The cytotoxicity against HepG2 cell line has been determined in the MTS and LDH assay for the six coumarins, some of which have been determined in previous study to have platelet antiaggregatory activities and to act as cyklooxygenase I inhibitors. Three of the coumarins did not decrease HepG2 cells viability at 30µM concentration after 48h of exposure. None of the other three coumarins, the important physicochemical properties determining the behaviour in biological systems have been calculated using the ADMET Predictor. The software has predicted four coumarins to have suitable drug-like properties (zero global risk) and the other two with the lowest risk in the ADMET Risk scale range. These two coumarins were identical with the coumarins showing certain cytotoxicity in the in vitro assays. Cytotoxicity in vitro has been also determined for the representative of the flavones' derivatives group the 3-hydroxyflavone. The 3-hydroxyflavone led to the decrease of HepG2 cells viability observed in MTS assay up to 80%, whereas no cytotoxicity has been observed in LDH assay. This may be explain by the cytostatic and not cytotoxic effect of 3-hydroxyflavone. Thus, the flavone derivative shall be further investigated.