

Supplementary figures

Figure S1. Evaluation of predictive accuracy and residual analysis for pIC50 values of *ADCY8*, *DDC*, and *PPP2R5C* with interacting ligands using a random forest regressor model

Figure S2. Applicability domain analysis of interacting ligands using principal component analysis (PCA).

Figure S3. Interactive Venn diagrams depicting the distribution and overlap of NCs across various food sources

Figure S4. Dotted vertical histogram of average molecular docking scores for nine target proteins and comparison of metabolic characteristics and bioactivity of natural compounds in docking with DDC.

Figure S5. pIC50 distribution across activity levels.

Figure S6. Maximum common substructures (MCS) across activity levels, segregated based on their bioactivity levels.

Supplementary Files

Supplementary File S1. Food sources of natural compounds to be selected.

Supplementary File S2. The binding energy between the target protein and selected natural compounds

Supplementary File S3. Binding energy between wild and mutated RNF213 protein (p.Arg4810Lys) and selected natural compounds