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Ant-inflammatory potential of secondary metabolites pectolinarin through their interaction with tumor necrosis factor- α (TNF- α), 5-lipoxygenase (5-LO), cyclooxygenase-2 (COX-2) and tyrosinase: Binding properties by virtual screening studies

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Objectives: Medicinal Plants contain numerous active phytoconstituents which provide food material but more specifically medicine to the human being in the world since very ancient time. Flavonoids represent a huge family of polyphenolic compounds which are major active nutraceuticals ingredients of plants, fruit, vegetables and beverages. In order to understand beneficial health effects of flavonoids, present work describe the biological properties of pectolinarin found in *Cirsium japonicum*. Inflammation is part of the non-specific immune response that subsequently develops cardiovascular diseases, diabetes, cancer etc.

Methods: In order to develop effective medicine for the treatment of inflammatory disorders, present work aim is to interpret the anti-inflammatory activity of the pectolinarin through in silico molecular modelling and other in-vitro and in vivo study. Based on their biological activity, the bioactive compounds pectolinarin was also studied through molecular modelling approach against tumor necrosis factor- α (TNF- α), 5-lipoxygenase (5-LO), cyclooxygenase-2 (COX-2) and tyrosinase to predict its structure-activity and molecular mechanism.

Results: Data analysis of information from various sources revealed that pectolinarin possesses anti-tumor, antioxidant, antidiabetic, anti-inflammatory and antifungal activities. Data interpretation showed that the pectolinarin exhibited variable degrees of binding with the different examined receptors that undoubtedly proved their anti-inflammatory activity. *In silico* molecular modelling study suggest that pectolinarin showed anti-inflammatory activity through interaction with the TNF- α , 5-LO, COX-2 and tyrosinase.

Conclusions: From the presented data we can conclude that pectolinarin could be a promising compound for the development of effective medicine in treatment of inflammatory disorders.