Detection of Possible Significant Metabolites by Comparison of Metabolic Simulation Profiles of Healthy and Breast Cancer Tissues

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Breast cancer is the most frequent malignancy in women worldwide and is curable in ~70–80% of patients with early- stage, non- metastatic disease. In Breast cancer there are pathways related to Luminal A breast cancer, Luminal B breast cancer, HER2 positive breast cancer, Basal like/Triple negative breast cancer. The crucial signal transduction pathways in a breast cancerous cell includes pathways like PKB (protein kinase B), MAPK (mitogen-activated protein kinase), MTOR (mammalian target of rapamycin), Fas ligand (Type-II transmembrane protein), Notch (single-pass transmembrane receptor), SHH (Sonic Hedgehog), Tnf (tumor necrosis factor), Wnt (wingless/integrated) pathways. The Systems Biology Markup Language (SBML) is a file format for representing computational models, helping to interpret data and understand biological functions, in a declarative form that different software systems can exchange. SBML is oriented towards describing biological processes, including metabolic pathways, cell signaling pathways, and many others. Therefore, differentially expressed pathways can be simulated by using SBML which contain metabolites in specific pathway. In order to calculate fold change expression levels of genes in breast cancer, GSE15852 (Expression data from human breast tumors and their paired normal tissues) containing 43 healthy tissue samples and 43 tumor tissue samples is used and analyzed in R via DeSeq2 packages. Gene Set Enrichment Analysis are carried out in R with clusterProfiler package. The pathway analysis is performed in KEGG pathways. According to the expression values of proteins and their forward and reverse reaction constant, pathway simulations in healthy tissues and tumor tissues are performed by PySB to indicate their changes in breast cancer. With ARIMA method significant chances in metabolite's amounts in a certain time interval are compared between healthy and tumor tissues.