Effect of methyl jasmonate on A-549 lung cancer cell line and docking with GLUT 1 and HK2 targeted proteins

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Abstract

Background: Methyl jasmonate (MJ) is a lipophilic volatile organic compound originated as stress hormone in plants. MJ is involved in plant defense and many other diverse metabolic pathways. This hormone is produced against biotic and abiotic stresses of plant through MAP kinase pathway. MJ has therapeutic potential in human having selective antiproliferative effect on cancerous cells without interfering normal cell growth.

Methods: Human lung cancer cell lines (A-549) were treated with different concentrations of MJ. Viability of cancer cells were measured by MTT assay. *In silico* docking of MJ was done with the involvement of Autodock tool 2.6, Marvin View 5.8.1, CLC Main WorkBench 3.0 and Discovery Studio 3.0.

Results: Sub-cytotoxicity of MJ with increasing concentration 0.31, 0.62, 1.25, 2.5, 5 and 10 mM have attenuated cell viability 91, 89, 87, 76, 50 and 21 percentages respectively. MJ was docked with the lung cancer cell glucose uptake channel transport protein named Glucose transporter 1 (GLUT1) and hexokinase 2 (HK2). Blocking of these two proteins in lung cancer cells are turned to hypoxic condition without primary source of glucose resulted into apoptosis of the cell.

Conclusions: MJ directly binds GLUT1 with free energy for binding -4.91 kcal/mol which blocks glucose uptake in high glycolytic tumor cell. MJ also binds with hexokinase-II (HK2) with free energy for binding +13.69 kcal/mol which detaches HK2 from voltage dependent anion channel (VDAC). MJ interferes active site of ATP in HK2 with overlapping the adenosine ring of nucleotide.

Biography

Samarth M Kansara completed his master's degree in Biotechnology course, affiliated to Sardar Patel University, India. The main subject of his Master's was Environmental Studies. He wrote a review on cytochrome p450 monoxygenase role and its application in oxygenation of xenobiotics and conversion into bioavailable form.

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