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Computational Investigation of Stevia Bioactives for Renal Anti-Fibrotic via Fibroblast Growth Factor Receptor 4 (FGFR4): In Silico Analysis

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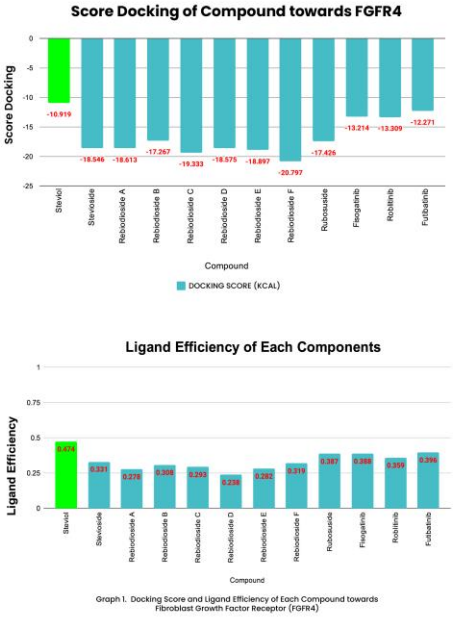
Objectives : CKD (Chronic Kidney Disease) is characterized by marked elevation of Fibroblast Growth Factor-23 (FGF23), which can activate Fibroblast Growth Factor Receptor (FGFR4) to promote renal fibroblast activation. This makes the FGF23-FGFR4 axis as a rational target for anti-fibrotic strategies. Stevia (Stevia rebaudiana) contains metabolites with reported anti-inflammatory and anti-fibrotic effects. Importantly, stevia may also add value in CKD complicated by diabetic comorbidity. By supporting glycemic control (as sugar substitute), stevia could address metabolic inflammation that accelerates fibrosis. Despite these promising signals, it remains unclear whether stevia bioactive can directly modulate FGFR4. Therefore, this study aims to evaluate the binding of stevia bioactives to FGFR4 using in silico analysis as an initial step toward anti-fibrotic strategies in CKD.
Methods : The three-dimensional structure of FGFR4 was retrieved from the Protein Data Bank, while ligand structures were obtained from PubChem. Stevia-derived compounds (steviol, stevioside, rebaudiosides A–F, and rubusoside) together with established FGFR4 inhibitors as positive controls were prepared by generating 3D conformations, assigning protonation states, and energy minimization to obtain stable geometries suitable for docking. Molecular docking then conducted against the FGFR4 binding site using Molecular Operating Environment (MOE) software. Compounds were ranked by docking score (DS) and ligand efficiency (LE) to reduce size-related bias.
Results : Steviol showed the highest ligand efficiency (LE = 0.474) with the most stable pose (DS= -10.919; RMSD = 0.67 Å), clearly outperforming all positive controls (fisogatinib LE = 0.388; roblitinib LE = 0.359; futibatinib LE = 0.396). Among the glycosides, rubusoside achieved LE (0.387) comparable to fisogatinib, whereas stevioside and rebaudiosides A-F had consistently lower LE values (0.238–0.331) despite some exhibiting strong absolute DS.
Conclusions : Steviol appears to be the most promising for further optimization and validation due to its highest ligand efficiency and most stable docking pose. However, FGFR4-focused experimental validation and more rigorous computational analysis are required.

DOCKING SCORE FGFR4.jpg.jpeg

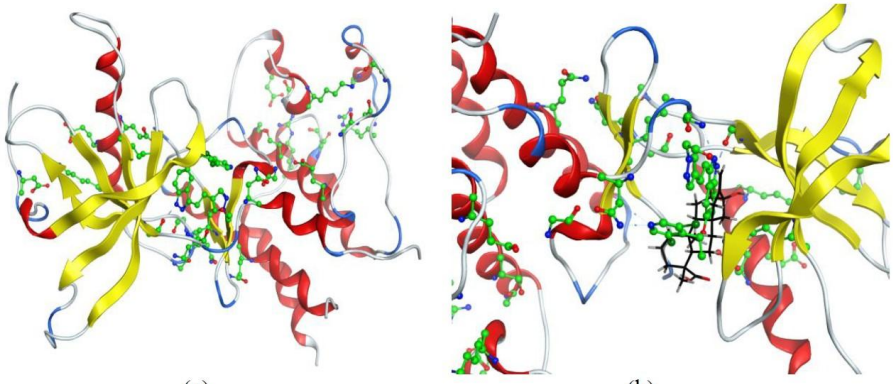
Table 1. Molecular Docking Result

NO	COMPOUND	DOCKING SCORE (KCAL)	RMSD (A)	Ligand Efficiency (LE)
1	Steviol	-10.919	0.67	0.474
2	Stevioside	-18.546	1.19	0.331
3	Rebiodioside A	-18.613	1.13	0.278
4	Rebiodioside B	-17.267	1.82	0.308
5	Rebiodioside C	-19.333	1.74	0.293
6	Rebiodioside D	-18.575	2.14	0.238
7	Rebiodioside E	-18.897	2.27	0.282
8	Rebiodioside F	-20.797	1.69	0.319
9	Rubosuside	-17.426	1.71	0.387
10	Fisogatinib	-13.214	1.12	0.388
11	Roblitinib	-13.309	1.13	0.359
12	Futibatinib	-12.271	1.17	0.396



Graph 1. Docking Score and Ligand Efficiency of Each Compound towards Fibroblast Growth Factor Receptor (FGFR4)

DOCKING SCORE FGFR4.jpg.jpeg



(a) (b)

Picture 1. (a) Biological Assembly of Fibroblast Growth Factor Receptor 4 (FGFR4) in Molecular Operating Environment; (b) Steviol Interaction Map within the FGFR4 Active Site