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Seaweed-Derived Bioactives as Potential Modulators of Inflammatory Signaling in Diabetic Kidney Disease

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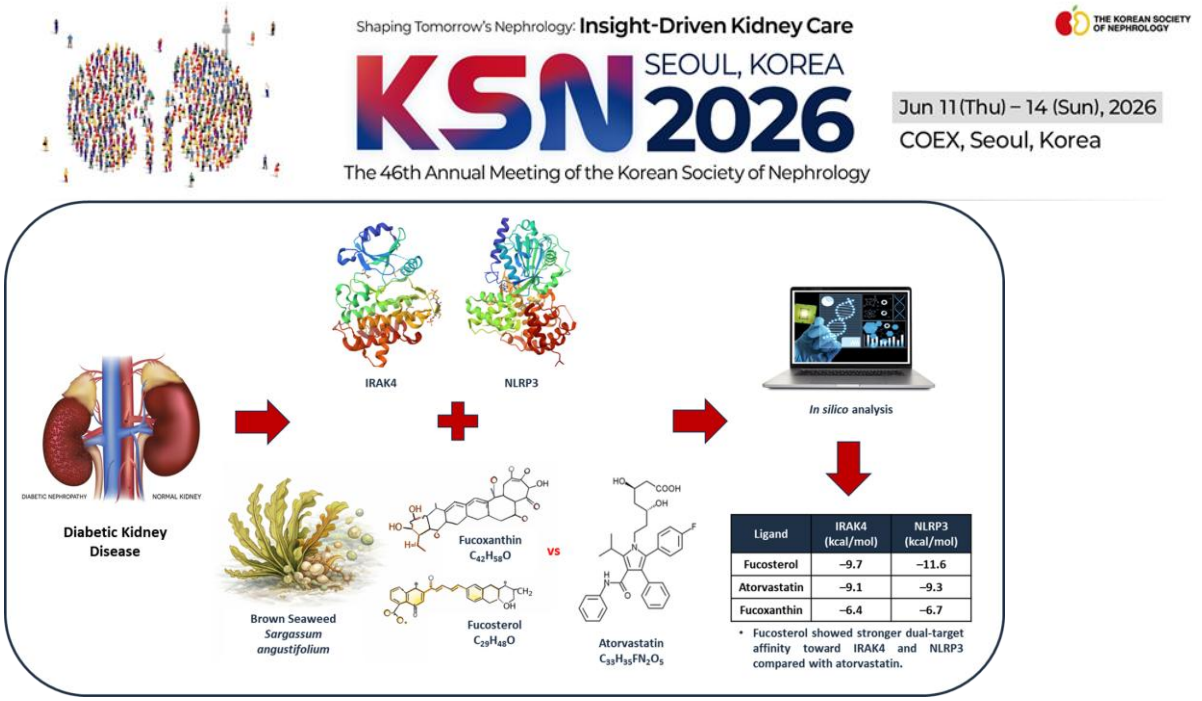
Objectives : Diabetic kidney disease (DKD) is a major cause of chronic kidney disease and is strongly associated with persistent low-grade inflammation that accelerates renal injury. The IRAK4–NF-κB–NLRP3 signaling axis plays a key role in innate immune activation and inflammasome signaling within renal tissues, contributing to inflammatory responses, fibrosis, and progressive decline in kidney function. Seaweed-derived bioactives such as fucosterol and fucoxanthin have demonstrated anti-inflammatory and antioxidant properties. Although atorvastatin is primarily used for lipid lowering, it also exhibits pleiotropic anti-inflammatory effects and has been investigated for potential renoprotective roles in diabetic complications. This study aimed to evaluate the molecular interactions of seaweed-derived bioactives with IRAK4 and NLRP3 in comparison with atorvastatin.
Methods : Virtual screening analysis was performed using validated human IRAK4 kinase and NLRP3 protein structures. Fucoxanthin and fucosterol were evaluated as candidate ligands, with atorvastatin included as a reference drug. Binding energies (kcal/mol) and interaction profiles, including hydrogen bonding and hydrophobic stabilization within key functional domains, were analyzed using Discovery Studio.
Results : Fucosterol demonstrated stronger binding affinity than atorvastatin toward both IRAK4 and NLRP3. For IRAK4, binding energies were –9.7 kcal/mol for fucosterol, –9.1 kcal/mol for atorvastatin, and –6.4 kcal/mol for fucoxanthin. For NLRP3, fucosterol exhibited the highest affinity (–11.6 kcal/mol), compared with –9.3 kcal/mol for atorvastatin and –6.7 kcal/mol for fucoxanthin. Interaction analysis revealed stable hydrophobic anchoring of fucosterol within both kinase and inflammasome domains, suggesting potential modulation of inflammatory priming and inflammasome activation involved in renal inflammatory signaling.
Conclusions : Fucosterol demonstrated consistent in silico affinity toward IRAK4 and NLRP3, key mediators implicated in inflammatory pathways associated with diabetic kidney disease progression. These findings highlight the potential of seaweed-derived bioactives as complementary therapeutic candidates targeting inflammatory signaling in DKD. Further experimental and clinical validation is warranted.

Figure 1_KSN.png



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