

Table S3 Analysis of the main differential active ingredients associated with neurodegenerative changes PPI in green tea (GT) compared to black tea (BT)

Compounds	Degree	Formula	Fold change	Family	MW	BBB permeant	Bioavailability Score
Prazepam	30	C19H17ClN2O	0.18	1,4-benzodiazepines	324.11	Yes	0.55
Fluconazole	17	C13H12F2N6O	0.08	Benzene and derivatives	306.10	No	0.55
Bilirubin	6	C33H36N4O6	0.07	Bilirubins	584.26	No	0.11
Naringenin	6	C15H12O5	0.27	Endogenous Metabolites	272.07	No	0.55
4-Hydroxycoumarin	4	C9H6O3	0.15	Coumarins and derivatives	162.03	Yes	0.55
4-tert-Amylphenol	4	C11H16O	0.05	Benzene and derivatives	164.12	Yes	0.55
Isoeugenol acetate	4	C12H14O3	0.29	Benzene and derivatives	206.09	Yes	0.55
Scopolin	4	C16H18O9	0.25	Coumarins	354.10	No	0.11
Tolmetin	4	C15H15NO3	0.20	Carbonyl compounds	257.10	Yes	0.85
3,5-Dicaffeoylquinic acid	3	C25H24O12	0.08	Alcohols	516.13	No	0.11
Adenosine	3	C10H13N5O4	0.07	Nucleic acids	267.10	No	0.55
Spiculisporic acid	3	C17H28O6	0.06	Others	328.19	No	0.56
Ubenimex	3	C16H24N2O4	0.26	Alkaloids	308.17	No	0.55
3-Methyladipic acid	2	C7H12O4	0.03	Endogenous Metabolites	160.07	No	0.85
Atractylenolide II	2	C15H20O2	0.17	Terpenoids	232.15	Yes	0.55
Microcystin-LR	2	C49H74N10O12	0.20	Endogenous Metabolites	994.53	No	0.11
Protostemonine	2	C23H31NO6	0.14	Alkaloids	417.22	Yes	0.55
3-Methylhistidine	1	C7H11N3O2	0.19	Amino acids, peptides, and analogues	169.09	No	0.55
Abscisic acid	1	C15H20O4	0.03	Others	264.14	Yes	0.85
Aspirin	1	C9H8O4	0.15	Benzene and derivatives	180.04	Yes	0.85
Bisphenol AP	1	C20H18O2	0.08	Extractables/Leachables	290.14	Yes	0.55
Dioxybenzone	1	C14H12O4	0.19	Extractables/Leachables	244.07	Yes	0.55
L-Glutathione (reduced)	1	C10H17N3O6S	0.03	Cofactors	307.08	No	0.11
Methyl salicylate	1	C8H8O3	0.13	Benzene and derivatives	152.05	Yes	0.55
Oxyresveratrol	1	C14H12O4	0.22	Polyketides[PK]	244.07	Yes	0.55
Pachymic acid	1	C33H52O5	0.23	Terpenoids	528.38	No	0.56
Silibinin	1	C25H22O10	0.20	Endogenous Metabolites	482.12	No	0.55
Uridine 5'-diphosphoglucuronic acid	1	C15H22N2O18P2	0.02	Gamma butyrolactones	580.03	No	0.11