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Molecular dynamics as a tool to discover novel endogenous systems: Lessons we learnt from opioid and endocannabinoid systems

All components and properties found in the greater world, the Universe, will be searched and found in the lesser world, human (AbūHāmidMuhammad ibn Muhammad al-Ghazālī (Algazelus), a Muslim Philosopher (c. 1058 – 1111)). More than two century ago, a German pharmacist Friedrich Wilhelm Adam Serturmer isolated morphine from Opium poppy (Papaver somniferum L.). Afterwards morphine congeners introduced into the market. After a long pause, by the 1973s, opioid receptors and endogenous opioids (endorphins) have been discovered by researchers at Johns Hopkins University. In a similar scenario, in 1964, a Bulgarian-descent Israeli Organic Chemist, Raphael Mechoulam, identified and synthetized Δg -tetrahydrocannabinol, the main psychoactive principle of hashish prepared from Cannabis sativa L. and his research team also discovered the endogenous cannabinoids, anandamide and 2-arachidonoyl glycerol (2-AG) under his supervision. Finally in 1990s, researchers in St. Louis University School of Medicine discovered cannabinoid receptors. After discovery of these two endogenous systems, we found that these systems are involving in many physiological functions besides their psychopharmacological activities. I hypothesize here, the story of opium and hashish can be repeated more quickly for other psychotropic herbs, because we are armed to cheminformatics nowadays. In this oration, I will describe a molecular dynamic methodology that generates a list of high-binding small molecule ligands found in psychoactive herbs like Passiflora incarnate, Turnera diffusa var. aphrodisiaca, Eschscholzia californica, Lobelia inflate, Aquilegia Canadensis, Juniperus virginiana, etc. for selected orphan G protein-coupled receptors.

Biography

Isaac Karimi is an Academic Member in the Razi University, Iran, which he joined in 2008. He received his Doctor of Veterinary Medicine (DVM; 1998-2004) from Shahr-e-Kord University, Iran, and his Doctorate of Veterinary Sciences (PhD; 2004-2008) in Physiology from Urmia University, Iran. At Razi University, he established Enzymology Laboratory, Laboratory of Molecular and Cellular Biology 1214, and Behavioral Neuroscience Laboratory. He has an interdisciplinary view; however he is concentrated on Ethnopharmacology, Translational Research, Safety Pharmacology and Nanotoxicology. Recently, he established the research ream in Computational Biology and Biomathematics. He supervised many theses and industrial R&D projects. He is Research Founder of Pars Ghousht Negin Company that produces and distributes protein products in Middle East. He received four distinguished researcher's awards from Razi University. He (co-)authored over 60 research papers and book chapters and served as a Senior Editor or an Editorial Board Member of 10 peer-reviewed journals and as a Reviewer of more than 20 peer-reviewed journals in the area of Pharmacoutics, Pharmacology, Pharmacognosy, and Biomedicines.

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