

Supplementary Data

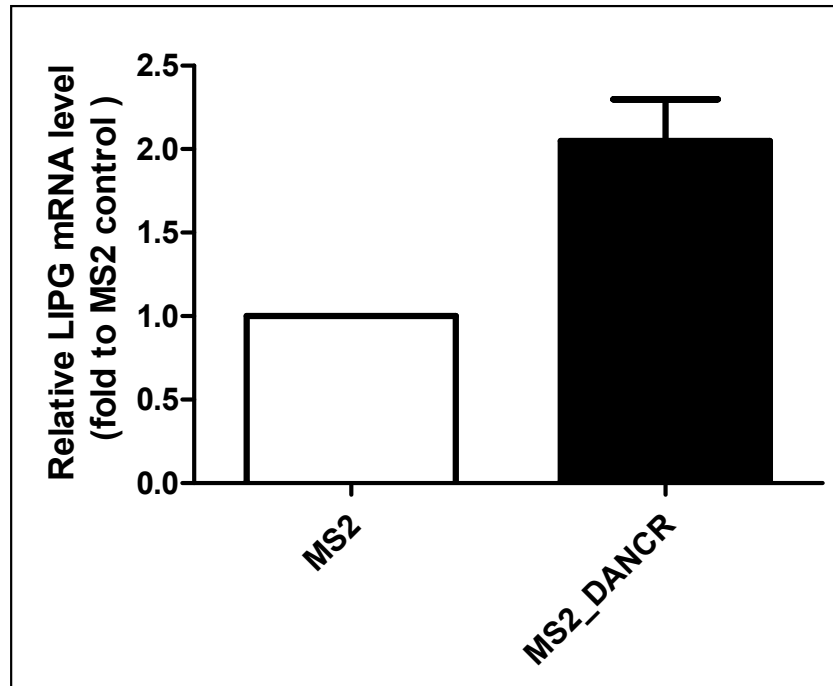


Figure S1. LIPG stable overexpressing MCF7 cells were co-transfected with p-NLS_MCP_GFP and pCDNA3-MS2 (negative control) or pCDNA3-MS2_hDANCR. Cells were collected 48 hours after transfection for RNA pulldown assay. A qRT-PCR analysis was performed to measure LIPG mRNA levels.

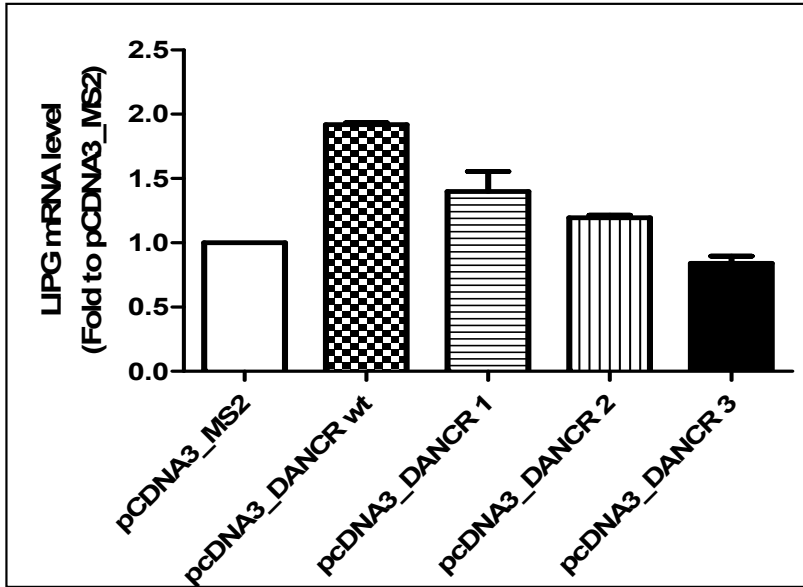
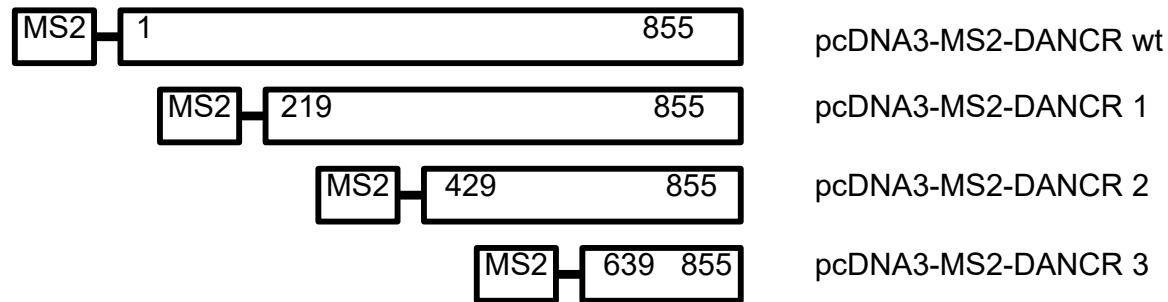


Figure S2. LIPG stable overexpressing MCF7 cells were co-transfected with p-NLS_MCP_GFP and pCDNA3-MS2 (negative control) or different length of pCDNA3-MS2_hDANCR. Cells were collected 48 hours after transfection for RNA pulldown assay. A qRT-PCR analysis was performed to measure LIPG mRNA levels.



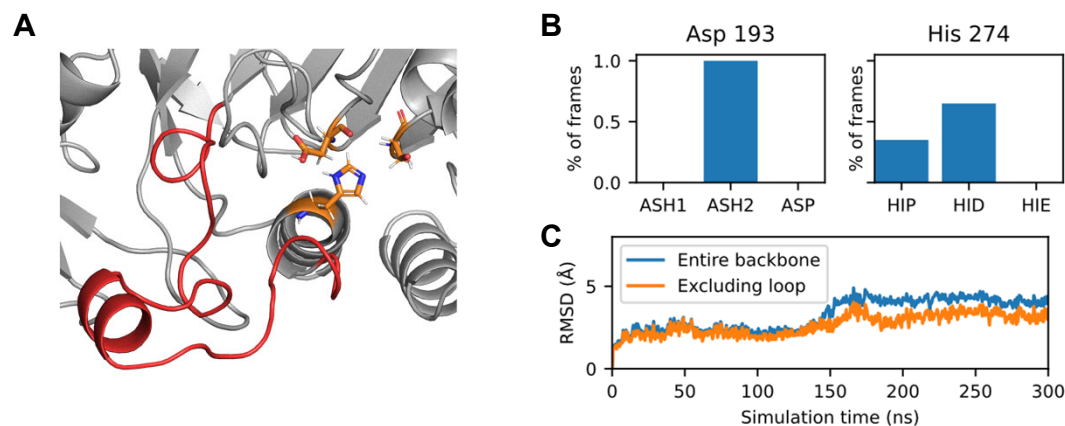


Figure S3: (A) Zoomed-in view of the binding pocket, with the catalytic triad (Ser169, Asp193, and His274) highlighted in orange and a nearby 29-residue dynamic loop in red. (B) Predicted protonation/tautomer state populations for Asp193 (protonated) and His274 (predominantly singly protonated as HID) from the continuous constant pH molecular dynamics simulations. (C) Root mean square deviation of the backbone atoms before (blue) and after (orange) removing the flexible loop near the binding site over a 300-ns conventional molecular dynamics simulation.

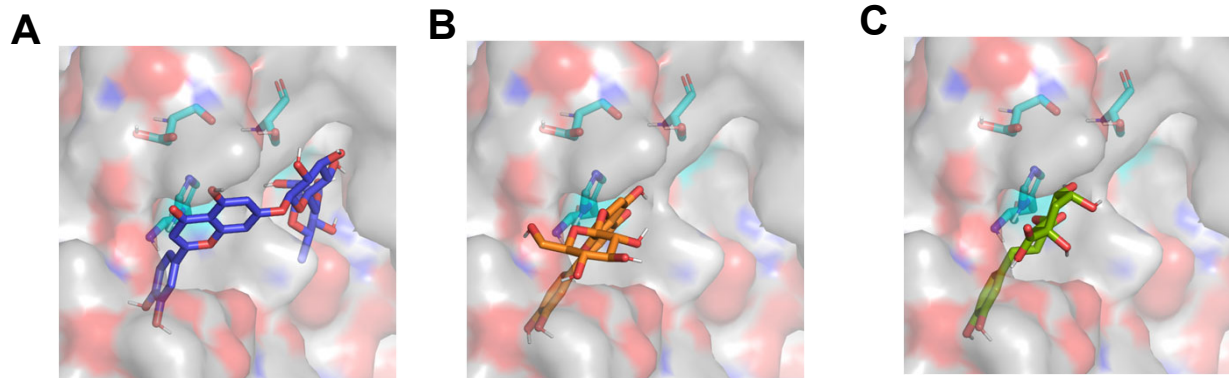


Figure S4: Binding poses of the top three compounds with the highest binding affinities: luteolin 7-O-beta-rutinoside (**A**), cynaroside (**B**), and luteolin (**C**). The catalytic triad Ser169, Asp193, and His274 highlighted as cyan sticks.

Figure S5

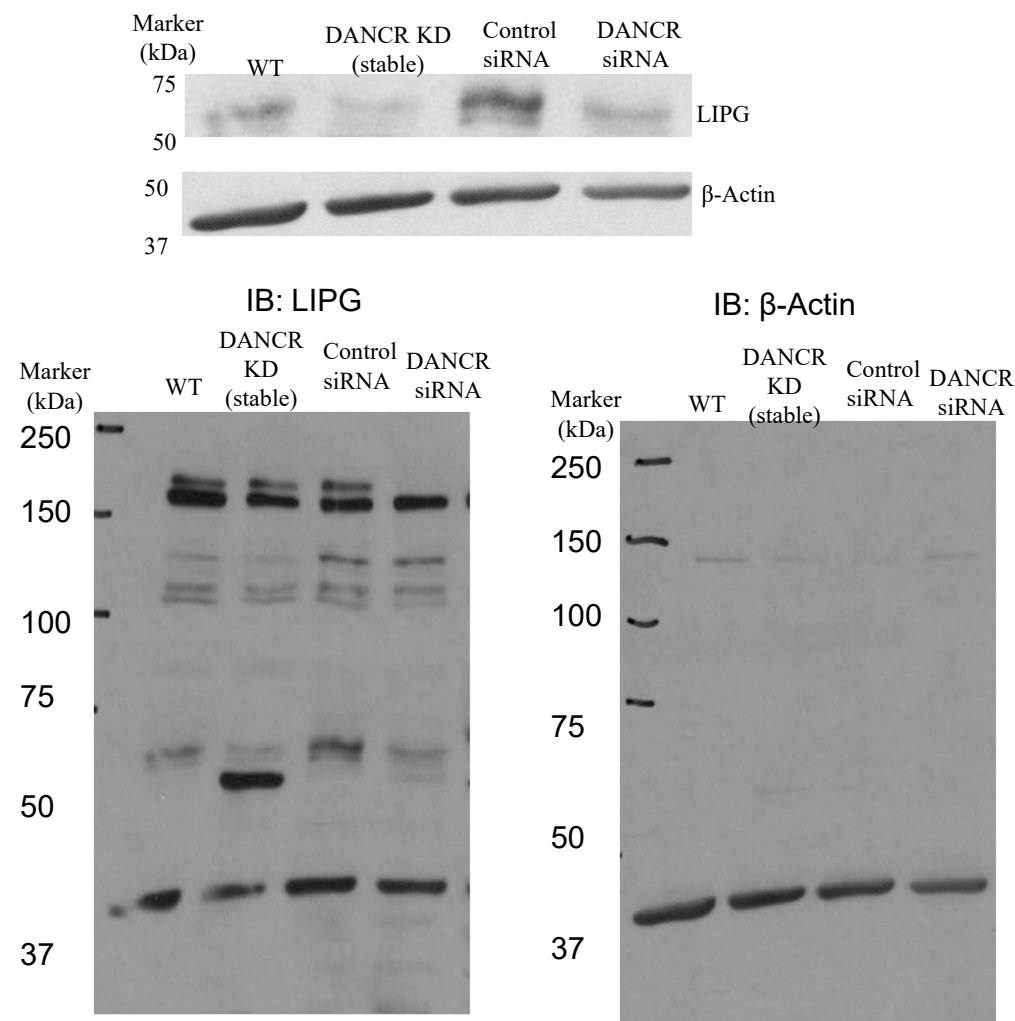


Figure S6

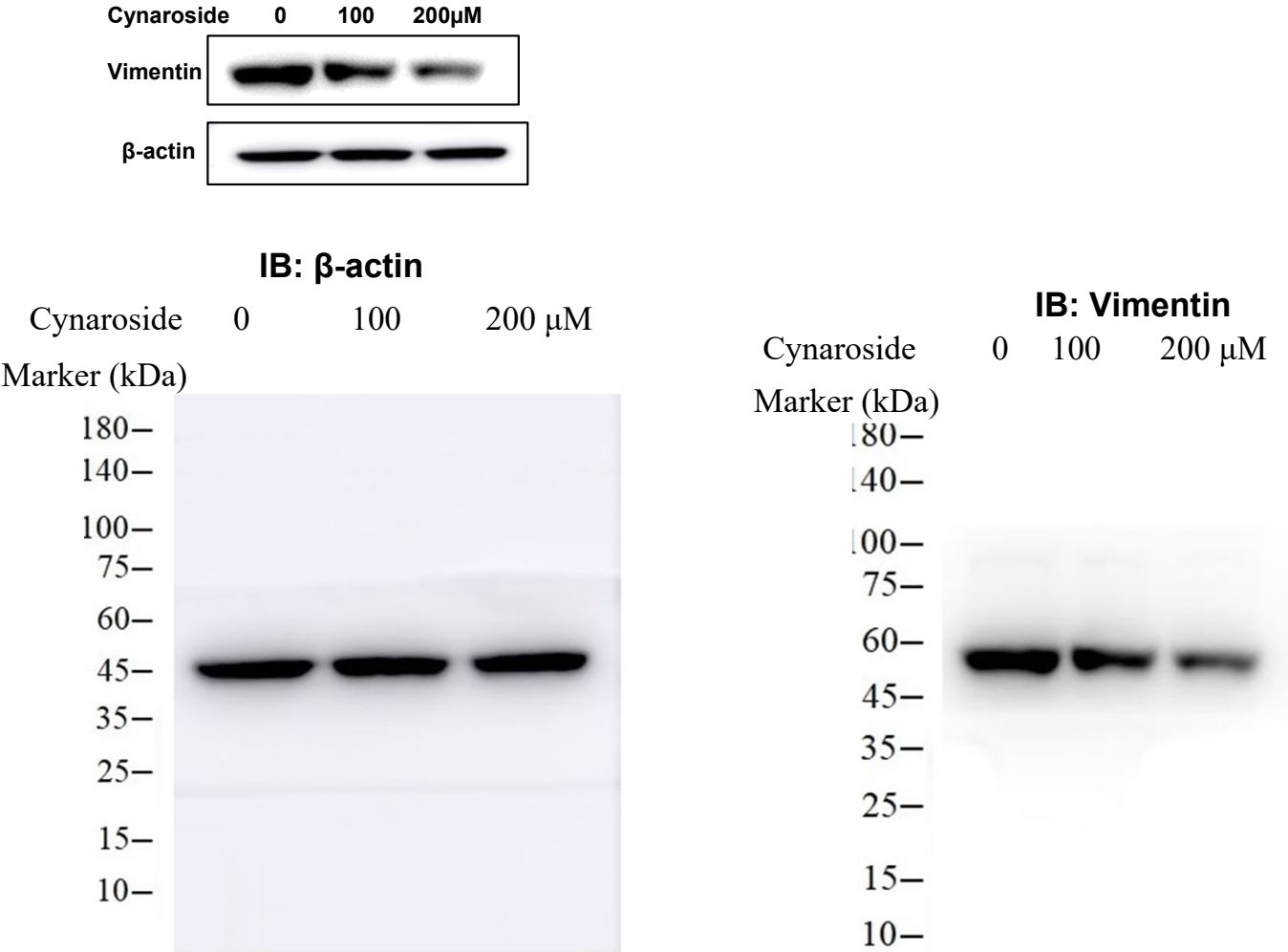


Figure S7

