In silico docking of Phytochemicals from *Ballota nigra* against Human Estrogen Receptor

Nishandhini M, Suganya J, RadhaMahendran*
Department of Bioinformatics, Vels University, Chennai- 600 117, India.
Corresponding author email: mahen.radha@gmail.com

From National Conference on Natural Products as therapeutics, Medical Microbiology, Nanobiology and System biology: Current Scenario & Emerging Trends, 'NATCON-2014'.
Post Graduate & Research Departments of Biochemistry, Microbiology, Biotechnology and Bioinformatics, Mohamed Sathak College of Arts & Science, Sholinganallur, Chennai-600119, India.
18-19 September 2014.

American J of Bio-pharm Biochem and Life Sci 2014 September, Vol. 4 (Suppl 1): P 04

ABSTRACT

Breast cancer is the most widespread cancer and foremost causes of death among women worldwide. About 70% of breast cancers are caused by Estrogen Receptor(ER). Estrogen and its receptor were responsible for the cell proliferation in large proportion of breast cancers. Binding of estrogens to the Estrogen Receptor promotes cancer growth in ERα positive breast cancer cells. Phytochemicals are proved to be very successful to reduce the possibility of cancer. The main aim of the study is to find better natural compounds with high binding affinity for breast cancer receptors, which pave the way to breast cancer treatment. Therefore, the main insight in understanding potential inhibitory effects of phytochemicals from *Ballota nigra* has been observed to target the breast cancer. *Ballota nigra* of the family Lamiaceae has been known for many eras as a traditional medicine. Human Estrogen Receptor was retrieved from the protein databank (PDB ID: 2iok) and active sites were analysed. Then the molecular docking studies of the sixteen phytochemicals was taken and docked into active site of Human Estrogen Receptor. Among those compounds, the three best compounds showed good binding energy of -11.3459, -11.0563 and -11.0399 kcal/mol. From this result, it is evident, that the three phytochemicals of the *Ballota nigra* will be the potent Human Estrogen inhibitor for the treatment of breast cancer.

©American Journal of Bio-pharmacology Biochemistry and Life Sciences [AJBBL].2014
Published: September 2014.