Designing Drugs by Artificial Intelligence: Novel Curcuminoids for the Treatment of Papillary Renal Cell Carcinoma Type II (PRCC2)

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Papillary type 2 renal cell carcinoma (CCRp2) is an aggressive type of kidney cancer that has been growing more rapidly in cells and can spread to other organs of the body. Curcumin, a compound found in turmeric, has shown anticarcinogenic potential in various diseases and cancers, suggesting that its analogues could be effective in treating CCRp2. In this study, the methodology consists of five steps. In Step I, a network of biological processes involving all proteins and genes related or predicted in the development of CCRp2 was constructed using artificial intelligence software. In Step II, a molecular docking simulation was performed with 10 curcumin-derived molecules generated by a script developed on targets found in the process network to evaluate the molecular interaction activity of these molecules. In Step III, a pharmacokinetic and toxicity assessment of these generated structures was conducted. In Step IV, molecular dynamics of the best compounds that passed docking were performed, evaluating RMSD, RMSF, ROG, and SASA, in addition to hydrogen bonds. In Step V, organic synthesis of the compounds with the best results from previous steps was performed. It was found that curcumin and its analogues acted on the identified targets, presenting a new promise of treatment for CCRp2. Additionally, the new network generated may contribute to the development of new therapies based on the identification of new proteins and genes identified by bioinformatics software.

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