Computational Exploration of *Amomum subulatum* Phytocompounds Through Network Pharmacology to Identify Hub Genes and Potential Therapeutics for Breast Cancer

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Abstract

Network pharmacology is a computational approach that can be used to identify bioactive phytocompounds and their interactions with specific target proteins for desired medical applications. In the present study, *In silico* network pharmacology was employed to study the molecular level relationship between phytocompounds of *Amomum subulatum* and core targets of breast cancer (BC). *Amomum subulatum* plant has 89 phytocompounds which were collected from the IMMPAT database and applied for ADME properties. Based on the pharmacokinetic properties, 38 phytocompounds have been elected for prediction of respective targets. The breast cancer target was retrieved from OMIM, GeneCards and Therapeutic Target Databases. A total 31 targets was found for common compounds and disease targets which have been utilized to identify the hub genes using Compound-Target-Disease network construction, GO analysis, gene expression, and survival analysis. From this study, five EGFR, ESR1, MAPK3, MAPK1 and AR hub genes have shown to involve in progression of breast cancer. Furthermore, Gene Expression and overall survival analysis were carried out to support in breast cancer development. Among the 38 phytocompounds, top 5 compounds have been identified based on the different parameters from network constructed. In addition, each phytocompounds were used to perform Molecular Docking analysis with five targets which exhibits good binding affinity. From this study, it inferred that the five phytocompounds from *Amomum subulatum* could be useful for further *In vitro* and *In vivo* biological experiments to develop a potential therapeutics in BC treatment.

Keyword: Breast Cancer, Herbal, Network Pharmacology, Phytocompounds.