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Prospective neuro-muscular protection of Theaflavin gallate and tea extract by suppressing acetylcholinesterase in rat, verified by *in vitro* and MD simulation studies

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Supplementary Data

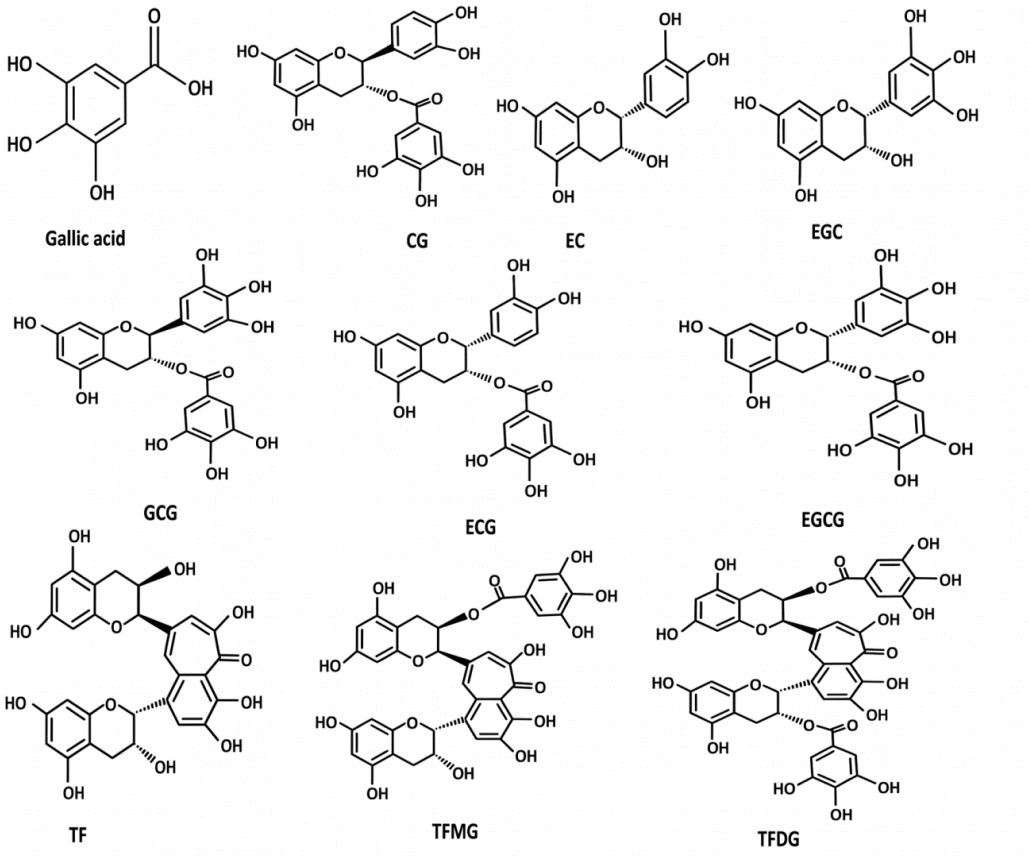

Fig. S1 — Caption is missing

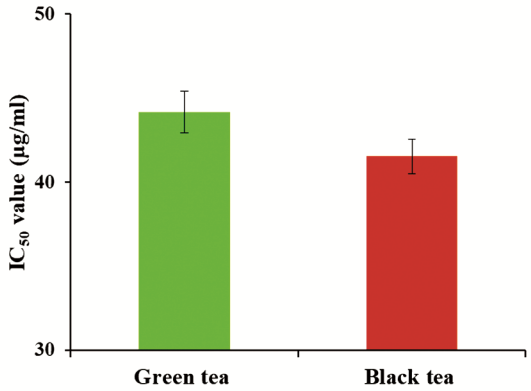

Fig. S2 — Comparative analysis of IC_{50} values (mg/mL) between green tea extractive and black tea extractives. Values are represented as mean ± SD where n = 3. The mean's differences were compared in one-way analysis of variance followed by Duncan's multiple range test (DMRT) with significant difference at $P \leq 0.05$. Mean values with same alphabetical letters are not significantly different at $P \leq 0.05$.

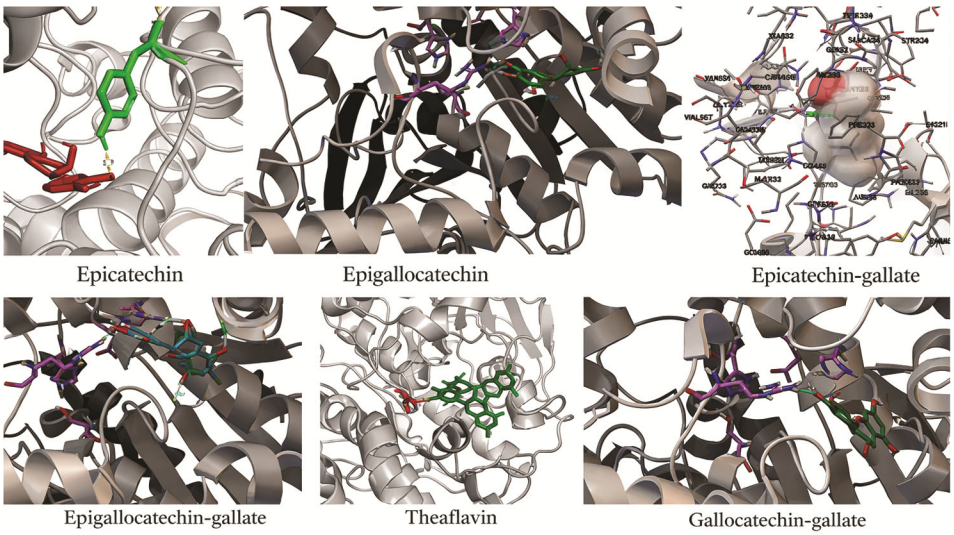

Fig. S3 — Molecular docking of several tea-flavonoids on AChE

Table S1 — Molecular docking parameters of Eserine, TFMG, TFDG and the substrate dihydrotanshinone.

Parameter	Specificity	Parameter	Specficity
npts 126 126 126	# num.grid points in xyz	map Protein.A.map	# atom-specific affinity map
gridfldProtein.maps.fld	# grid_data_file	map Protein.C.map	# atom-specific affinity map
spacing 0.641666666667	# spacing(A)	map Protein.HD.map	# atom-specific affinity map
receptor_types A C HD N NA OA SA	# receptor atom types	map Protein.OA.map	# atom-specific affinity map
ligand_types A C HD OA N	# ligand atom types	map Protein.N.map	# atom-specific affinity map
receptor Protein.pdbqt	# macromolecule	elecmapProtein.e.map	# electrostatic potential map
gridcenter auto	# xyz-coordinates or auto	dsolvmapProtein.d.map	# desolvation potential map
smooth 0.5	# store minimum energy w/in rad(A)	dielectric -0.1465	# <0, AD4 distance-dep.diel;>0, constant

Table S2 — Docking parameters between Acetylcholinesterase and TFMG

Parameters	SET1	SET2	SET3	SET4	SET5	SET6	SET7	SET8	SET9	SET10
Binding energy	-9.84	-8.32	-6.4	-8.05	-9.92	-7.11	-5.82	-7.89	-6.29	-7.76
Ligand efficiency	-0.19	-0.16	-0.12	-0.15	-0.19	-0.14	-0.11	-0.15	-0.12	-0.15
Inhibitory constant	61.15 nM	797.98 nM	20.28 μM	1.27 μM	53.28 nM	6.17 μM	54.19 μM	1.66 μM	24.66 μM	2.04 μM
Intermol energy	-11.33	-9.81	-7.89	-9.54	-11.41	-8.6	-7.31	-9.38	-7.78	-9.25
Vdw_hb_desolv_energy	-11.24	-9.8	-7.66	-9.61	-11.74	-8.61	-7.18	-9.25	-7.71	-9.15
Electrostatic energy	-0.1	-0.01	-0.24	0.07	0.32	0.01	-0.13	-0.13	0.07	-0.1
Total_internal	-3.53	-3.07	-4.14	-3.96	-2.98	-4.02	-3.67	-4.05	-4.13	-3.87
Tortional energy	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49
Unbound energy	-3.53	-3.07	-4.14	-3.96	-2.98	-4.02	-3.67	-4.05	-4.13	-3.87
clRMS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
refRMS	48.41	50.14	69.22	48.21	52.22	52.12	70.5	35.09	38.97	46.53
Rseed1	None	None	None	None	None	None	None	None	None	None
Rseed2	None	None	None	None	None	None	None	None	None	None
H-bonding	PHE295	PHE346	ALA497	VAL73	THR383, GLN527	THR383, ALA528	ALA497, LEU518	ARG219	GLU292 GLN369	GLY342, HIS287, TYR341

Table S3 — Docking parameters between Acetylcholinesterase and TFDG

Parameters	SET1	SET2	SET3	SET4	SET5	SET6	SET7	SET8	SET9	SET10
Binding energy	-1.07	-0.85	0.47	-1.14	0.2	-2.54	-2.0	-1.39	-3.3	0.67
Ligand efficiency	-0.03	-0.03	0.01	-0.04	0.01	-0.08	-0.06	-0.04	-0.1	0.02
Inhibitory constant	164.11 mM	237.85 mM	-	145.95 mM	-	13.76 mM	34.47 mM	95.16 mM	3.81 mM	-
Intermol energy	-7.93	-7.71	-6.39	-8.0	-6.66	-9.4	-8.86	-8.25	-10.16	-6.19
Vdw_hb_desolv_energy	-7.65	-7.56	-6.04	-7.7	-6.51	-9.31	-8.76	-8.02	-9.98	-6.13
Electrostatic energy	-0.28	-0.15	-0.35	-0.3	-0.14	-0.09	-0.09	-0.23	-0.18	-0.06
Total_internal	-3.9	-4.18	-4.97	-4.16	-5.27	-3.54	-5.0	-3.92	-4.1	-5.15
Tortional energy	6.86	6.86	6.86	6.86	6.86	6.86	6.86	6.86	6.86	6.86
Unbound energy	-3.9	-4.18	-4.97	-4.16	-5.27	-3.54	-5.0	-3.92	-4.1	-5.15
clRMS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
refRMS	51.05	59.38	75.18	53.1	45.04	52.72	53.6	51.06	49.33	54.21
Rseed1	None	None	None	None	None	None	None	None	None	None
Rseed2	None	None	None	None	None	None	None	None	None	None
H-bonding	ARG296	PRO108, GLU185	LYS23	ARG525, ARG522, ALA526, ARG525	VAL370, GLU292, ARG364	HIS287, PHE295, TYR124		ASP384, ASP400	TYR341	GLN527

Table S4 — Docking parameters between Acetylcholinesterase and dihydrotanshinone (pubchem id. 5316743)

Parameters	SET1	SET2	SET3	SET4	SET5	SET6	SET7	SET8	SET9	SET10
Binding energy	-6.48	-8.82	-6.55	-6.54	-6.07	-6.07	-6.51	-8.39	-8.84	-6.55
Ligand efficiency	-0.31	-0.42	-0.31	-0.31	-0.29	-0.29	-0.31	-0.4	-0.42	-0.31
Inhibitory constant	17.83 μM	343.03 nM	15.9 μM	15.99 μM	35.34 μM	35.63 μM	16.77 μM	703.92 nM	332.6 nM	15.84 μM
Intermol energy	-6.48	-8.82	-6.55	-6.54	-6.07	-6.07	-6.51	-8.39	-8.84	-6.55
Vdw_hb_desolv_energy	-6.39	-8.78	-6.61	-6.61	-6.07	-6.06	-6.57	-8.36	-8.79	-6.61
Electrostatic energy	-0.08	-0.04	0.06	0.06	0.0	0.0	0.06	-0.03	-0.04	0.06
Total_internal	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Tortional energy	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Unbound energy	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
clRMS	0.0	0.15	0.02	0.02	0.0	0.03	0.07	0.0	0.0	0.0
refRMS	19.83	0.68	30.8	30.82	27.86	27.88	30.82	2.45	0.66	30.8
Rseed1	None	None	None	None	None	None	None	None	None	None
Rseed2	None	None	None	None	None	None	None	None	None	None
H-bonding	ARG463	PHE295	ARG219	ARG219	HIS381, TRP385	HIS381, TRP385	ARG219	ARG296	PHE295	ARG219

Table S5 — Docking parameters between Acetylcholinesterase and Physostigmine (pubchem id. 5983)

Parameters	SET1	SET2	SET3	SET4	SET5	SET6	SET7	SET8	SET9	SET10
Binding energy	-7.85	-5.99	-7.82	-7.83	-5.88	-6.1	-5.94	-5.93	-7.15	-7.85
Ligand efficiency	-0.39	-0.3	-0.39	-0.39	-0.29	-0.31	-0.3	-0.3	-0.36	-0.39
Inhibitory constant	1.75 μM	40.4 μM	1.84 μM	1.83 μM	49.29 μM	33.81 μM	44.36 μM	45.02 μM	5.76 μM	1.75 μM
Intermol energy	-8.45	-6.59	-8.42	-8.42	-6.47	-6.7	-6.54	-6.53	-7.74	-8.45
Vdw_hb_desolv_energy	-7.95	-5.8	-7.91	-7.97	-5.68	-6.09	-5.75	-5.74	-7.12	-7.97
Electrostatic energy	-0.5	-0.79	-0.51	-0.45	-0.79	-0.61	-0.79	-0.79	-0.62	-0.48
Total_internal	-0.26	-0.23	-0.24	-0.25	-0.23	-0.22	-0.24	-0.25	-0.25	-0.22
Tortional energy	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6
Unbound energy	-0.26	-0.23	-0.24	-0.25	-0.23	-0.22	-0.24	-0.25	-0.25	-0.22
clRMS	0.0	0.0	1.15	0.43	0.65	0.0	0.19	0.0	0.0	0.0
refRMS	50.79	57.69	50.65	50.86	58	39.88	57.79	55.99	50	50.73
Rseed1	None	None	None	None	None	None	None	None	None	None
Rseed2	None	None	None	None	None	None	None	None	None	None
H-bonding		ASP384, TRP385	SER293	SER293	ASP384, TRP385	ARG296	ASP384, TRP385		PHE295	SER293