Yellow K2 – Potential Next Generation NSAID

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One of the main imperatives of medicine and pharmacy is the treatment of pain, inflammation, and fever [1]. Non-steroidal anti-inflammatory drugs (NSAIDs) are leading medicines for treatment, yet current NSAIDs suffer from various limitations (such as efficacy, adverse effects, and/or potential abuse) [2,3]. The relatively recent development of precise *in silico* bioinformatic and chemoinformatic tools can substantially optimize and fast-track the process of drug development. Along with exponentially increasing knowledge of molecular mechanisms underlying pathological states, it enables proper ground for engineering and development of better NSAIDs with more precise targeting without undesired side effects.

A newly developed compound "Yellow K2", with potential use as an NSAID with a functional group of increased cyclooxygenase-2 (COX-2) affinity, has been engineered and developed using contemporary chemoinformatic and bioinformatic methodologies of *in silico* molecular engineering. The lead compound development and optimization included *in silico* design, pharmacokinetic and pharmacodynamic studies, molecular docking simulations, and structural studies with the use of Virtual reality (VR), followed by a computer-assisted exploration of reverse synthesis – possible pathways of organic synthesis from economically viable constituent reagents.

The project was wrapped up by conducting ground *in vitro* cytotoxicity studies on human embryonic kidney 293 cell lines using MTT assay to test the *in silico* obtained projections.

Building upon promising results of this small, economically viable molecule, the research is scheduled to proceed into the second phase of preclinical trials – *in vitro* immunofluorescence pharmacokinetic and pharmacodynamic studies on a wider array of mammalian cell cultures – traditional liquid cultures and novel 3D cell cultures (organs-on-a-chip and organoids).

References:

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