Pharmacophore based inhibitors designing and molecular interaction studies on bioactive leads-An attempt to explore the new inhibitors for human epidermal growth factor receptor

Annie Absala Trace, Barani kumar*
Department of Bioinformatics, Sathyabama University, Chennai- 600 119, India.
Corresponding author email: absalabommy@gmail.com

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Post Graduate & Research Departments of Biochemistry, Microbiology, Biotechnology and Bioinformatics, Mohamed Sathak College of Arts & Science, Sholinganallur, Chennai-600119, India.
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ABSTARCT

The malignant is considered an important killer and threat to human in various ways. Malignant breast neoplasm or Breast cancer is a type of cancer originating from tissues of breast and it occurs mostly in inner lining of milk ducts which is responsible for supplying the milk. The key factor involved in cell growth, proliferation and cell differentiation is epidermal growth factor (EGF). EGF is generally responsible for malignancy. Several drugs are discovered for breast cancer and most of them are synthetic in origin and a few plant origin. Several drugs were designed for cancer using rational drug design approach but it has several drawbacks and it also time consuming practice. The recent years an alternative approaches are being used for drug designing to explore the efficient drug molecules. Pharmacophore based inhibitor designing is one of the effective and successful technique used in lead discovery. Several bioactive compounds were derived from various plant species namely vinblastin from species *Catharanthus roseus*, paclitaxel from species *Pacific yew*, montamine from species *Centaure centauriam*, gossypol from species *Thunbergia grandiflor*, vincristine from species *Catharanthus roseus*. Based on the plant compounds, pharmacophore model were generated using HipHop program and then selected compounds were used for molecular interaction studies with EGF protein using Discovery studio-LigandFit program. As a result of docking we have identified that montamine showed better interaction with target protein. Thus, *in silico* studies will help us to predict the potential anticancer compounds in future using Pharmacophore modeling and mapping techniques.

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