

Table S1 Compound information in green tea (GT)

Fold Change	Formula	Name	Family	MW	BBB permeant	Bioavailability Score
0.18	C19H17CIN2O	Prazepam	1,4-benzodiazepines	324.8	Yes	0.55
0.15	C6H6N4O2	3-Methylxanthine	Alkaloids	166.14	No	0.55
0.14	C23H31NO6	Protostemonine	Alkaloids	417.5	Yes	0.55
0.26	C16H24N2O4	Ubenimex	Alkaloids	308.37	No	0.55
0.19	C7H11N3O2	3-Methylhistidine	Amino acids, peptides, and analogues	169.18	No	0.55
0.05	C11H16O	4-tert-Amylphenol	Benzene and derivatives	164.24	Yes	0.55
0.15	C9H8O4	Aspirin	Benzene and derivatives	180.16	Yes	0.85
0.08	C13H12F2N6O	Fluconazole	Benzene and derivatives	306.27	No	0.55
0.29	C12H14O3	Isoeugenol acetate	Benzene and derivatives	206.24	Yes	0.55
0.13	C8H8O3	Methyl salicylate	Benzene and derivatives	152.15	Yes	0.55
0.16	C12H13N3O4S	N4-Acetylsulfamethoxazole	Benzene and derivatives	295.31	No	0.55
0.25	C7H6O3	3,4-Dihydroxybenzaldehyde	Carbonyl compounds	138.12	Yes	0.55
0.05	C6H6O3	5-Hydroxymethylfurfural	Carbonyl compounds	126.11	No	0.55
0.20	C15H15NO3	Tolmetin	Carbonyl compounds	257.28	Yes	0.85
0.25	C16H18O9	Scopolin	Coumarins	354.31	No	0.55
0.15	C9H6O3	4-Hydroxycoumarin	Coumarins and derivatives	162.14	Yes	0.55
0.03	C7H12O4	3-Methyladipic acid	Endogenous Metabolites	160.17	No	0.85
0.27	C15H12O5	Naringenin	Endogenous Metabolites	272.25	No	0.55
0.20	C25H22O10	Silibinin	Endogenous Metabolites	482.44	No	0.55
0.08	C20H18O2	Bisphenol AP	Extractables/Leachables	290.36	Yes	0.55
0.19	C14H12O4	Dioxybenzone	Extractables/Leachables	244.24	Yes	0.55
0.11	C22H18O10	(-)-Catechin gallate	Flavonoids	442.37	No	0.55
0.02	C15H14O6	(-)-Epicatechin	Flavonoids	290.27	No	0.55
0.04	C15H14O6	Catechin	Flavonoids	290.27	No	0.55
0.03	C19H18O8	Chrysofenetin B	Flavonoids	374.34	No	0.55
0.13	C15H14O6	Epicatechin	Flavonoids	290.27	No	0.55

0.05	C15H14O7	Epigallocatechin	Flavonoids	306.27	No	0.55
0.03	C15H12O6	Eriodictyol	Flavonoids	288.25	No	0.55
0.05	C21H20O10	Genistin	Flavonoids	432.38	No	0.55
0.06	C22H22O10	Glycitin	Flavonoids	446.4	No	0.55
0.17	C15H10O7	Quercetin	Flavonoids	302.24	No	0.55
0.16	C25H22O10	Silibinin	Flavonoids	482.44	No	0.55
0.14	C25H22O10	Silychristin	Flavonoids	482.44	No	0.55
0.07	C10H13N5O4	Adenosine	Nucleic acids	267.24	No	0.55
0.03	C15H20O4	Abscisic acid	Others	264.32	Yes	0.85
0.06	C17H28O6	Spiculisporic acid	Others	328.4	No	0.56
0.13	C8H8O3	4-Hydroxyphenylacetic acid	Phenols and derivatives	152.15	Yes	0.85
0.24	C16H16O6	Oxypeucedanin hydrate	Phenylpropanoids	304.29	No	0.55
0.16	C20H22O9	Astringin	Polyketides[PK]	406.38	No	0.55
0.07	C9H8O4	Caffeic acid	Polyketides[PK]	180.16	No	0.56
0.06	C8H8O4	Orsellinic acid	Polyketides[PK]	168.15	No	0.56
0.22	C14H12O4	Oxyresveratrol	Polyketides[PK]	244.24	No	0.55
0.17	C15H20O2	Atractylenolide II	Terpenoids	232.32	Yes	0.55
0.25	C20H22O9	Ginkgolide K	Terpenoids	406.38	No	0.55
0.23	C33H52O5	Pachymic acid	Terpenoids	528.76	No	0.56
0.04	C6H8O6	Ascorbic acid	Vitamins	176.12	No	0.56