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ADMET ANALYSIS OF SELECTED PHYTOCHEMICAL COMPOUNDS FROM TRIFOLIUM PRATENSE AGAINST OSTEOSARCOMA

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ABSTRACT

Bone cancer, also known as osteosarcoma or osteogenic sarcoma, is a malignant tumour in a bone. It is a very aggressive malignant tumour (and hence a sarcoma) that demonstrates osteoblastic differentiation and gives rise to malignant osteoid. It develops from primitive altered cells of mesenchymal origin. Important villous forage herb Trifolium pratense is an upright biennial or perennial. It is traditionally used to treat cancer, sedative, hard swelling, gout, psoriasis, and eczema. The efficacy of several red clover (Trifolium pratense L.) extracts to enhance the activity of osteoblastic osteosarcoma cells was investigated. Alkaline phosphatase (ALP), or cellular protein synthesis, was selected as a critical indicator of osteoblasticity because it showed a considerable increase in activity when incubated with chloroform extracts. Based on research, formononetin, biochanin A, quercetin, kaempferol, luteolin, rutin and myricetin were selected for pharmacokinetics analysis. The pharmacokinetics analysis done through 18 important ADMET properties and were calculated using admetSAR, including Ames mutagenicity (Ames), acute oral toxicity (AO), Caco-2 permeability (Caco-2), P-glycoprotein substrate (P-gps), P-glycoprotein inhibitor (P-gpi), CYP substrates and inhibitors (CYP1A2, CYP2C9, CYP2D6, CYP2C19 and CYP3A4), human intestinal absorption (HIA), CYP inhibitory promiscuity (CYPPRO), carcinogenicity (CARC), human ether-a-go-go-related gene inhibition (hERG), and the organic cation transporter protein 2 inhibitor (OCT2i). For acute oral toxicity models, category 1 ($LD_{50} \leq 50$ mg kg^{-1}) and category 2 (50 mg kg^{-1} < $LD_{50} \leq 500$ mg kg^{-1}) were considered as toxic while category 3 (500 mg kg^{-1} < $LD_{50} \leq 5000$ mg kg^{-1}) and category 4 (5000 mg kg^{-1} < LD_{50}) were considered to be nontoxic. In the meantime, compounds with the prediction of non-carcinogenic (inactive) or weakly carcinogenic (TD_{50} > 10 mg kg^{-1} per day) were considered as non-carcinogenic and the others were considered as carcinogenic. After analyzing the ADMET results of selected seven phytochemical compounds. We found that formononetin shows the best ADMET scoring function.

Keywords: *Osteosarcoma of Bone, ADMET, Pharmacokinetics, Trifolium Pratense, Cancer.*