

Supplementary Materials for:

**Exploring the Potential Molecular Targets and Therapeutic Mechanisms of
Cyperi Rhizoma in Treating Diabetic Cardiomyopathy: A Computational
Approach**

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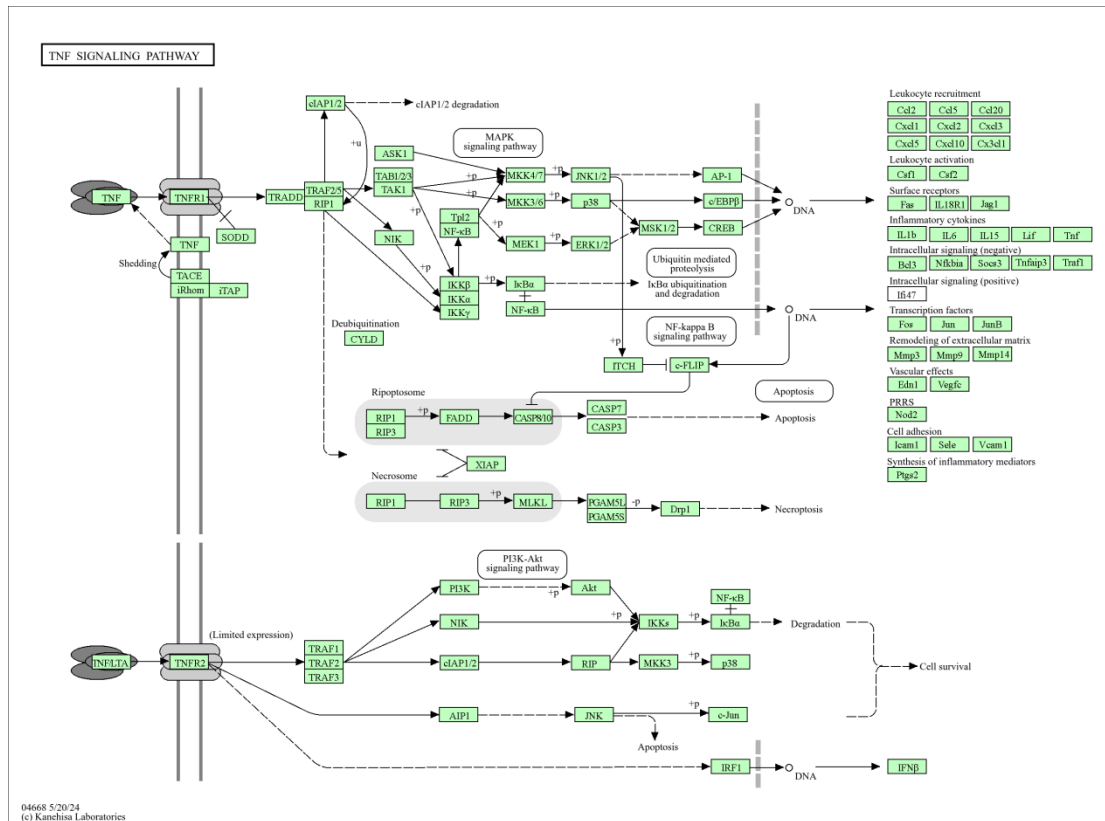


Figure S1 Map of TNF signaling pathway

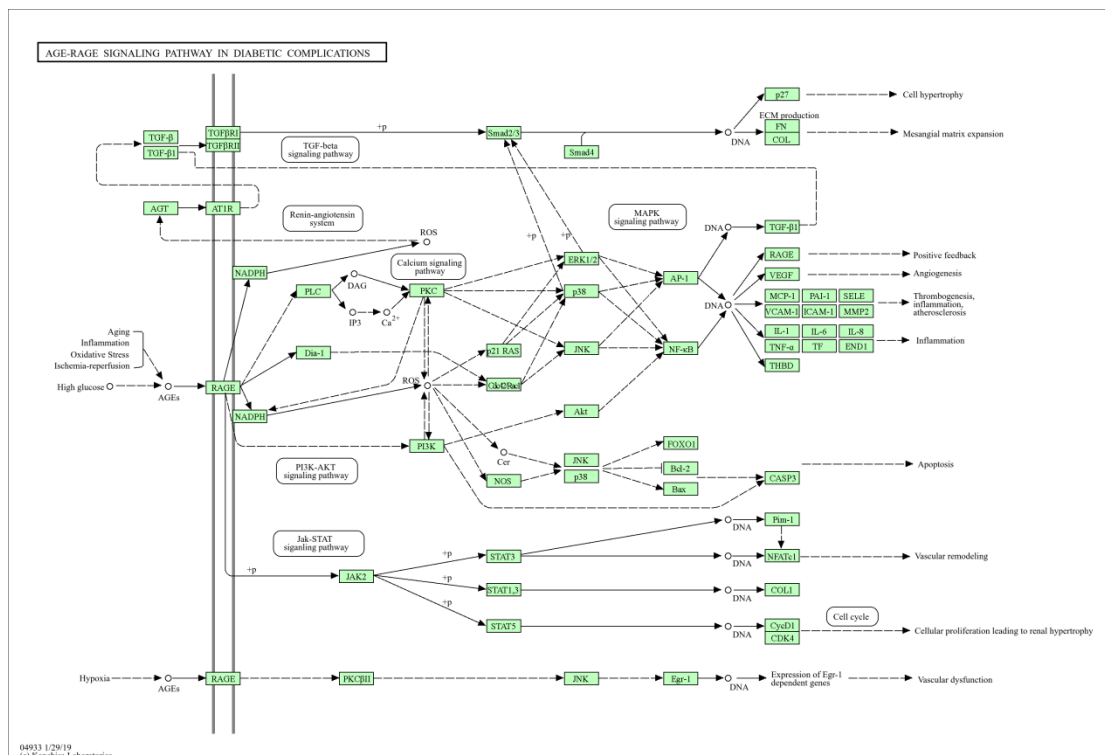
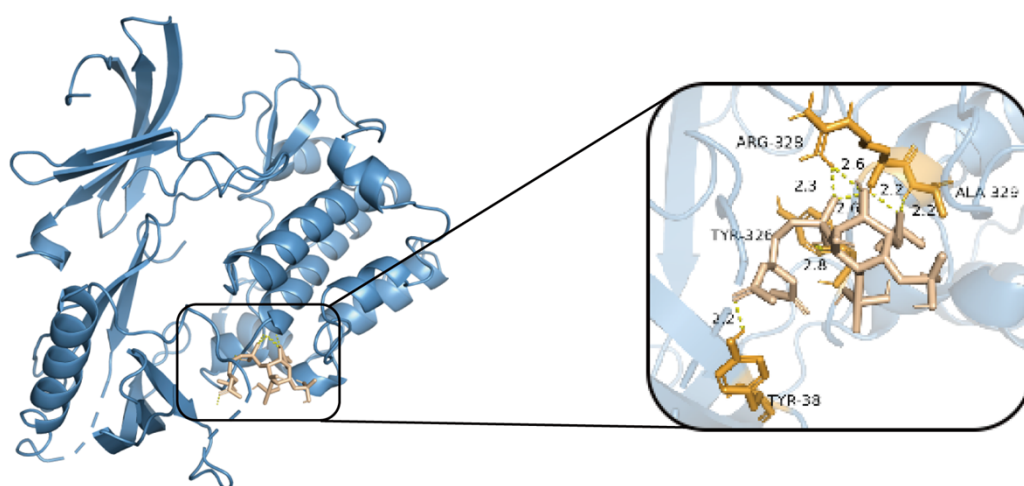


Figure S2 Map of AGE-RAGE signaling pathway in diabetic complications



center_X = 6.29 center_Y = -7.941 center_Z = 17.261 Binding energy = -5.6
 size_X = 75.25 size_Y = 75.25 size_Z = 75.25

Figure S3 Molecular docking between AKT1 and its natural ligand PIP3

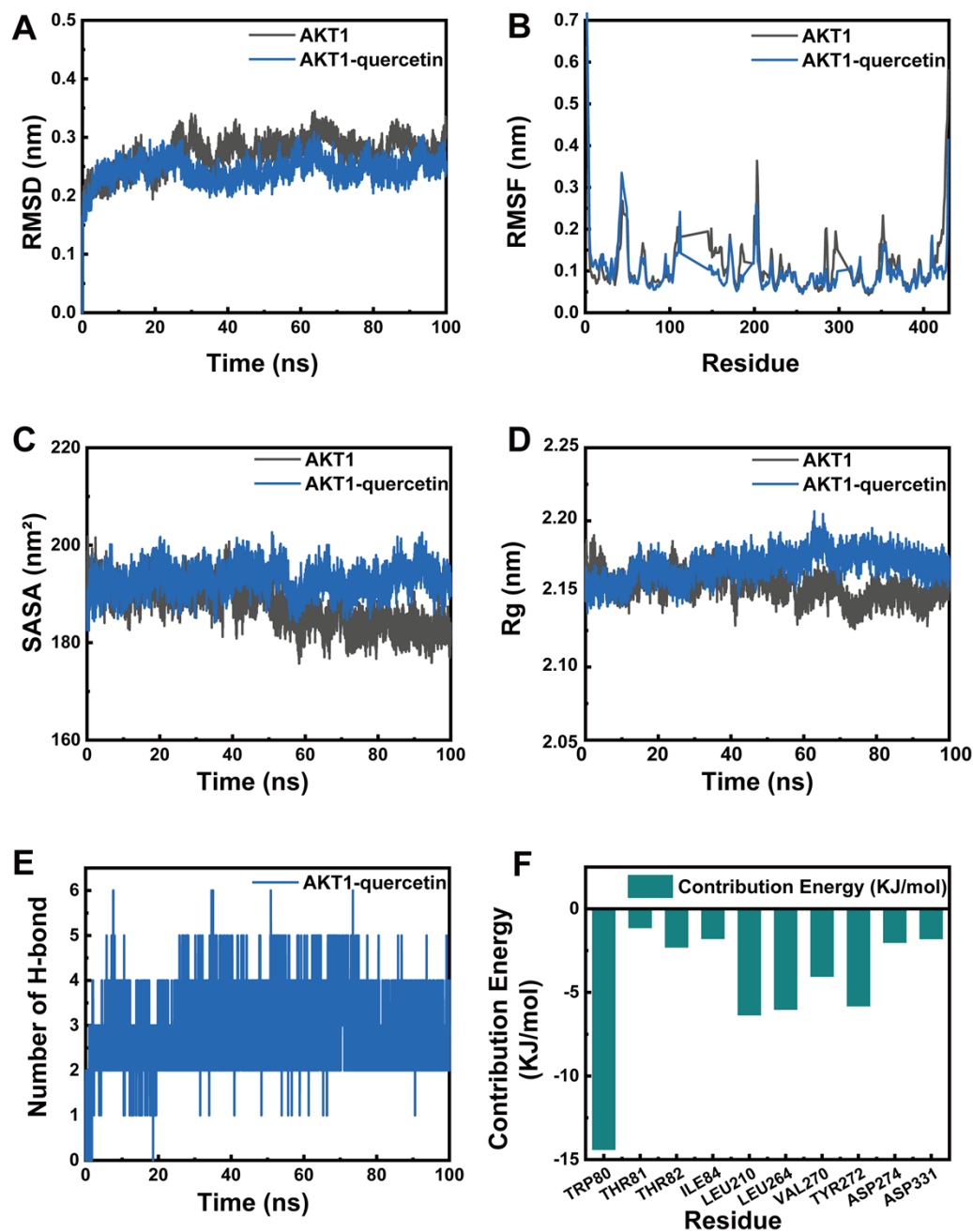


Figure S4 Analysis of MDS Results

(A) RMSD of AKT1-querceetin.(B) RMSF of AKT1-querceetin.(C) SASA of AKT1-querceetin.(D) Rg changes of AKT1-querceetin.(E) Number of Hydrogen Bonds (HBNUM) of AKT1-querceetin.(F) Free Energy Decomposition of Amino Acids for AKT1-querceetin.

Table S1 Protein ligand MMPBSA analysis

Energy	complex
Van der Waals Energy (KJ/mol)	-156.766
Electrostatic energy (kJ/mol)	-75.610
Polar solvation energy (KJ/mol)	161.970
Nonpolar solvation Energy(KJ/mol)	-19.120
Total Binding Energy(KJ/mol)	-89.526
-TΔS(KJ/mol)	4.473
Total Binding Free Energy(KJ/mol)	-85.053

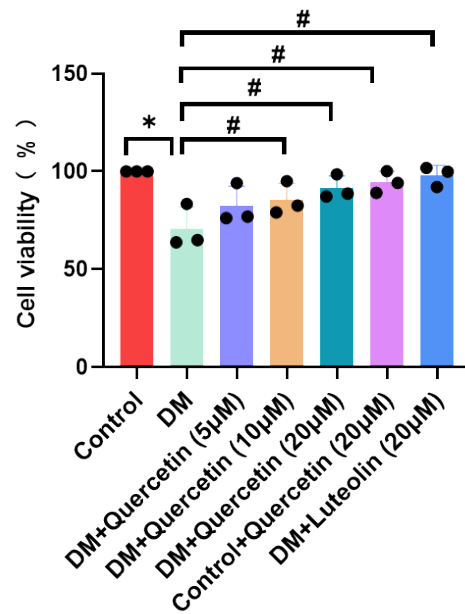


Figure S5 Impact of quercetin and luteolin on H9c2 cardiomyocytes in a diabetic environment

Influence of quercetin and luteolin on the survival rate of H9c2 myocardial cells subjected to injury from high glucose and PA, as relative to the Control group, * $P < 0.05$; and relative to the DM group, # $P < 0.05$, $n=3$ different cell batches. * indicates that there is a correlation between two variables and a $P < 0.05$ is considered to indicate statistical significance.