

Supplementary material:

Table 1: Docking result of fisetin against three targets of AD using FlexX and iGEMDOCK.

Docking result of fisetin against three targets of AD using FlexX								Docking result of fisetin against three targets of AD using iGEMDOCK				
Sl No	Name of the Target	Score	Match	Lipo	Ambig	Clash	Rot	Energy	vdW	H-Bond	Elec	Interacting residues
1.	AChE (1EVE)	-28.2652	-27.0709	-8.3948	-8.8656	5.0661	5.6000	-112.042	-86.8547	-25.1877	0	GLN-69, TYR-70, ASP-72, TRP-84, ASN-85, TYR-130, SER-200, HIS-440, TRP-84, TRP-84, GLY-117, GLY-118, TYR-121, SER-122.
2.	ABAD (ISO8)	-15.0147	-20.0799	-4.2368	-5.3236	3.5356	5.6000	-103.006	-80.7207	-22.2853	0	SER-20, LEU-22, GLY-2, ALA-63, VAL-65, GLY-93, GLY-17, ASP-41, LEU-42, VAL-65, ALA-92, ILE-94.
3.	BACE1 (2QP8)	-31.4957	-30.1429	-8.9555	-8.3419	3.5445	7.0000	-70.9739	-42.0566	-28.9173	0	ARG-68, ASN-89, HIS-110, ARG-111, ARG-68, ASN-175, LEU-228.

Table 2: ADMET predicted profile of fisetin.

Model	Result	Probability
Absorption		
Blood-Brain Barrier	BBB+	0.5116
Human Intestinal Absorption	HIA+	0.9833
Caco-2 Permeability	Caco2-	0.8367
P-glycoprotein Substrate	Substrate	0.5510
P-glycoprotein Inhibitor	Non-inhibitor	0.9018
	Non-inhibitor	0.8259
Renal Organic Cation Transporter	Non-inhibitor	0.9242
Distribution		
Metabolism		
CYP450 2C9 Substrate	Non-substrate	0.8088
CYP450 2D6 Substrate	Non-substrate	0.9110
CYP450 3A4 Substrate	Non-substrate	0.6630
CYP450 1A2 Inhibitor	Inhibitor	0.9249
CYP450 2C9 Inhibitor	Inhibitor	0.8949
CYP450 2D6 Inhibitor	Non-inhibitor	0.9230
CYP450 2C19 Inhibitor	Non-inhibitor	0.6965
CYP450 3A4 Inhibitor	Non-inhibitor	0.7054
CYP Inhibitory Promiscuity	Low CYP Inhibitory Promiscuity	0.5409
Excretion		
Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	Weak inhibitor	0.9774
	Non-inhibitor	0.8374
AMES Toxicity	Non AMES toxic	0.5905
Carcinogens	Non-carcinogens	0.9390
Fish Toxicity	High FHMT	0.9766
TetrahymenaPyriformis Toxicity	High TPT	0.9971
Honey Bee Toxicity	High HBT	0.6228
Biodegradation	Not ready biodegradable	0.8902
Acute Oral Toxicity	II	0.7187
Carcinogenicity (Three-class)	Non-required	0.5926

Table 3: ADMET predicted profile of fisetin based on regression analysis.

Model	Value	Unit
Absorption		
Aqueous solubility	-3.0804	LogS
Caco-2 Permeability	0.4029	LogPapp, cm/s
Distribution		
Metabolism		
Excretion		
Toxicity		
Rat Acute Toxicity	3.1831	LD50, mol/kg
Fish Toxicity	0.2432	pLC50, mg/L
TetrahymenaPyriformis Toxicity	0.5944	pIGC50, ug/L