

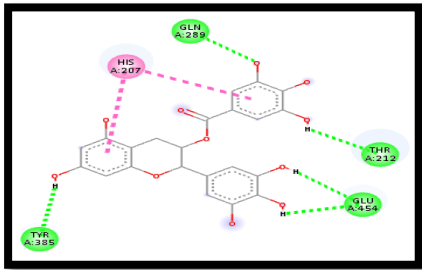
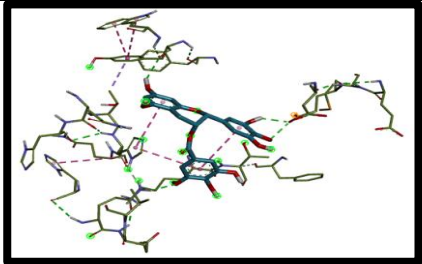
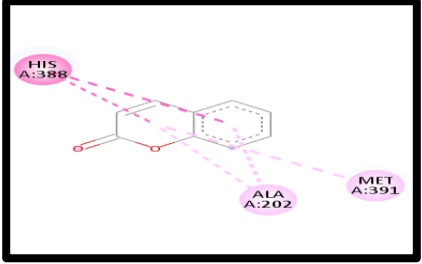
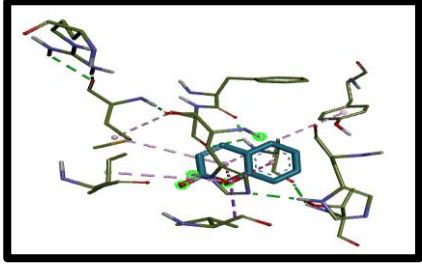
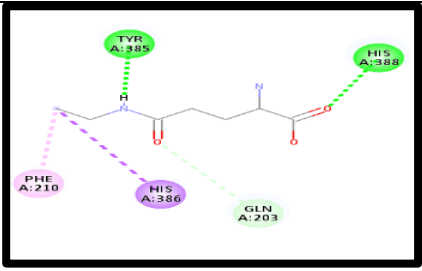
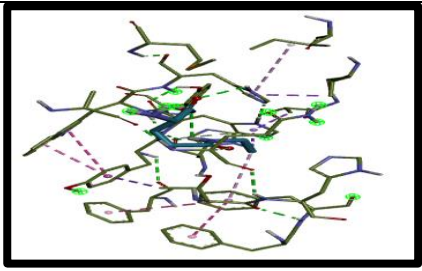
# Green Tea Augments Cognitive Function: An *In Silico* Model

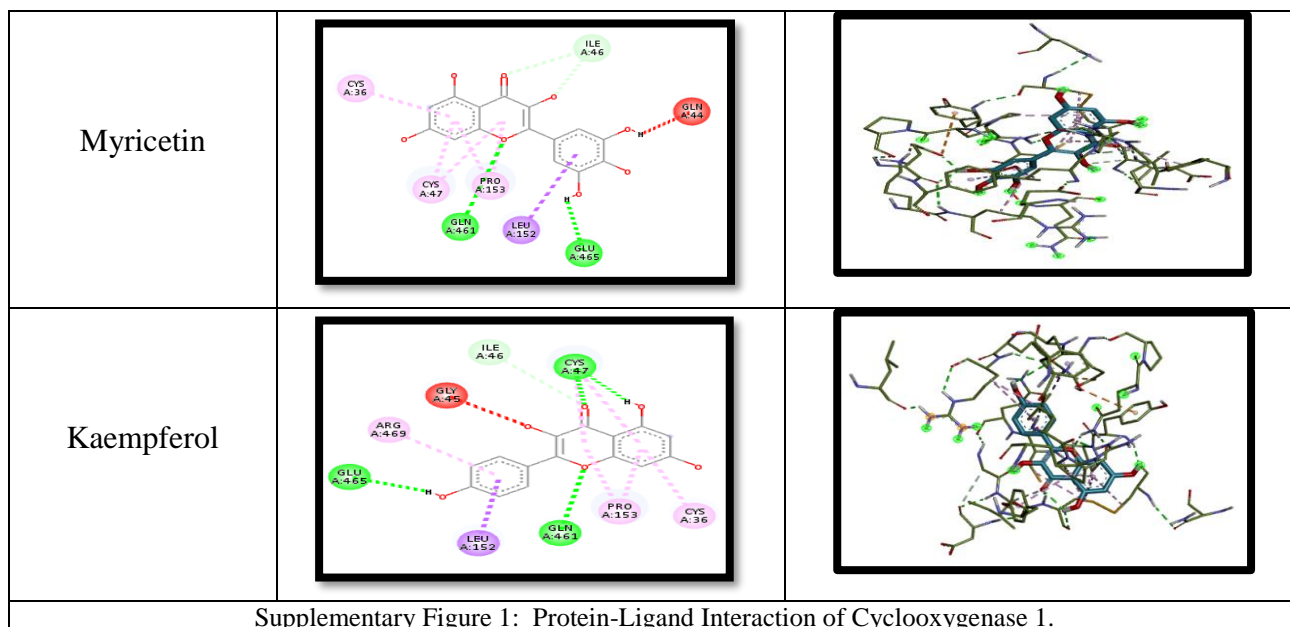
Aditya Sabhayasachi Khan<sup>1,2</sup>, Rezowana Mannan<sup>1,3</sup>, Laila Anjuman Banu<sup>4</sup>, Sohidul Islam<sup>2\*</sup>  
and Mahmud Hossain<sup>1\*</sup>

## Supplementary Figures

Two-dimensional structures simplify the interactions, whereas three-dimensional models amalgamate molecular interactions in ligand binding to the stimulation of the proteins. In the following models, deep green represents conventional hydrogen bonds, light green represents pi-donor hydrogen bond, pink represents a pi-alkyl bond, violet represents pi-sigma, and red represents an unfavorable donor-donor bond. It also simplifies the number of hydrogen bonds and polar interactions favored by ligand-protein interaction.

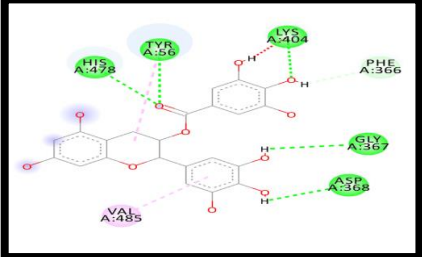
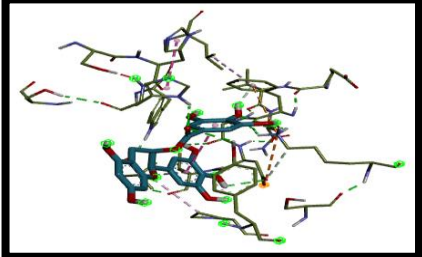
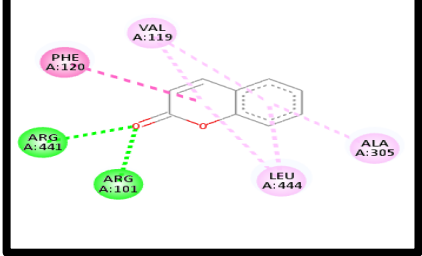
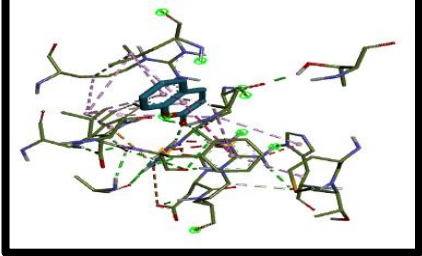
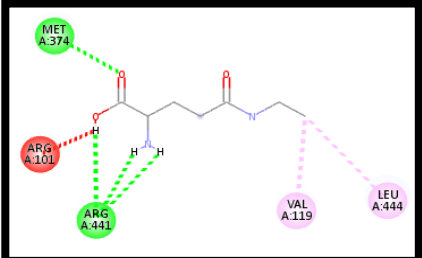
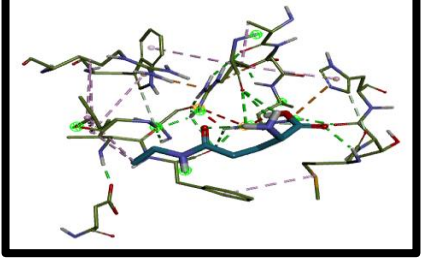
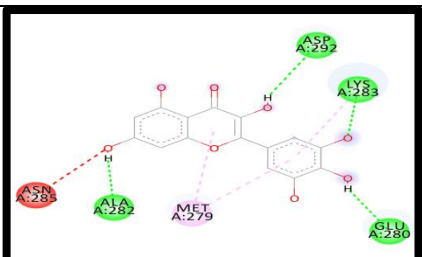
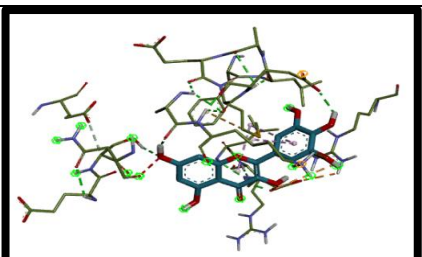
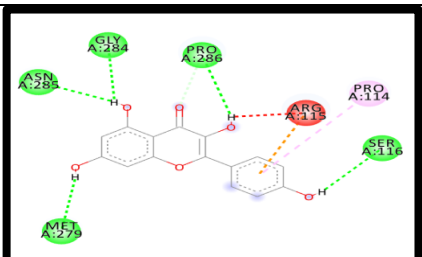
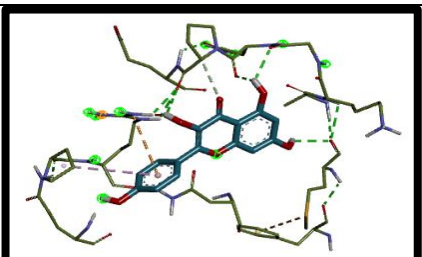
The ligands' two-dimensional and three-dimensional interaction with Cox 1 (Supplementary Figure 1)

Ligands With Cox1 Protein	2D Interactions	3D Interactions
Epigallocatechin Gallate (EGCG)		
Coumarin		
L-Theanine		



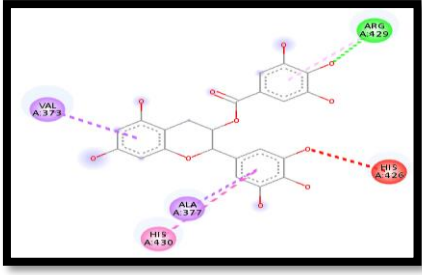
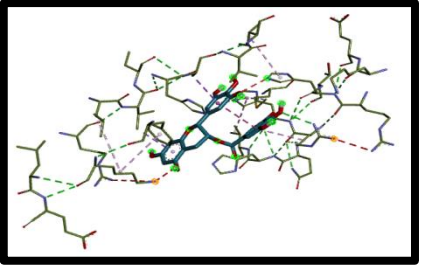
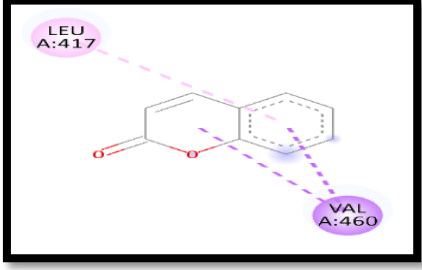
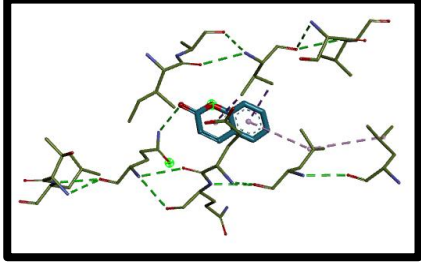
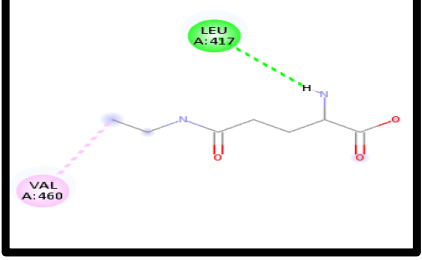
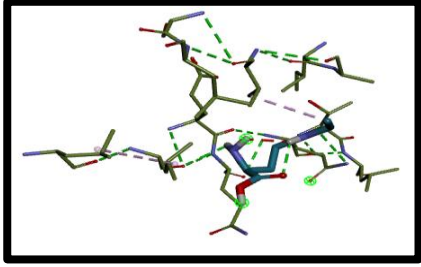
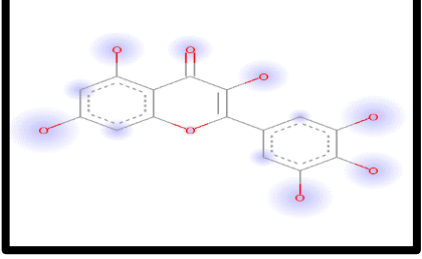
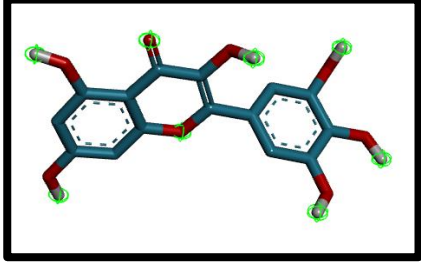
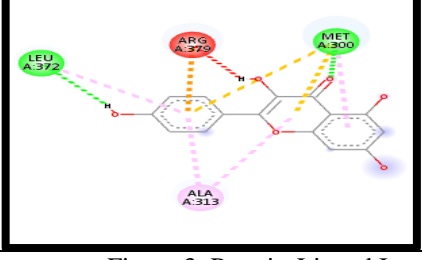
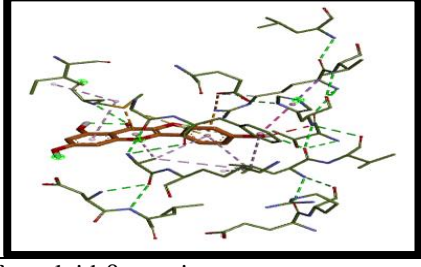
Supplementary Figure 1: Protein-Ligand Interaction of Cyclooxygenase 1.

The ligands' two-dimensional and three-dimensional interaction with Cyp4502d6 (Supplementary Figure 2).

Ligands With Cyp4502d6 Protein	2D Interactions	3D Interactions
Epigallocatechin gallate (EGCG)		
Coumarin		
L- Theanine		
Myricetin		
Kaempferol		

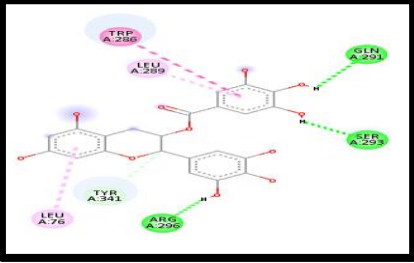
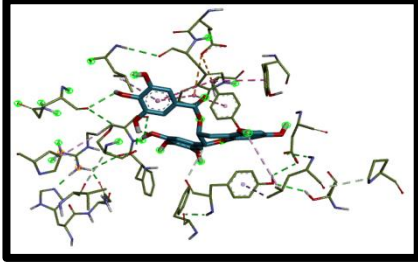
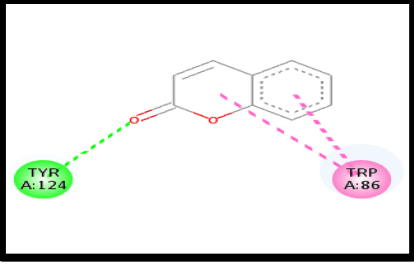
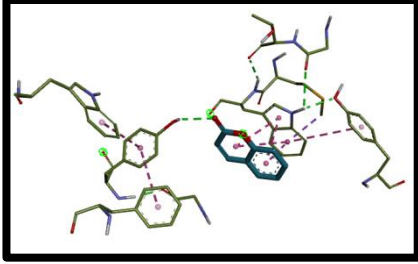
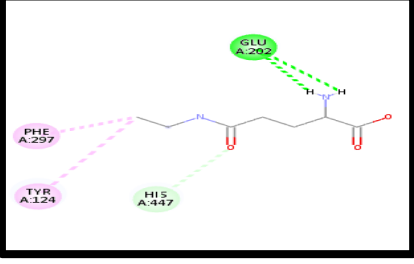
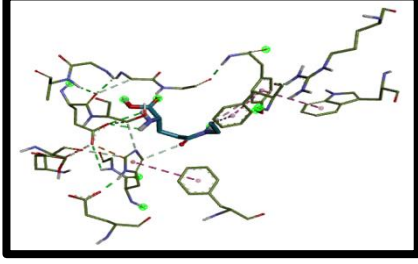
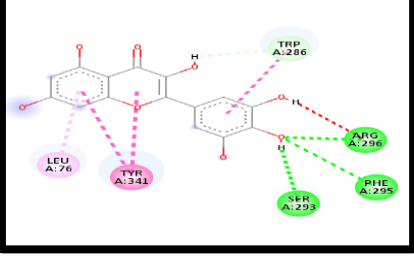
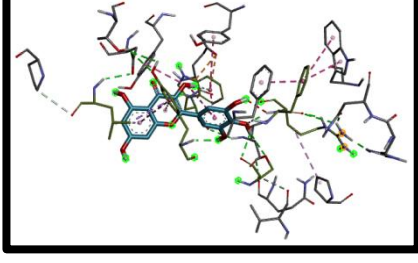
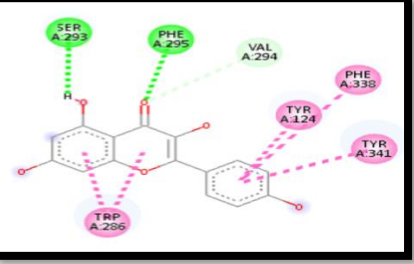
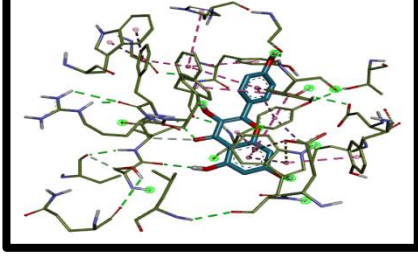
Supplementary Figure 2: Protein-Ligand Interaction of Cytochrome P4502d6.

The ligands' two-dimensional and three-dimensional interactions with App1 (Supplementary Figure 3).

Ligands With Amyloid- $\beta$ Protein	2D Interactions	3D Interactions
Epigallocatechin gallate (EGCG)		
Coumarin		
L-Theanine		
Myricetin		
Kaempferol		

Supplementary Figure 3: Protein-Ligand Interaction of amyloid- $\beta$  protein.

The ligands' two-dimensional and three-dimensional interactions with AChE (Supplementary Figure 4)

Ligands With AChE Protein	2D Interactions	3D Interactions
Epigallocatechin Gallate (EGCG)		
Coumarin		
L-Theanine		
Myricetin		
Kaempferol		

Supplementary Figure 4: Protein-Ligand Interaction of acetylcholinesterase.