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Design, synthesis, docking and QSAR studies of novel 3,5-diaryl pyrazole derivatives and their evaluation as antioxidants and as immunomodulators, inhibitors of TNF-, IL-2, IL-6

Dalia Hussein Soliman
Al-Azhar University, Egypt

Tumor necrosis factor- α (TNF- α) is one of the major pro-inflammatory cytokines which regulates further cytokine induction, especially IL-1, IL-6, IL-2 and IL-8. The overexpression of these cytokines has been implicated in many diseases including cancer, immune disorders as well as inflammatory diseases like septic shock, rheumatoid arthritis (RA), multiple sclerosis and Crohn's disease. An example of the small molecules is the pyrazole-derived scaffolds which have been identified as immunomodulators. The pyrazole core possesses radical-scavenging ability and even its modulation in inflammatory response was related to its considerable antioxidant activity. Moreover, it has been reported that certain antioxidants reduce LPS-induced inflammation and fever. In this work, a new series of pyrazole-derived immune suppressants, through IL-2, IL-6 and TNF- α inhibition, has been synthesized and evaluated for their antioxidant capacities as well. The results showed that the new compounds had good anticytokine activity comparable to the reference Dexamethasone especially against IL-2. They also demonstrated promising antioxidant activities. Docking of the compounds into the active site of p38MAPKinase was also studied in addition a 2D QSAR model was generated in order to correlate the anticytokine activity with the physicochemical properties of the target compounds.

Biography

Dalia Hussein Soliman has completed her at the age of 35 years from AL-Azhar University and Postdoctoral studies from the same University in addition to Ain-Shams University. She is currently working as an Associate Professor of Pharmaceutical Chemistry, Pharmaceutical Chemistry Department at the Egyptian Russian University. She has published more than 12 papers in reputed journals.

odihss2@gmail.com

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