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In silico study of the biological activities of the saharan medicinal plant *Limoniastrum feei*

Ouahab Ammar
University of Batna 2, Algeria

In-silico study was performed to find the pharmacodynamics, toxicity profiles and biological activities of three phytochemicals isolated from *Limoniastrum feei* (Plumbagenaceae). Online pharmacokinetic tools were used to estimate the potential of Quercetin, kaempferol-3-O-β-D-glucopyranoside (astragalin) and quercitin-7-O-β-D-glucopyranoside as specific drugs. Then the prediction of potential targets of these compounds were investigated using PharmMapper. Auto-Dock 4.0 software was used to investigate the different interactions of these compounds with the targets predicted earlier. The permeability of quercetin was found within the range stated by Lipinski's rule of five. Hematopoietic prostaglandin (PG) D synthase (HPGDS), farnesyl diphosphate synthetase (FPPS) and the deoxycytidine kinase (DCK) were potential targets for quercetin, astragalin and quercetin 7, respectively. Quercetin showed antiallergic and anti-inflammatory activity, while astragalin and quercetin 7 were predicted to have anticancer activities. The activity of Astragalin appeared to be mediated by FPPS inhibition. The inhibition of DCK was predicted as the anticancer mechanisms of quercetin 7. The compounds showed interesting interactions and satisfactory binding energies when docked into their targets. These compounds are proposed to have activities against a variety of human aliments such as allergy, tumors, muscular dystrophy, and diabetic cataracts.

e: a.ouahab@univ-batna2.dz

A personalized approach for the delivery of nanomaterial-based cancer therapeutics

Bella B Manshian, Uwe Himmelreich and **Stefaan J Soenen**
KU Leuven, Belgium

To date, cancer drug concentrations are calculated based on individual weight. This does not always lead to optimal therapeutic results. Thus, in this work, we aimed to correlate the nanoparticle (NP) concentration to the size and metabolic activity of the individual tumor. For this aim, the cytotoxicity of CdTe NPs was evaluated over a broad range of concentrations using an in house developed high content imaging approach for evaluating bio-nano interactions. Exposure of the mouse lung tumor cells (KLN 205) to 13.91x107 NPs/cell resulted in 20% acute (at 24 h) cell death while 10% acute cell death was achieved with 10.43x107 NPs/cell. We then used non-invasive optical imaging (IVIS spectrum) to determine the metabolic activity of the individual tumor, in a syngeneic tumor model (in DBA2 mice), based on which we provided fluorescent CdTe NPs at toxic levels at personalized concentration of at a general average dose. A series of 5 groups of mice with subcutaneous KLN 205 tumors were generated. The animals were either given 100 µl of saline (control animals) or 100 µl saline containing 435 or 318 µg CdTe quantum dots (standard reference groups GHequal (20% cell death) and GLequal, (10% cell death) respectively, or 362–480 or 269–361 µg CdTe personalized medicine groups GHRel (20% cell death) and GLRel, (10% cell death), respectively.

The results showed an impeded growth for all CdTe-treated tumors compared to control animals. Only those animals with personalized dosages displayed significant effects even at low NP concentrations, while at average dosages, these results were obscured due to the high level of variability. Additionally, the therapeutic activity could be monitored, *in-vivo*, as anticancer efficacy correlated with loss in fluorescence intensity. In conclusion, this work demonstrates the advantages of noninvasive imaging for monitoring therapeutic delivery and optimal NP-mediated cancer treatment via personalized medicine.

e: bella.manshian@kuleuven.be