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5'-desmethoxyyatein: Potential key inhibitor of proteins for cancer inhibition

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5'-desmethoxyyatein, a natural lignan, has shown potent cytotoxic activity in many cancer cell lines including melanoma, leukemia, breast, colon and brain cancers. Molecular docking is a powerful computational tool to predict the binding mode and binding affinity of a ligand with the specific proteins. In this study, we aimed to investigate molecular targets of 5'-desmethoxyyatein from 80 proteins, which relate to cancer cell proliferation, cell cycle progression, apoptosis, or cell migration. Binding affinity evaluation of 5'-desmethoxyyatein to these proteins was carried out using Molecular docking method. Results showed that 5'-desmethoxyyatein may inhibit activin receptor 2 (ACTVR2), prostaglandin G/H synthase 2, human epidermal growth factor receptor 2 (HER-2), janus kinase 3 (JAK3), protein kinase C (PKC), heat shock protein 90-beta (Hsp90-beta), transforming growth factor receptor I (TGF- β receptor I), androgen receptor and NF-kappa-B-inducing kinase (NIK) proteins. This information was derived from better predicted binding affinity of 5'-desmethoxyyatein, compared to its known inhibitors. Moreover, 5'-desmethoxyyatein may hinder cell cycle progression via binding to cyclin A, polo-like kinase 1 (PLK1) and aurora A proteins with binding energy and inhibition constant lower than its known inhibitors. X-linked inhibitor of apoptosis protein (XAIP) and glycogen synthase kinase 3 (GSK-3 β) proteins, involved in apoptosis and migration in cancer cells, also may better interact with 5'-desmethoxyyatein than their inhibitors. This study suggests 5'-desmethoxyyatein would be anti-tumor agent with anti-proliferation, cell cycle arrest inducing, apoptosis induction and anti-migration activities. However, further studies such as Western blot analysis are needed.

Biography

Aman Tedasen is a PhD student at Department of Biomedical Sciences, Faculty of Medicine, Prince of Songkla University, Thailand. He received his Medical Technology training and earned his Bachelor's degree in 2012. He received a scholarship from the Royal Golden Jubilee PhD Program of Thai government. His research interest has focused on developing effective treatment strategies from herbal medicine for breast cancer.

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