

Table S2 Compound information in black tea (BT)

Fold Change	Formula	Name	Family	MW	BBB	Bioavailability
					permeant	Score
5.70	C10H9NO3	3-Furfuryl 2-pyrrolicarboxylate	Alkaloids	191.18	Yes	0.55
5.29	C25H41NO9	Aconine	Alkaloids	499.59	No	0.55
10.77	C15H24N2O2	Ammothamine	Alkaloids	264.36	Yes	0.55
26.27	C35H39N5O5	Ergocristine	Alkaloids	609.71	No	0.55
7.68	C10H9NO2	Indole-3-acetic acid	Alkaloids	175.18	Yes	0.85
4.10	C27H39NO3	Jervine	Alkaloids	425.6	Yes	0.55
8.25	C38H44N2O6	Neferine	Alkaloids	624.77	No	0.55
16.95	C21H30BrNO4	Scopolamine butylbromide	Alkaloids	440.37	No	0.55
12.28	C25H32N2O6	Vindoline	Alkaloids	456.53	No	0.55
6.24	C20H37NO2	Linoleoyl ethanolamide	Amines	323.51	Yes	0.55
7.85	C20H39NO2	Oleoyl ethanolamide	Amines	325.53	Yes	0.55
5.79	C20H35NO2	α -Linolenoyl ethanolamide	Amines	321.5	Yes	0.55
5.45	C4H8N2O3	Asparagine	Amino acids	132.12	No	0.55
26.65	C9H11NO3	L-Tyrosine	Amino acids	181.19	No	0.55
34.76	C6H11NO3	4-Acetamidobutanoic acid	Amino acids, peptides, and analogues	145.16	No	0.85
4.05	C16H28N4O4S	Biocytin	Amino acids, peptides, and analogues	372.48	No	0.55
7.06	C11H18N2O2	Cyclo(leucylprolyl)	Amino acids, peptides, and analogues	210.27	No	0.55
24.13	C6H12N2O4S2	L-Cystine	Amino acids, peptides, and analogues	240.3	No	0.55
57.86	C18H34N2O6S	Lincomycin	Amino acids, peptides, and analogues	406.54	No	0.55
13.29	C8H15NO3	N-Acetyl-L-leucine	Amino acids, peptides, and analogues	173.21	No	0.85
8.03	C11H13NO3	N-Acetyl-L-phenylalanine	Amino acids, peptides, and analogues	207.23	No	0.85
36.66	C7H13NO3	N-Isovalerylglycine	Amino acids, peptides, and analogues	159.18	No	0.85
19.46	C10H11NO3	Phenylac-Gly-OH	Amino acids, peptides, and analogues	193.2	No	0.85
20.36	C8H15NO2	Tranexamic Acid	Amino acids, peptides, and analogues	157.21	No	0.55
104.64	C9H12O3	1,3,5-Trimethoxybenzene	Benzene and derivatives	168.19	Yes	0.55

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5.21	C7H6O4	2,4-Dihydroxybenzoic Acid	Benzene and derivatives	154.12	No	0.56
9.74	C8H8O3	2-Anisic acid	Benzene and derivatives	152.15	Yes	0.85
11.47	C9H10O3	3,4'-Dihydroxyphenylacetone	Benzene and derivatives	166.17	Yes	0.55
13.12	C9H10O2	3,4-Dimethylbenzoic acid	Benzene and derivatives	150.17	Yes	0.85
6.88	C7H6O3	3-Hydroxybenzoic acid	Benzene and derivatives	138.12	Yes	0.85
88.23	C8H9NO	Acetanilide	Benzene and derivatives	135.16	Yes	0.55
7.58	C29H41NO4	Buprenorphine	Benzene and derivatives	467.64	Yes	0.55
16.07	C9H10O5	Ethyl gallate	Benzene and derivatives	198.17	No	0.55
7.19	C10H14O4	Guaifenesin	Benzene and derivatives	198.22	No	0.55
43.68	C25H28N6O	Irbesartan	Benzene and derivatives	428.53	No	0.55
22.93	C13H18O2	Methyl p-tert-butylphenylacetate	Benzene and derivatives	206.28	Yes	0.55
32.53	C17H19NO4	Oxymorphone	Benzene and derivatives	301.34	No	0.55
13.27	C19H20N2O3S	Pioglitazone	Benzene and derivatives	356.44	No	0.55
11.80	C18H14N4O5S	Sulfasalazine	Benzene and derivatives	398.39	No	0.56
4.15	C14H17NO6	(R)-Prunasin	Carbohydrates	295.29	No	0.55
30.57	C6H13NO5	D-(+)-Glucosamine	Carbohydrates	179.17	No	0.55
8.14	C8H8O4	2,4,6-Trihydroxyacetophenone	Carbonyl compounds	168.15	No	0.55
4.51	C6H6O3	5-Hydroxymethyl-2-furaldehyde	Carbonyl compounds	126.11	No	0.55
9.49	C10H12N2O3	L-Kynurenine	Carbonyl compounds	208.21	No	0.55
3.70	C10H12O4	Xanthoxylone	Carbonyl compounds	196.2	Yes	0.55
123.95	C9H6O4	Esculetin	Coumarins	178.14	No	0.55
16.38	C10H8O4	4-Methyl-6,7-dihydroxycoumarin	Coumarins and derivatives	192.17	Yes	0.55
13.07	C15H8O7	Demethylwedelolactone	Coumarins and derivatives	300.22	No	0.55
11.07	C22H37NO3	(+/-)5(6)-EET Ethanolamide	Endogenous Metabolites	363.53	Yes	0.55
157.73	C12H16N2O4	Alanyltyrosine	Endogenous Metabolites	252.27	No	0.55
9.13	C20H33NO	Arachidonoyl amide	Endogenous Metabolites	303.48	Yes	0.55
10.10	C12H14N2O3	DL-5-Methoxytryptophan	Endogenous Metabolites	234.25	No	0.55
11.21	C21H44NO7P	Glycerophospho-N-palmitoyl ethanolamine	Endogenous Metabolites	453.55	No	0.56

25.96	C25H34O6	Ingenol-3-angelate	Endogenous Metabolites	430.53	No	0.55
4.23	C20H26O3	Kahweol	Endogenous Metabolites	314.42	Yes	0.55
36.41	C20H39NO3	N-Acetylspingosine	Endogenous Metabolites	341.53	Yes	0.55
95.19	C22H36O4	Prostaglandin A1 ethyl ester	Endogenous Metabolites	364.52	Yes	0.55
16.03	C20H20O7	Tangeritin	Endogenous Metabolites	372.37	Yes	0.55
60.59	C18H34O4	(+/-)12(13)-DiHOME	Fatty acyls[FA]	314.46	No	0.56
7.99	C10H20O3	10-Hydroxydecanoic acid	Fatty acyls[FA]	188.26	Yes	0.85
56.96	C18H31NO4	10-Nitrolinoleate	Fatty acyls[FA]	325.44	No	0.56
5.65	C12H24O3	12-Hydroxydodecanoic acid	Fatty acyls[FA]	216.32	Yes	0.85
9.08	C18H28O3	12-Oxophytodienoic acid	Fatty acyls[FA]	292.41	Yes	0.85
25.45	C18H30O3	13(S)-HOTrE	Fatty acyls[FA]	294.43	Yes	0.85
16.42	C20H32O4	15(s)-hpete	Fatty acyls[FA]	336.47	No	0.85
7.28	C16H32O3	16-Hydroxyhexadecanoic acid	Fatty acyls[FA]	272.42	Yes	0.85
10.63	C5H11NO2	5-Aminovaleric acid	Fatty acyls[FA]	117.15	No	0.55
7.76	C20H30O3	5-OxoETE	Fatty acyls[FA]	318.45	Yes	0.85
14.23	C11H16O	5-Phenyl-1-pentanol	Fatty acyls[FA]	164.24	Yes	0.55
9.71	C18H30O3	9-Oxo-10(E),12(E)-octadecadienoic acid	Fatty acyls[FA]	294.43	Yes	0.85
18.49	C18H30O3	9-Oxo-ODE	Fatty acyls[FA]	294.43	Yes	0.85
41.05	C20H32O2	Arachidonic acid	Fatty acyls[FA]	304.47	No	0.85
31.54	C23H39NO3	Arachidonoylserinol	Fatty acyls[FA]	377.56	Yes	0.55
32.61	C18H32O5	Corchorifatty acid F	Fatty acyls[FA]	328.44	No	0.56
11.37	C22H32O2	Docosahexaenoic acid	Fatty acyls[FA]	328.49	No	0.85
6.92	C20H32O4	Prostaglandin B1	Fatty acyls[FA]	336.47	No	0.85
15.77	C9H6O4	5,7-Dihydroxychromone	Flavonoids	178.14	No	0.55
46.41	C27H30O10	Baohuoside I	Flavonoids	514.52	No	0.55
4.19	C21H22O10	Engeletin	Flavonoids	434.39	No	0.55
20.49	C16H12O7	Eupafolin	Flavonoids	316.26	No	0.55
9.63	C16H12O4	Formononetin	Flavonoids	268.26	Yes	0.55
6.01	C19H18O7	Gardenin B	Flavonoids	358.34	No	0.55

8.74	C16H12O5	Glycitein	Flavonoids	284.26	No	0.55
8.94	C23H28O10	Isomucronulatol 7-O-glucoside	Flavonoids	464.46	No	0.55
20.19	C25H26O6	Mulberrin	Flavonoids	422.47	No	0.55
7.09	C21H22O8	Nobiletin	Flavonoids	402.39	No	0.55
8.38	C21H22O8	Noreugenin	Flavonoids	402.39	No	0.55
16.20	C15H14O5	Phloretin	Flavonoids	274.27	No	0.55
123.60	C21H20O9	Puerarin	Flavonoids	416.38	No	0.55
15.51	C16H12O7	Rhamnetin	Flavonoids	316.26	No	0.55
4.58	C15H12O7	Taxifolin	Flavonoids	304.25	No	0.55
13.23	C21H39NO6	Myriocin	G Protein-coupled receptors	401.54	No	0.55
5.83	C21H41O7P	Oleoyl-L- α -lysoph osphatidic acid	Glycerophospholipids[GP]	436.52	No	0.56
15.73	C12H18O2	Sedanolide	Isobenzofurans	194.27	Yes	0.55
13.45	C5H5N5	Adenine	Nucleic acids	135.13	No	0.55
32.05	C9H13N3O5	Cytidine	Nucleic acids	243.22	No	0.55
79.89	C9H12O7S	4-Hydroxy-3- methoxyphenylglyc ol sulfate	Organic acids	264.25	No	0.56
57.11	C18H37NO2	Palmitoyl ethanolamide	Organic acids	299.49	Yes	0.55
7.21	C6H13NO3	4-Hydroxyisoleucin e	Others	147.17	No	0.55
11.34	C31H38O7	5,15-Diacetyl-3-be nzoyllathyrol	Others	522.63	No	0.55
23.68	C15H20O4	Abscisic acid	Others	264.32	Yes	0.85
10.62	C16H32O5	Aleuritic acid	Others	304.42	No	0.56
12.61	C12H13NO2	Ethyl 3-Indoleacetate	Others	203.24	Yes	0.55
9.31	C30H26O10	Hypocrellin A	Others	546.52	No	0.56
45.86	C14H19NO8	Lithosprmoside	Others	329.3	No	0.55
449.48	C21H26O10	Sec-O-Glucosylha maudol	Others	438.43	No	0.55
8.83	C12H16O2	Senkyunolide A	Others	192.25	Yes	0.55
14.90	C17H28O6	Spiculisporic acid	Others	328.4	No	0.56
12.02	C12H18O3	trans-Jasmonic Acid	Others	210.27	Yes	0.85
82.40	C22H28O6	Gomisin J	Phenols and derivatives	388.45	No	0.55
8.95	C10H12O3	Isopropyl 4-Hydroxybenzoate	Phenols and derivatives	180.2	Yes	0.55
8.59	C8H8O5	Methyl gallate	Phenols and derivatives	184.15	No	0.55
40.54	C20H24N2OS	Propiomazine	Phenothiazines	340.48	Yes	0.55
6.97	C13H18O2	Ibuprofen	Phenylpropanoic acids	206.28	Yes	0.85

9.63	C14H16O9	Bengenin	Phenylpropanoids	328.27	No	0.55
88.70	C11H12O4	Ethyl caffeate	Phenylpropanoids	208.21	Yes	0.55
10.51	C10H10O3	Ferulaldehyde	Phenylpropanoids	178.18	Yes	0.55
4.42	C12H14O5	3,4,5-Trimethoxycinnamic acid	Polyketides[PK]	238.24	Yes	0.85
201.60	C17H26O4	6-Gingerol	Polyketides[PK]	294.39	Yes	0.55
14.95	C22H30O4	Cannabidiolic acid	Polyketides[PK]	358.47	No	0.56
7.11	C15H10O5	Galangin	Polyketides[PK]	270.24	No	0.55
12.88	C15H20O	Hexylcinnamaldehyde	Polyketides[PK]	216.32	Yes	0.55
4.27	C18H16O8	Irigenin	Polyketides[PK]	360.31	No	0.55
13.13	C21H22O9	Liquiritin	Polyketides[PK]	418.39	No	0.55
8.21	C14H12O3	Resveratrol	Polyketides[PK]	228.24	Yes	0.55
12.64	C15H24O	(-)-Caryophyllene oxide	Prenol lipids[PR]	220.35	Yes	0.55
4.61	C8H9NO4	4-Pyridoxic acid	Pyridine and derivatives	183.16	No	0.56
47.12	C22H23ClN2O2	Loratadine	Pyridine and derivatives	382.88	Yes	0.55
29.75	C11H16N2O3	Butalbital	Pyrimidines and pyrimidine derivatives	224.26	No	0.55
23.98	C24H30O3	Drospirenone	Steroids and derivatives	366.49	Yes	0.55
113.35	C20H32O2	Mesterolone	Steroids and derivatives	304.47	Yes	0.55
16.44	C27H41NO3	Peimisine	Steroids and derivatives	427.62	Yes	0.55
12.91	C25H36O8	Epitestosterone glucuronide	Steroids/Vitamins/Hormones	464.55	No	0.56
26.34	C19H24O3	2-Methoxyestrone	Sterol lipids[ST]	300.39	Yes	0.55
77.96	C21H29FO5	Fludrocortisone	Sterol lipids[ST]	380.45	No	0.55
4.61	C27H44O4	Gitogenin	Sterol lipids[ST]	432.64	Yes	0.55
5.66	C24H34O5	Telocinobufagin	Sterol lipids[ST]	402.52	No	0.55
5.13	C21H30O3	Testosterone acetate	Sterol lipids[ST]	330.46	Yes	0.55
5.28	C25H36O8	Testosterone glucuronide	Sterol lipids[ST]	464.55	No	0.56
10.57	C15H22O5	Artemisinin	Terpenoids	282.33	Yes	0.55
31.27	C30H48O5	Asiatic acid	Terpenoids	488.7	No	0.56
14.64	C20H28O3	Cafestol	Terpenoids	316.43	Yes	0.55
5.50	C16H26O2	Clareolide	Terpenoids	250.38	Yes	0.55
3.76	C10H12O	Cuminaldehyde	Terpenoids	148.2	Yes	0.55
18.39	C15H24O5	Dihydroartemisinin	Terpenoids	284.35	Yes	0.55
8.56	C30H48O7	Dihydrocucurbitacin	Terpenoids	520.7	No	0.55
6.38	C20H24O9	Eurycomanone	Terpenoids	408.4	No	0.55
33.05	C15H28O7P2	Farnesyl pyrophosphate	Terpenoids	382.33	No	0.56
6.43	C30H52O4	Panaxtriol	Terpenoids	476.73	No	0.55

8.05	C15H20O3	Parthenolide	Terpenoids	248.32	Yes	0.55
14.13	C10H14O	Perillene	Terpenoids	150.22	Yes	0.55
7.13	C29H44O6	Polygalic acid	Terpenoids	488.66	No	0.56
7.59	C30H40O4	Pristimerin	Terpenoids	464.64	No	0.55
7.72	C22H28O5	Pyrethrin II	Terpenoids	372.45	Yes	0.55
57.04	C18H30O2	α -Eleostearic acid	Fatty acyls[FA]	278.43	Yes	0.85
