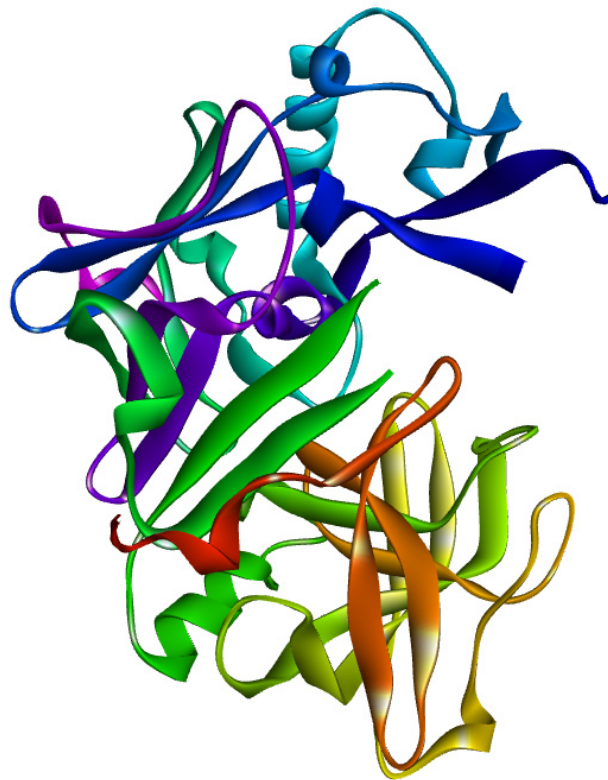


Supplementary Materials

***Caesalpinia mimosoides* Leaf Extract Promotes Neurite Outgrowth and Inhibits BACE1 Activity in Mutant APP-Overexpressing Neuronal Neuro2a Cells**

Panthakarn Rangsinth, Chatrawee Duangjan, Chanin Sillapachaiyaporn, Ciro Isidoro, Anchalee Prasansuklab and Tewin Tencomnao

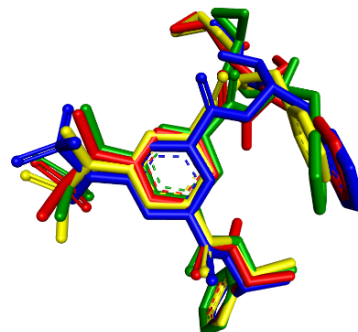
A



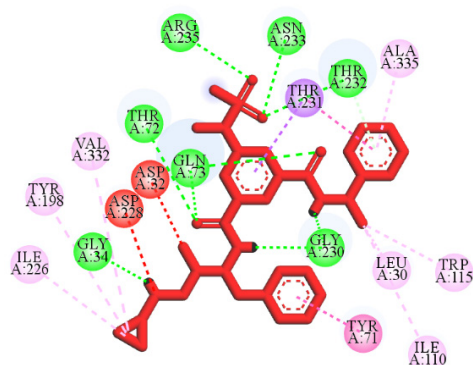
B



C



D

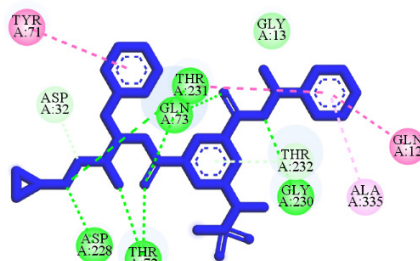


Interactions

Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Donor Hydrogen Bond
Pi-Sigma

Pi-Pi T-shaped
Amide-Pi Stacked
Alkyl
Pi-Alkyl

E

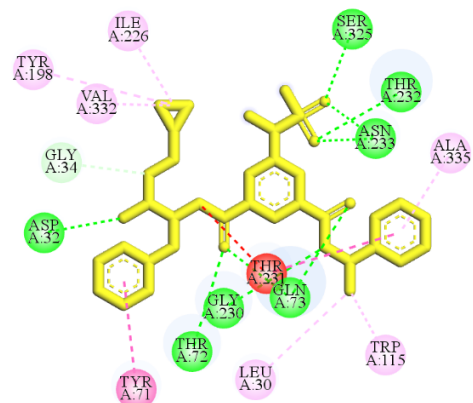


Interactions

van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Donor Hydrogen Bond

Pi-Pi T-shaped
Amide-Pi Stacked
Alkyl
Pi-Alkyl

F

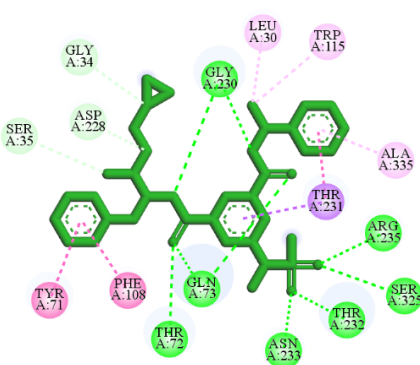


Interactions

Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Donor-Donor
Pi-Pi T-shaped

Amide-Pi Stacked
Alkyl
Pi-Alkyl

G



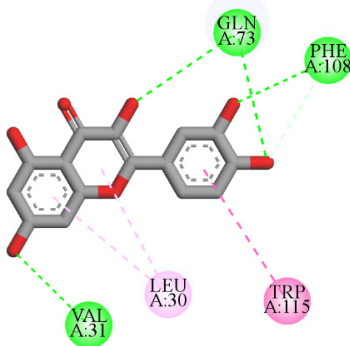
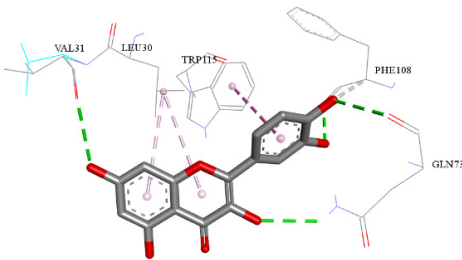
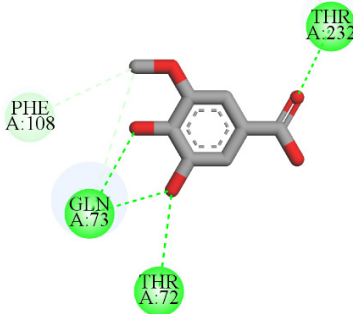
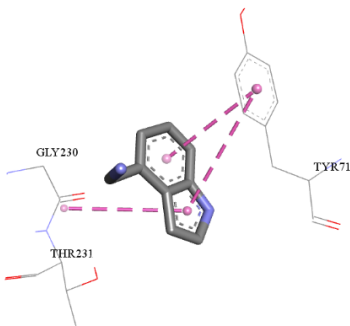
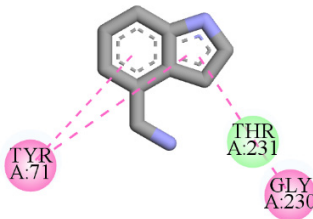
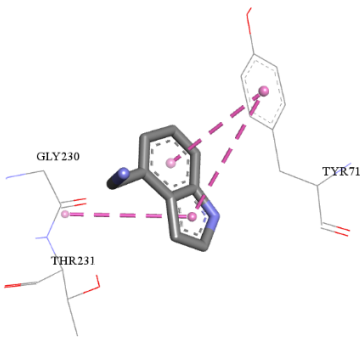
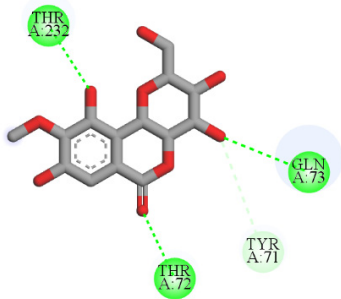
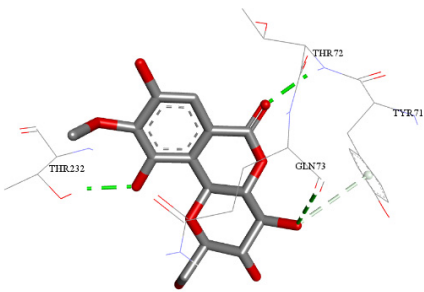
Interactions

Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Sigma
Pi-Pi T-shaped

Amide-Pi Stacked
Alkyl
Pi-Alkyl

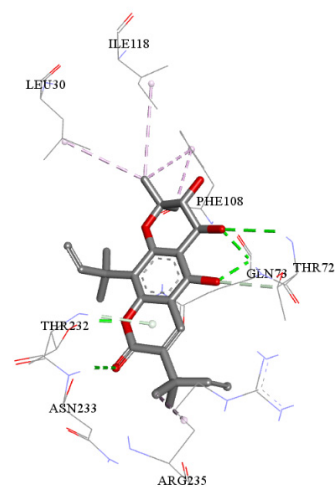
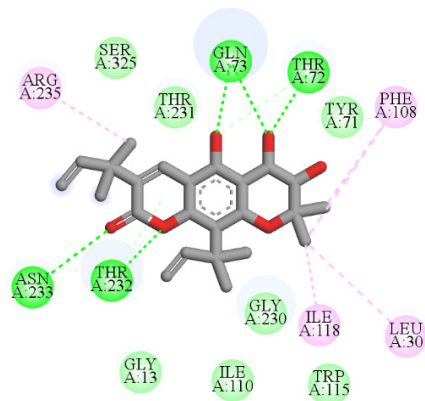
Figure S1. Diagrams represent protein-ligand interactions. (A) BACE1 structure (PBB ID 3TPP) (B-C) Overlapping structures of 5HA original crystal structure (red) and re-docking conformation on BACE1 (blue, yellow, and green are from redocking run 1-3, respectively). Schematics of amino acid interactions of BACE1 and 5HA: (D) 5HA from crystal structure, (E) 5HA from re-docking run 1, (F) 5HA from re-docking run 2, and (G) 5HA from re-docking run 3.

Table S1. Diagrams of protein-ligand interactions of BACE1 and candidate ligands.

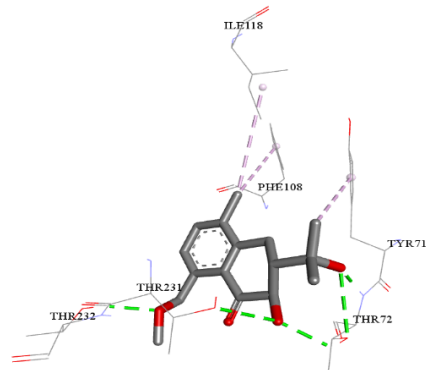
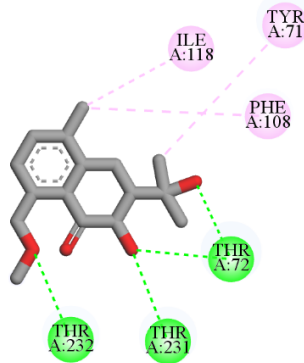
Ligand	Protein-ligand interactions
Quercetin (reference inhibitor)	 
3-O-Methylgallate	 
4-Aminomethylindole	 
Bergenin	 

Ligand **Protein-ligand interactions**

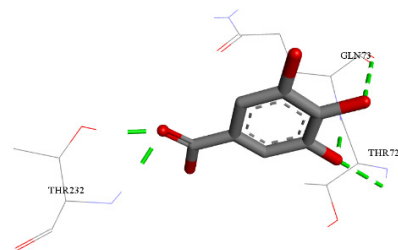
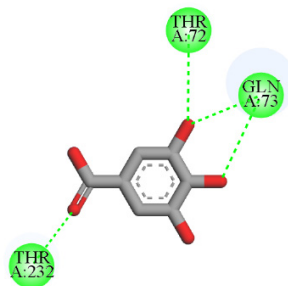
Clausarinol



Emmotin A

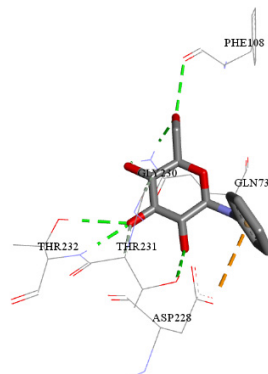
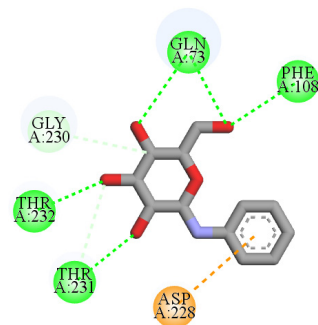


Gallic acid

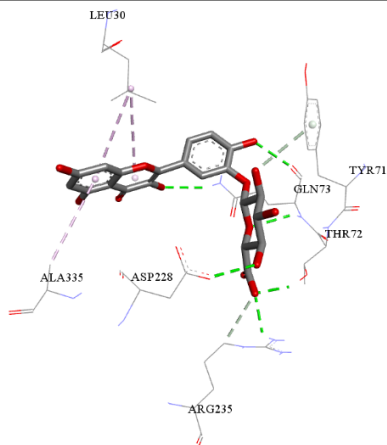
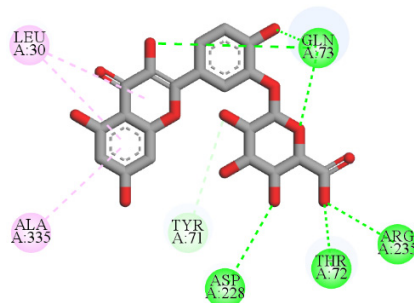


Ligand **Protein-ligand interactions**

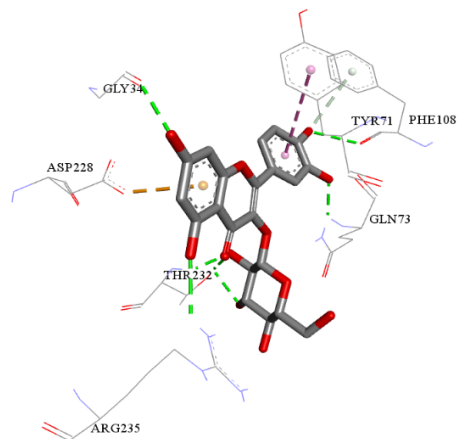
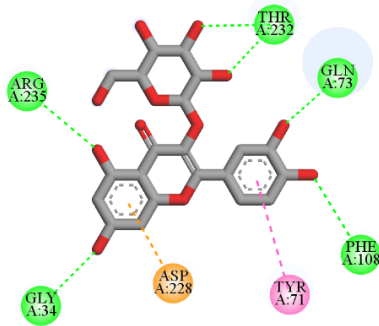
N-D-Glucosylarylamine



Quercetin-3'-glucuronide

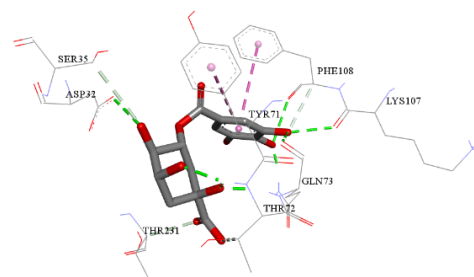
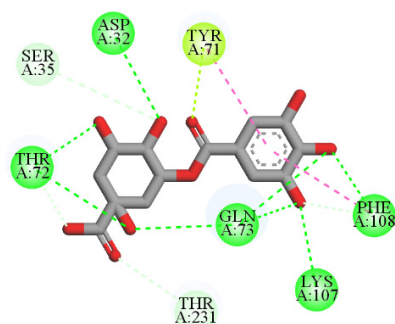


Quercetin-3-O-glucoside



Ligand**Protein-ligand interactions**

Theogallin



Green-dashes indicate hydrogen bonds. Pink-dashes indicate hydrophobic bonds. Orange-dashes indicate electrostatic bonds.