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In vitro and *in silico* approaches to unveil the mechanisms underlying the cytotoxic effect of juncunol on human hepatocarcinoma cells

Maria João Rodrigues[1], Catarina Vizetto-Duarte[1], Katkam N. Gangadhar[1], Gokhan Zengin[2], Adriano Mollica[3], João Varela[1], Luísa Barreira[1] and Luísa Custódio[1]

[1] Centre of Marine Sciences, University of Algarve, Faculty of Sciences and Technology, Ed. 7, Campus of Gambelas, Faro, Portugal.

[2] Selcuk University, Science Faculty, Department of Biology, Campus, 42250, Konya, Turkey

[3] Department of Pharmacy, University "G. d'Annunzio" of Chieti-Pescara, 66100, Chieti-Italy

Abstract

Background: Juncunol is a phenanthrene isolated from the halophyte species *Juncus acutus,* with selective cytotoxic activity towards human hepatocarcinoma (HepG2) cells. However, its mechanism of action is unknown.

Methods: The *in vitro* cytotoxic mechanism of juncunol was evaluated on HepG2 cells through several methods to elucidate its potential to induce apoptotic features, decrease mitochondrial membrane potential, promote internal ROS production and influence cell cycle. We also report its haemolytic activity on human erythrocytes and *in silico* DNA-binding studies.

Results: Juncunol induced an increase in the number of apoptotic cells in a concentration-dependent manner, accompanied by a decrease in the mitochondrial membrane potential. No significant differences were observed in production of reactive oxygen species (ROS). Moreover, juncunol application at the IC_{50} value significantly induced cell cycle arrest in the G0/G1 phase comparatively