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*Asia-Pacific Journal of Molecular Medicine 2017, 7 (SUPP 1)*

**Abstracts for 7th Regional Conference on Molecular Medicine (RCMM)**

**in Conjunction with 3rd National Conference for Cancer Research 2017**

**10-12th November 2017, Auditorium UMBI, Kuala Lumpur**

**In silico analysis and molecular docking studies of thymoquinone in STAT3, NF-κβ and PI3K isoforms**

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**ABSTRACT**

Protein kinases such as PI3K and AKT isoforms are important in the regulation of cell survival, growth and proliferation. Both kinases are closely linked to tumorigenesis, whereby inhibition of PI3K and AKT is relevant in the treatment of cancer. Thymoquinone, a bioactive compound of *Nigella sativa* is well known for its anticancer activity. However, its target molecule and mechanism of action are still being studied. This study aims to analyse the inhibitory activity of thymoquinone by elucidating its binding mode in PI3K and AKT proteins using computational docking studies. The 3D structure of thymoquinone was docked into the ATP binding site of PI3K and AKT proteins using AutoDock 4.2 program. Docking analysis was performed using scoring strategy and the types of interaction formed by the docking complexes. The binding modes of thymoquinone in PI3K and AKT isoforms were compared to potent PI3K and AKT inhibitors; LY294002 and AZD5363 respectively. Thymoquinone demonstrated a hydrogen bond interaction with Val882 of PI3Kγ, a critical interaction for potency. However, such interaction with respective amino acids in other PI3K isoforms (αVal851, βVal855 and δVal822) was not observed. Similarly, critical interaction for inhibitor potency was not observed in AKT isoforms. These results indicate that thymoquinone could be a potential PI3Kγ inhibitor to treat cancer and inflammatory diseases.