Assessing molecules from some Indian Medicinal Plants against breast cancer

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Abstract

The cornerstone of breast cancer hormonal therapy is estrogen receptors (ERα and ERβ)[1]. Estrogen binds to ERs, causing DNA synthesis and cellular proliferation in hormone-responsive breast cancer. About 75% of breast tumours express ERα and may be cured with drugs that inhibit estrogen-mediated signalling. In this work, we propose to use Indian medicinal plants: Neem, Tulsi and Turmeric[2], to design ERα Inhibitors as these plants have extensively been used in Ayurveda. We prepared a database of 360 molecules from these plants and performed virtual screening using in-house developed RASPD+[3]. The top 100 molecules from screening were put through molecular docking using in-house developed ParDock[4], and finally, the top 10 molecules were assessed with molecular simulations and free energy estimations. The molecules with the favourable free energy of binding are proposed to be tested on ERα (MCF-7) and ERβ (MDA-MB-231) cell lines to study their biological activity and cytotoxicity and siRNA silencing analysis to verify the ERα selectivity. This study is expected to add to the success stories of *Sanjeevini*[5] and revalidate the idea that understanding the magical cures that Indian Medicinal Plants offer at a molecular level will help in disseminating the knowledge and cures to the whole world.

References

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