

ORAL ABSTRACTS

Molecular mechanism of anti-inflammatory effects of flavonoids

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Phospholipase A2 (PLA2) catalyzes the rate limiting step of production of pro-inflammatory compounds and hence form a target for anti-inflammatory agents. Increased levels of human non-pancreatic secretory PLA2 have been reported in various pathophysiological conditions. Hence a selective and potent inhibitor of this enzyme may have therapeutic values. Flavonoids have enormous range of biological effects including anti-inflammatory. But their mechanism of action is not fully understood. In order to understand the mechanism of action of flavonoids, we have performed *in vitro* binding studies, which indicated strong affinity of seven flavonoids with hnpS-PLA2. To evaluate the molecular recognition of PLA2, flavonoids were docked on hnpS-PLA2 structure and their interactions were analysed. The binding affinities of flavonoids and PLA2 were observed in the range of 10mM- 100mM. All the flavonoids were found to interact with the substrate binding hydrophobic channel of PLA2. Most of the flavonoids additionally made polar interactions with the catalytic Asp 48 and His 47 residues of PLA2. The binding of flavonoids is comparable with the binding of other inhibitors of PLA2, which indicated the possible similar mechanism of anti-inflammatory effects of flavonoids. The binding of flavonoids may also provide idea about development of more potent and effective inhibitors of hnpS-PLA2, which may have therapeutic relevance.

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