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# Insilico Drug Design Approach for Identification of Putative Inhibitor against Follistatin

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## ABSTRACT

Polycystic ovary syndrome (PCOS) is a complex endocrine disorder in women of reproductive age which is characterized by polycystic ovaries, chronic anovulation and hyperandrogenism. Symptoms include irregular menstrual cycle, hirsutism, acne and infertility. Follistatin is a glycoprotein involved primarily in reproductive health of women, which can bind to activin. Activin stimulates the secretion of Follicle Stimulating Hormone (FSH) but when follistatin binds to the activin it suppresses the role of activin to stimulate FSH and inhibits it. FSH is very important in folliculogenesis, decreased FSH arrests the follicle development. In the present study, an in silico virtual screening and docking study was performed for identification of potential inhibitor. A compound library of 105 phytochemicals from PubChem and DrugBanks was generated and virtually screened for the pharmacokinetic properties like absorption, distribution, metabolism, excretion and toxicity (ADMET) using PreADMET tool. Molecular docking was performed to study the binding efficacy of the phytochemicals and follistatin protein. The compound Browniine, an extract from brown rice showed good binding energy of -9.42 kcal/mol with strong interactions with the target protein. Hence the screened molecule can be considered as a potential lead compound against follistatin.

**Keywords:** Follistatin, PCOS, Virtual screening, PreADMET

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