligands were analysed using Molinspiration [2]. Pharmacokinetics, Drug-likeness and Toxicity of the compounds was performed using SwissADME (<http://www.swissadme.ch/>)

Results:

From the docking result it was observed that the docked compounds have low docking energy and thus have potential to inhibit the activity of anti-proliferation and apoptosis of the prostate cancer cell targets. The result from the swissADME shows that most of the docked compounds are not toxic to the human. The result also shows that most of the compounds analysed for drug likeliness also passed the Lipinski's Rule of 5.

Conclusions:

The results indicate that the docked mushroom compounds have effective anticancer activities against prostate cancer, Low toxicity and also can be used in drug development for treatment and prevention of prostate cancer.

References:

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