Abstract

Natural products including phytochemicals have been recently proposed as tumor suppressors. In this paper, docking study is presented to use these phytochemicals for their prospective role in cancers including breast and prostate cancer. The most common type of cancer in women all over the world is breast cancer. The breast cells including cancerous breast cells have receptors for binding with estrogen and progesterone to stimulate a growth response. This crucial property has been exploited to investigate binding properties of phytochemicals with these receptors to generate an antagonist response in order to resolve uncontrolled cancerous growth. The most commonly used breast cancer drugs mainly work against the effects of estrogen on these cells. In this context groups of different set of phytochemicals (3-IMG-Glucosinolates, Anthocyanins, Apigenin, Carnosol, Daidzein, Genistein, Isoflavones and Quercetin) were taken and docked into the active site of Human estrogen receptor (PDB ID: 2IOK). In this study, based on molecular docking, potential phytochemicals have successfully been identified which may be used as anticancer drugs against breast cancer. These studies based on binding energy, docking energy, drug likeness and other relevant scores show that Daidzein, Genistein and Quercetin could be the potential lead molecule for
the inhibition of signals potent for Human breast cancer and Leu346, Leu384, Leu387, Phe404 and Leu525 are the most important residues for potential drug targets. This paper is the initial step towards a rational design of novel selective and potent Human estrogen inhibitors for the treatment of cancer.

References
Docking Studies reveal Phytochemicals as the long searched Anticancer Drugs for Breast Cancer


Index Terms

Computer Science  Biomedical

Keywords
docking binding energy phytochemicals estrogen drug design