Depression, the Great Evil of the Century: Evaluation of the Antidepressant Effect of the Macromolecule WRKY26 from Musa Paradisiaca Peel through Computer Programs

Rossa Burato, Ana (School: Colegio Murialdo)
Daniel, Artur (School: Colegio Murialdo)

Depression is a severe, complex and multifactorial neuropsychiatric disorder. Recent research indicates that Musa paradisiaca peel is rich in dopamine and other substances, such as WRKY26. Thus, the aim of the study was to evaluate molecular interactions and the possible antidepressant and neuroprotective effects of Musa paradisiaca peel in the computational model of depression. Structure modeling and optimization was performed by homology technique using SWISS-MODEL server and ascertained by SAVES v5.0 server in order to verify the structural feasibility of the macromolecule. To test other structures with antidepressant effects, the ligands milnacipran, duloxetine and pregabalin available in the ChemSpider chemical structure bank were used. Subsequently, the targets CRF, eNOS, IGF1, D2 and D3 found in biological process networks by String server and confirmed by KEGG. It was possible to observe that WRKY26 showed 78.87% similarity with other model structures. Through molecular docking analysis it was evidenced that the WRKY26 ligand presented similar/superior results to duloxetine, being that milnacipran and pregabalin presented inferior results to the other interactions. In the network of biological processes, new targets related to depression were discovered, such as AKT2, RPS6KB2, INSR, JAK2, AKT2, GRB10, SRC, PTPN1, EGFR, IGF2 and CRHR2. WRKY26 may be an important ally in the treatment of depression, acting through the eNOS pathway and the dopaminergic system (D2R and D3R). In summary, the results exemplified by bioinformatics were sufficient to demonstrate the potential of WRKY26 protein and newly discovered targets in the mechanism of depression development.