

Table S1. Analysis of the composition of BREE-Ea into the blood.

No.	RT/time	Ionisation mode	Measured	Theoretical	Molecular formula	Primary secondary ion fragments /MS ²	Compound
1	0.82	[M+H] ⁺	179.1067	179.1013	C ₁₀ H ₁₀ O ₃	147.0439,91.0548,179.1061,119.0855,161.0594	Coniferaldehyde
2	1.15	[M-H] ⁻	133.0132	133.0137	C ₄ H ₆ O ₅	115.0024,133.0132,71.0124,72.9917,89.0228	L-Malic acid
3	1.75	[M-H] ⁻	115.0752	115.0724	C ₄ H ₄ O ₄	71.0488,115.0748	Maleic acid
4	2.81	[M+H] ⁺	103.0546	103.0518	C ₅ H ₁₂ NO ⁺	102.1281,74.0971,58.0659,84.9602	Betaine aldehyde
5	4.18	[M-H] ⁻	128.0342	128.0348	C ₅ H ₇ NO ₃	128.0342	L-Pyroglutamic acid
6	4.89	[M+H] ⁺	139.0459	139.0458	C ₅ H ₄ N ₄ O	137.0457,138.0558	Allopurinol*
7	4.96	[M+H] ⁺	188.0706	188.0706	C ₁₁ H ₉ NO ₂	170.0598,188.0703,171.0631,189.0742	3-Indoleacrylic acid* N-
8	5.10	[M+H] ⁺	214.0894	214.0896	C ₁₀ H ₁₅ NO ₂ S	141.003,158.0268,142.0040,142.9946,159.0304	Butylbenzenesulfonamide*
9	5.41	[M+H] ⁺	178.0343	178.0360	C ₆ H ₁₁ NOS ₂	113.9644,119.0855	sulforaphane
10	5.43	[M-H] ⁻	178.1705	178.1700	C ₉ H ₉ NO ₃	134.0597,132.9707,77.0124	Hippuric acid*
11	5.59	[M-H] ⁻	179.054 2	179.0555	C ₉ H ₈ O ₄	179.0551,161.0429,151.0755,135.0439,103.9190	Caffeic acid
12	5.93	[M+H] ⁺	199.1615	199.1601	C ₉ H ₁₀ O ₅	140.6081,125.0236,97.1016,77.0392,95.0496	Syringic acid
13	6.06	[M-H] ⁻	153.0112	153.0188	C ₇ H ₆ O ₄	109.0281,153.0187,108.0193	3,4-Dihydroxybenzoic acid
14	7.05	[M+H] ⁺	233.1585	233.1524	C ₁₅ H ₂₀ O ₂	105.0339,115.0275,103.2808,129.0669,131.0686	Alantolactone
15	7.40	[M-H] ⁻	187.0018	187.0000	C ₉ H ₁₆ O ₄	125.0959,187.0973,97.0643,123.0801	Azelaic acid
16	7.43	[M+H] ⁺	130.0403	130.0425	C ₅ H ₇ NO ₃	130.05,113.9	D-Pyroglutamic acid
17	7.61	[M+H] ⁺	479.1190	479.1184	C ₂₂ H ₂₂ O ₁₂	318.0692,317.0658,302.0422,274.0457,153.0186,97.921,85.0291,69.0344,55.1870	Isorhamnetin 3-O-glucoside*

18	7.79	[M+H] ⁺	171.1290	171.1257	C ₇ H ₆ O ₅	171.1490,126.0	Gallic acid
19	7.81	[M-H] ⁻	489.1290	489.1250	C ₂₀ H ₂₆ O ₁₄	325.225,207.4384,192.0726	Bergenin glucoside
20	8.52	[M-H] ⁻	301.1116	301.1107	C ₁₆ H ₁₄ O ₆	286.0484,269.1815,191.6895,150.4503	3,3',4,4'-Tetrahydroxy-2-methoxychalcone
21	9.82	[M-H] ⁻	417.1191	417.1180	C ₂₁ H ₂₂ O ₉	417.2132,135.0739,119.0488	Isoglycoside
22	10.07	[M-H] ⁻	221.1026	221.1019	C ₁₂ H ₁₄ O ₄	77.0382,71.0488134.0364,147.0078	Monoisobutyl phthalic acid
23	10.51	[M+H] ⁺	355.0897	355.0867	C ₁₆ H ₁₈ O ₉	135.1166,163.1108,145.1012,117.0700	Chlorogenic acid
24	11.03	[M-H] ⁻	821.5965	821.5934	C ₄₂ H ₆₂ O ₁₆	821.5693,822.5854	Glycyrrhizin
25	11.08	[M+H] ⁺	318.2901	318.2998	C ₁₈ H ₃₉ NO ₃	318.2999,300.2898	2-Amino-1,3,4-octadecanetriol*
26	11.37	[M+H] ⁺	419.2601	419.2608	C ₂₆ H ₄₂ O ₄	71.0863,85.1017,57.0707,149.02229	Bis(3,5,5-trimethylhexyl)phthalate*
27	14.65	[M+H] ⁺	282.5179	282.5152	C ₁₈ H ₃₅ NO	282.2794,247.24,191.18,135.11	Oleamide*
28	14.66	[M+H] ⁺	415.3917	415.3934	C ₂₉ H ₅₀ O	57.0334,79.0005,119.0858,59.0449	β-sitosterol
29	14.75	[M+H] ⁺	329.2778	329.2714	C ₁₄ H ₁₆ O ₉	329.2478,233.1514,205.1226,159.1386,193.1223,191.1077,181.1277,177.1638,159.1171,133.1013	Bergenium
30	14.83	[M+H] ⁺	287.2862	287.2806	C ₁₆ H ₁₄ O ₅	170.1665,150.1325,121.1015,107.0860	Licorice chalcone B
31	14.83	[M+H] ⁺	329.2473	329.2475	C ₂₂ H ₃₂ O ₂	329.2472,311.2354,293.2254,269.2251	Docosahexaenoic Acid*
32	15.64	[M+H] ⁺	317.2674	317.2656	C ₁₆ H ₁₂ O ₇	317.2472,302.0421,285.2210,257.1900,275.2000	Isorhamnetin
33	16.25	[M+H] ⁺	271.2830	271.2819	C ₁₆ H ₁₄ O ₄	161.1336,137.1328,123.1127,109.1015	Medicarpin
34	16.25	[M+H] ⁺	271.2630	271.2638	C ₁₇ H ₃₄ O ₂	271.2629,103.0757,117.0910,83.0861,97.1015	Methyl palmitate*
35	16.45	[M+H] ⁺	271.2430	271.2461	C ₁₅ H ₁₀ O ₅	271.2630,215.4698,137.1334,253.1287	7,3',4'-

36	16.49	[M+H] ⁺	265.2125	265.2185	C ₁₃ H ₁₆ N ₂ O ₄	136.1202178.1658,160.0756,188.0370	Trihydroxyflavone Acetyl-N-formyl-5- methoxykynurenamine
37	17.15	[M-H] ⁻	137.0288	137.0239	C ₇ H ₆ O ₃	137.0288,136.0904	3,4- Dihydroxybenzaldehyde
38	18.22	[M-CH ₃] ⁻	687.5443	687.5434	C ₃₉ H ₇₉ N ₂ O ₆ P	687.5410,168.0421	Palmitoyl sphingomyelin*
39	18.70	[M+H] ⁺	158.0270	158.0270	C ₆ H ₇ NO ₂ S	141.0003,95.0495,105.0450	Benzenesulfonamide*
40	21.83	[M-H] ⁻	255.2337	255.2333	C ₁₆ H ₃₂ O ₂	255.2324,203.8189	Palmitic Acid*
41	27.36	[M+H] ⁺	195.1800	195.1810	C ₁₀ H ₁₀ O ₄	195.008,193.12,178.16,149.13, 135.11	Ferulic acid
42	30.72	[M-H] ⁻	141.0004	141.0000	C ₆ H ₆ O ₄	59.2349	cis,cis-Muconic acid

* represents entry into the blood as metabolites.

Table S2. Analysis of the composition of BREE-Ea into the brain.

No.	RT/Ti me	Ionisation mode	Measured	Theoretical	Molecular formula	Primary secondary ion fragments /MS ²	Compound
1	1.75	[M-H]-	115.0752	115.0724	C ₄ H ₄ O ₄	71.0488,115.0748	Maleic acid [#]
2	4.96	[M+H] ⁺	188.0706	188.0706	C ₁₁ H ₉ NO ₂	170.0598,188.0703,171.0631,189.0742	3-Indoleacrylic acid [#]
3	5.41	[M+H] ⁺	178.0343	178.0360	C ₆ H ₁₁ NOS ₂	113.9644,119.0855	sulforaphane
4	5.43	[M-H]-	178.1705	178.1700	C ₉ H ₉ NO ₃	134.0597,132.9707,77.0124	Hippuric acid
5	5.93	[M+H] ⁺	199.1615	199.1601	C ₉ H ₁₀ O ₅	140.6081,125.0236,97.1016,77.0392,95.0496	Syringic acid
6	7.40	[M-H]-	187.0018	187.0000	C ₉ H ₁₆ O ₄	125.0959,187.0973,97.0643,123.0801	Azelaic acid [#]
7	7.43	[M+H] ⁺	130.0403	130.0425	C ₅ H ₇ NO ₃	130.05,113.9	D-Pyroglutamic acid
8	7.61	[M+H] ⁺	479.1190	479.1184	C ₂₂ H ₂₂ O ₁₂	318.0692,317.0658,302.0422,274.0457,153.018 6,97.921,85.0291,69.034455.1870	Isorhamnetin 3-O- glucoside
9	7.79	[M+H] ⁺	171.1290	171.1257	C ₇ H ₆ O ₅	171.1490,126.0	Gallic acid
10	10.51	[M+H] ⁺	355.0897	355.0867	C ₁₆ H ₁₈ O ₉	135.1166,163.1108 145.1012,117.0700	Chlorogenic acid [#]
11	11.08	[M+H] ⁺	318.2901	318.2998	C ₁₈ H ₃₉ NO ₃	318.2999,300.2898	2-Amino-1,3,4- octadecanetriol [#]
12	14.65	[M+H] ⁺	282.5179	282.5152	C ₁₈ H ₃₅ NO	282.2794,247.24,191.18,135.11	Oleamide
13	14.66	[M+H] ⁺	415.3917	415.3934	C ₂₉ H ₅₀ O	57.0334,79.0005,119.0858,59.0449 329.2478,233.1514,205.1226,159.1386	β-sitosterol
14	14.75	[M+H] ⁺	329.2778	329.2714	C ₁₄ H ₁₆ O ₉	193.1223,191.1077,181.1277,177.1638,159.117 1,133.1013	Bergeninum
15	14.83	[M+H] ⁺	329.2473	329.2475	C ₂₂ H ₃₂ O ₂	329.2472,311.2354,293.2254,269.2251	Docosahexaenoic Acid [#]
16	15.64	[M+H] ⁺	317.2674	317.2656	C ₁₆ H ₁₂ O ₇	317.2472,302.0421,285.2210,257.1900,275.200 0	Isorhamnetin [#]
17	16.25	[M+H] ⁺	271.2630	271.2638	C ₁₇ H ₃₄ O ₂	271.2629,103.0757 , 117.0910,83.0861,97.1015	Methyl palmitate [#]

18	18.70	[M+H] ⁺	158.0270	158.0270	C ₆ H ₇ NO ₂ S	141.0003,95.0495,105.0450	Benzene sulfonamide [#]
19	27.36	[M+H] ⁺	195.1800	195.1810	C ₁₀ H ₁₀ O ₄	195.008,193.12,178.16,149.13,135.11	Ferulic acid

[#] indicates that the substance was able to enter the brain through the blood-brain barrier in AD mice (Compared with the blank group).

Table S3. Summary of biomarkers of model group versus BREE-Ea group.

No.	Compound	RT/time	m/z	Type	Formula	Change
1	6-Aminonicotinic acid	139.0499	173.3	POS	C ₆ H ₆ N ₂ O ₂	↑
2	Nicotinamide	121.0405	28.2	NEG	C ₆ H ₆ N ₂ O	↑
3	4-Guanidinobutyric acid	146.0921	214.5	POS	C ₅ H ₁₁ N ₃ O ₂	↑
4	Taurine	124.007	179.8	NEG	C ₂ H ₇ NO ₃ S	↑
5	N-Acetylneuraminic acid	308.0979	215.8	NEG	C ₁₁ H ₁₉ NO ₉	↑
6	3-Hydroxy-3-methylglutaric acid	161.045	213.7	NEG	C ₆ H ₁₀ O ₅	↑
7	beta-Guanidinopropionic acid	130.0619	208.4	NEG	C ₄ H ₉ N ₃ O ₂	↑
8	Hexaethylene glycol	283.1748	31.2	POS	C ₁₂ H ₂₆ O ₇	↓
9	Creatine	130.0619	208.4	NEG	C ₄ H ₉ N ₃ O ₂	↑
10	Thiamine monophosphate	345.0775	287.9	POS	C ₁₂ H ₁₇ N ₄ O ₄ PS	↑
11	Glycerophosphoethanolamine	216.0623	232.5	POS	C ₅ H ₁₄ NO ₆ P	↑
12	Glycerophosphocholine	258.1088	229.9	POS	C ₈ H ₂₀ NO ₆ P	↑
13	Homoserine	118.0505	209.9	NEG	C ₄ H ₉ NO ₃	↑
14	N,N-Diethyl-2-aminoethanol	100.1118	141	POS	C ₆ H ₁₅ NO	↑
15	Urocanic acid	139.0499	173.3	POS	C ₆ H ₆ N ₂ O ₂	↑
16	Prostaglandin D2 (PGD2)	351.2161	36.8	NEG	C ₂₀ H ₃₂ O ₅	↑
17	SM(d18:1/17:0)	715.5744	114.3	NEG	C ₄₀ H ₈₁ N ₂ O ₆ P	↑
18	2'-Deoxyuridine	227.067	42.1	NEG	C ₉ H ₁₂ N ₂ O ₅	↑
19	PC(16:0/16:0)	734.5646	18.5	POS	C ₄₀ H ₈₀ NO ₈ P	↑
20	2-Pyrimidinylacetic acid	139.0499	173.3	POS	C ₆ H ₆ N ₂ O ₂	↑
21	Acetylcarnitine (Car(2:0))	204.122	187.7	POS	C ₉ H ₁₇ NO ₄	↑
22	N-Acetylglucosamine 1-phosphate	300.0488	256.7	NEG	C ₈ H ₁₆ NO ₉ P	↑
23	3-AMINO-2-PIPERIDONE	115.0862	122.5	POS	C ₅ H ₁₀ N ₂ O	↑
24	Prostaglandin E2 (PGE2)	351.2161	36.8	NEG	C ₂₀ H ₃₂ O ₅	↑
25	2-Hydroxyethanesulfonic acid	124.991	92.5	NEG	C ₂ H ₆ O ₄ S	↑
26	Lauramine oxide	230.2469	55.9	POS	C ₁₄ H ₃₁ NO	↑
27	PC(18:0/14:0)	734.5673	103.3	POS	C ₄₀ H ₈₀ NO ₈ P	↑
28	Butyllactate	145.0868	36.4	NEG	C ₇ H ₁₄ O ₃	↑
29	2-Aminonicotinic acid	139.0499	173.3	POS	C ₆ H ₆ N ₂ O ₂	↑

30	15-keto-Prostaglandin_E2	349.2019	17.4	NEG	C ₂₀ H ₃₀ O ₅	↑
31	3-(2-Oxocyclohexyl)propanoic acid	169.0868	201.3	NEG	C ₉ H ₁₄ O ₃	↑
32	Tetraethylammonium cation	130.1587	65.4	POS	C ₈ H ₂₀ N	↑
33	8-Oxononanoic acid	171.1023	53.6	NEG	C ₉ H ₁₆ O ₃	↑
34	Artemoin_C	551.503	25.2	POS	C ₃₅ H ₆₆ O ₄	↑
35	Flavonol base + 4O, 1MeO	331.0446	179.8	NEG	C ₂₈ H ₃₂ O ₁₈	↑
36	n-Dodecylamine	186.221	60	POS	C ₁₂ H ₂₇ N	↑
37	(-)-Jasmonic_acid	209.1177	30	NEG	C ₁₂ H ₁₈ O ₃	↑
38	L-Isoserine	104.035	228.9	NEG	C ₃ H ₇ NO ₃	↑
39	Succinic semialdehyde	101.0242	212.1	NEG	C ₄ H ₆ O ₃	↑
40	Methyl 5-methylnicotinate	152.0701	157	POS	C ₈ H ₉ NO ₂	↓
41	D-Ribose	149.045	100.1	NEG	C ₅ H ₁₀ O ₅	↑
42	5(S),14(R)-Lipoxin_B4	375.2149	46.5	POS	C ₂₀ H ₃₂ O ₅	↑
43	Decenediethylcarnitine	326.1959	159.7	POS	C ₁₇ H ₂₉ NO ₆	↑
44	1-Methyl-2-imidazolidinethione	117.0476	169.2	POS	C ₄ H ₈ N ₂ S	↓
45	2-Amino-1-(4-aminophenyl)-1H-pyrrolo[2,3-b]quinoxaline-3-carbonitrile	301.1203	113.8	POS	C ₁₇ H ₁₂ N ₆	↑
46	2-Amino-6-(methylsulfanyl)-3,5-pyridinedicarbonitrile	191.0395	220	POS	C ₈ H ₆ N ₄ S	↑
47	2-(Benzylamino)-5,6,7,8-tetrahydro[1]benzothien[2,3-d]pyrimidin-4(3H)-one	312.1153	162.8	POS	C ₁₇ H ₁₇ N ₃ OS	↑
48	LPC(32:0)	720.5865	38.5	POS	C ₄₀ H ₈₂ NO ₇ P	↑
49	Cyclocytidine	226.0833	231.3	POS	C ₉ H ₁₁ N ₃ O ₄	↑
50	4-Hydroxy-4'-chlorobiphenyl	203.0281	214.2	NEG	C ₁₂ H ₉ ClO	↑
51	Diethyl 2-((3-((3-ethoxy-2-(ethoxycarbonyl)-3-oxo-1-propenyl)amino)anilino)methylene)malonate	244.0824	116.3	NEG	C ₁₀ H ₁₅ NO ₆	↑

52	Hematoxylin	301.0699	115.5	NEG	C ₁₆ H ₁₄ O ₆	↑
53	Dehydro-L-(+)-ascorbic acid dimer	347.0241	26.9	NEG	C ₁₂ H ₁₂ O ₁₂	↓
54	5-Nitro-N-(3- pyridinylmethyl)-2- furamide	248.0647	230.6	POS	C ₁₁ H ₉ N ₃ O ₄	↑
55	PC(33:1)	746.5638	104.5	POS	C ₄₁ H ₈₀ NO ₈ P	↑
56	3-Hydroxyglutaric_acid	147.0296	207.7	NEG	C ₅ H ₈ O ₅	↑
57	Tanshinone I	277.0882	194.1	POS	C ₁₈ H ₁₂ O ₃	↑
58	1-Phenyl-3- (trifluoromethyl)-1H- pyrazol-5-ol	229.0602	111.8	POS	C ₁₀ H ₇ F ₃ N ₂ O	↓
59	Artocarpin	437.1925	17.2	POS	C ₂₆ H ₂₈ O ₆	↑
60	2,4-Bis(2- acetoxymethyl)benz oic acid	298.0695	115	NEG	C ₁₆ H ₁₃ NO ₅	↑
61	4-(1H-Benzimidazol-2- yl)-1,2,5-oxadiazol-3- ylamine	202.0705	217.3	POS	C ₉ H ₇ N ₅ O	↑
62	4-Hydroxynonenal glutathione	464.2055	199.7	POS	C ₁₉ H ₃₃ N ₃ O ₈ S	↑
63	7-Amino-2- methylpyrazolo[1,5- a]pyrimidine-6- carbonitrile	174.0757	159.8	POS	C ₈ H ₇ N ₅	↑
64	8-Geranyl-7- hydroxycoumarin	297.1525	14.8	NEG	C ₁₉ H ₂₂ O ₃	↓
65	Haplamine	258.115	36.1	POS	C ₁₅ H ₁₅ NO ₃	↓
66	S- Acetyldihydrolipoamide- E	250.093	35.7	POS	C ₁₀ H ₁₉ NO ₂ S ₂	↓
67	Tolmetin	258.1096	245.7	POS	C ₁₅ H ₁₅ NO ₃	↑
68	5-[(2- Phenylethyl)amino]- 1,3,4-thiadiazole-2(3H)- thione	238.0446	232	POS	C ₁₀ H ₁₁ N ₃ S ₂	↑
69	3-Hydroxy-4- iodobenzonitrile	245.9439	208.3	POS	C ₇ H ₄ INO	↑
70	5-Amino-1-(2- pyridinyl)-1H-pyrazole- 4-carbonitrile	186.0754	182.7	POS	C ₉ H ₇ N ₅	↑
71	.alpha.- Naphthoflavanone	275.1053	131.5	POS	C ₁₉ H ₁₄ O ₂	↑
72	Thieno[3,2-b]pyridin-7-	152.0217	208.3	POS	C ₇ H ₅ NOS	↑

	ol					
73	2'-Chloro-2-hydroxy-5-methylbenzophenone	245.0421	203.2	NEG	C ₁₄ H ₁₁ ClO ₂	↑
74	(E)-2-Phenylethanesulfonic acid	183.0153	57	NEG	C ₈ H ₈ O ₃ S	↑
75	4-Chloro-5,6,7,8-tetrahydroquinazolin-2-amine	184.0599	22.9	POS	C ₈ H ₁₀ ClN ₃	↓
76	N,N'-Diphenyl-p-phenylenediamine	261.1435	238.3	POS	C ₁₈ H ₁₆ N ₂	↑
77	4-(1H-Indol-3-yl)-1,3-thiazol-2-ylamine	214.0483	232.3	NEG	C ₁₁ H ₉ N ₃ S	↑
78	Triamifos	295.1393	195.6	POS	C ₁₂ H ₁₉ N ₆ OP	↑
79	Trifluoroperazine	408.177	161.7	POS	C ₂₁ H ₂₄ F ₃ N ₃ S	↑
80	Naphtho[2,3-b]furan-2(4H)-one, 4a,5,6,7,8,8a,9,9a-octahydro-3,8a-dimethyl-5-methylene-	233.1486	273.1	POS	C ₁₅ H ₂₀ O ₂	↑
81	2-Amino-1-(4-chlorophenyl)ethanone	170.0321	208.3	POS	C ₈ H ₈ ClNO	↑
82	Maslinic_acid_3-O-b-D-glucoside	635.4115	206.4	POS	C ₃₆ H ₅₈ O ₉	↑
83	Fenoxaprop	334.0525	287.2	POS	C ₁₆ H ₁₂ ClNO ₅	↑
84	N-Acetylsulfamethoxazole	296.0653	230.6	POS	C ₁₂ H ₁₃ N ₃ O ₄ S	↑
85	PA(20:4(5Z,8Z,11Z,14Z)/18:0)	725.5175	29.1	POS	C ₄₁ H ₇₃ O ₈ P	↓
86	PC(18:3(9Z,12Z,15Z)/16:0) (2S,4S,6S)-2-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]tetrahydro-6-(4,5-dihydroxy-3-methoxyphenyl)-2H-pyran-4-ol	756.5471	19.5	POS	C ₄₂ H ₇₈ NO ₈ P	↑
87	9(Z),11(E)-Conjugated_Linoleic_Acid	391.1733	153.5	POS	C ₂₁ H ₂₆ O ₇	↑
88	3b-Hydroxy-6b-(3-chloro-2-hydroxy-2-methylbutanoyloxy)-	279.2318	19.3	NEG	C ₁₈ H ₃₂ O ₂	↑
89		401.1726	121.3	POS	C ₂₀ H ₂₉ ClO ₆	↑

	7(11)-eremophilen- 12,8b-olide					
90	3,5-Dichlorotyrosine	247.9894	275.9	NEG	C ₉ H ₉ Cl ₂ NO ₃	↑
91	His-His	291.1207	30.6	NEG	C ₁₂ H ₁₆ N ₆ O ₃	↑
92	2-Hydroxy-2-(2-methoxy-2-oxoethyl)butanedioic acid	205.0348	26.7	NEG	C ₇ H ₁₀ O ₇	↓
93	2-Acetylthiazole	128.0174	180.1	POS	C ₅ H ₅ NOS	↑
94	Quercetin_3-beta-D-glucoside	918.0544	179.8	NEG	C ₂₁ H ₂₀ O ₁₂	↓
95	Daidzein	251.0358	180.1	POS	C ₁₅ H ₁₀ O ₄	↑
96	Daucic_acid	205.0335	99.7	POS	C ₇ H ₈ O ₇	↑
97	Met-Asn	262.0926	116.1	NEG	C ₉ H ₁₇ N ₃ O ₄ S	↑
98	Benzenesulfonic acid	156.9905	207.7	NEG	C ₆ H ₆ O ₃ S	↑
99	4-Chloro-5,6-dimethyl-2-[(4-methylpiperidin-1-yl)methyl]thieno[2,3-d]pyrimidine	310.1123	215.9	POS	C ₁₅ H ₂₀ ClN ₃ S	↑
100	Lorazepam glucuronide	495.0407	208.6	NEG	C ₂₁ H ₁₈ Cl ₂ N ₂ O ₈	↑
101	Naphthalene_epoxide	143.0478	180.1	POS	C ₁₀ H ₈ O	↑
102	2-[4-(Hydroxycarbamoyl)phenyl]-N-(2-hydroxyethyl)-N-phenylacetamide	315.1359	107.7	POS	C ₁₇ H ₁₈ N ₂ O ₄	↑
103	2-Chloro-3-oxo-N-phenylbutanamide	212.0423	249.6	POS	C ₁₀ H ₁₀ ClNO ₂	↑
104	N-Cyclopropyl-N'-(3,4-dichlorophenyl)urea	245.0262	100.9	POS	C ₁₀ H ₁₀ Cl ₂ N ₂ O	↑
105	Pipltartine	316.1155	230.2	NEG	C ₁₇ H ₁₉ NO ₅	↑
106	3-[(Methylsulfonyl)amino]-2-thiophenecarboxylic acid	219.9768	173.7	NEG	C ₆ H ₇ NO ₄ S ₂	↓
107	2-Methylthiophene-3-carbaldehyde	127.025	180.1	POS	C ₆ H ₆ OS	↑
108	2-Phenyl-1,3-benzoxazole-5-carboxylic acid	240.0706	99.6	POS	C ₁₄ H ₉ NO ₃	↑
109	Nylidrin	300.2011	30.7	POS	C ₁₉ H ₂₅ NO ₂	↓
110	CARBADOX	263.0732	183.5	POS	C ₁₁ H ₁₀ N ₄ O ₄	↑
111	19-Aldoandrost-4-ene-3,17-dione	301.1748	143	POS	C ₁₉ H ₂₄ O ₃	↑

112	2'-Cyano[1,1'-biphenyl]- 2-carboxylic acid	224.0756	27.9	POS	C ₁₄ H ₉ NO ₂	↓
113	4- Methylthioamphetamine	182.1029	82.8	POS	C ₁₀ H ₁₅ NS	↑
114	6-Fluoro-4-oxo-1- propyl-1,4-dihydro-3- quinolinecarboxylic acid	248.0786	35.6	NEG	C ₁₃ H ₁₂ FNO ₃	↓
115	phellopterin	339.0573	208.4	POS	C ₁₇ H ₁₆ O ₅	↑
116	Carboxymethyloxysucci nate	191.0194	208.4	NEG	C ₆ H ₈ O ₇	↑
117	5-Guanidino-2- oxopentanoate	174.0869	215.9	POS	C ₆ H ₁₀ N ₃ O ₃ ⁻	↓
118	Styrene	141.0165	52.5	NEG	C ₈ H ₈	↑
119	Nopaline	341.0825	176.4	NEG	C ₁₁ H ₂₀ N ₄ O ₆	↓
120	6-Deoxy-5-ketofructose 1-phosphate	260.0525	269.4	POS	C ₆ H ₁₁ O ₈ P	↑
121	Glyceraldehyde	71.0137	128.7	NEG	C ₃ H ₆ O ₃	↑

Table S4. BREE-Ea Active Ingredients

No.	Compound	Formula	CAS	RT	M/Z	Type
1	1-Cyano-2-hydroxy-3-butene	C ₄ H ₅ NO	7451-85-6	12.44	98.06	POS
2	2-Hydroxyadipic acid	C ₆ H ₁₀ O ₅	18294-85-4	30.36	161.05	NEG
3	(-)-3-Cyanomethyl-3-hydroxy-1H-indol-2(3H)-one	C ₁₀ H ₈ N ₂ O ₂	137761-24-1	38.18	189.07	POS
4	sn-Glycerol3-phosphate	C ₃ H ₇ O ₆ P	17989-41-2	40.62	173.02	POS
5	L-Cysteic acid	C ₃ H ₅ NO ₄ S	498-40-8	41.13	168	NEG
6	Dehydrochorismic acid	C ₁₇ H ₁₅ NO ₄	81757-66-6	41.21	225.04	POS
7	L-Threonic acid	C ₄ H ₆ O ₅	7306-96-9	43.39	135.03	NEG
8	7-Methylxanthine	C ₅ H ₆ N ₄ O	552-62-5	43.39	165.04	NEG
9	Glyceric acid	C ₃ H ₄ O ₄	473-81-4	44.11	105.02	NEG
10	Graveoline	C ₁₇ H ₁₇ NO ₂	485-61-0	44.57	280.09	POS
11	4-Aminobutyric acid	C ₄ H ₉ NO ₂	1956/12/2	45.28	104.07	POS
12	Glycerophosphocholine	C ₅ H ₁₂ NO ₆ P	28319-77-9	45.29	258.11	POS
13	L-Asparagine	C ₄ H ₈ N ₂ O ₃	70-47-3	45.46	133.06	POS
14	D-Glutamine	C ₅ H ₁₀ N ₂ O ₃	5959-95-5	45.64	147.08	POS
15	L-Threonine	C ₄ H ₉ NO ₃	72-19-5	46	120.07	POS
16	2-Oxovaleric acid	C ₅ H ₈ O ₃	1821-02-9	46	117.05	POS
17	D-(+)-Allose	C ₆ H ₁₂ O ₆	2595-97-3	46.92	239.08	NEG
18	D-Tagatose	C ₆ H ₁₂ O ₆	87-81-0	46.92	163.06	POS
19	2-Furancarboxaldehyde	C ₅ H ₄ O ₂	1998/1/1	46.92	97.03	POS
20	2-Furanmethanol	C ₅ H ₆ O ₂	98-00-0	46.92	99.04	POS
21	D-Arabinose	C ₅ H ₁₀ O ₅	147-81-9	47.95	149.05	NEG
22	1,2,3-Trihydroxybenzene	C ₆ H ₆ O ₃	87-66-1	47.95	125.02	NEG
23	Alpha-D-Glucose	C ₆ H ₁₂ O ₆	492-62-6	47.98	179.06	NEG
24	Citric acid	C ₆ H ₈ O ₇	77-92-9	48.23	191.02	NEG

25	Norvaline	$C_5H_{11}NO_2$	760-78-1	48.86	118.09	POS
26	D-Proline	$C_5H_9NO_2$	344-25-2	48.93	116.07	POS
27	Choline	$C_5H_{14}NO^+$	62-49-7	48.95	104.11	POS
28	2-Ketobutyric acid	$C_4H_6O_3$	600-18-0	49.47	101.02	NEG
29	Ascorbic acid	$C_6H_8O_6$	50-81-7	49.92	175.02	NEG
30	L-Arginine	$C_6H_{14}N_4O_2$	74-79-3	50.58	175.12	POS
31	Sucrose	$C_{12}H_{22}O_{11}$	57-50-1	50.96	341.11	NEG
32	Pyrrolidine	C_4H_9N	123-75-1	51.86	72.08	POS
33	Mesaconic acid	$C_5H_6O_4$	498-24-8	52.14	129.02	NEG
34	Nigelllic acid	$C_{18}H_{30}O_2$	91897-25-5	52.44	281.14	POS
35	L-Valine	$C_5H_{11}NO_2$	72-18-4	52.96	116.07	NEG
36	Gallic acid	$C_7H_6O_5$	149-91-7	54.45	169.02	NEG
37	Murrayacine	$C_{11}H_{15}NO_3$	27300-29-4	63.52	278.12	POS
38	Trehalose	$C_{12}H_{22}O_{11}$	99-20-7	67.23	401.13	NEG
39	Isonicotinic acid	$C_6H_5NO_2$	55-22-1	77.31	122.02	NEG
40	D-Glucose	$C_6H_{12}O_6$	50-99-7	81.59	179.06	NEG
41	D-Xylose	$C_5H_{10}O_5$	58-86-6	84.77	149.05	NEG
42	L-Tyrosine	$C_9H_{11}NO_3$	60-18-4	86.14	180.07	NEG
43	D-2-Amino-4-methylpentanoic acid	$C_6H_{13}NO_2$	328-38-1	86.71	132.1	POS
44	L-Leucine	$C_6H_{13}NO_2$	61-90-5	86.94	130.09	NEG
45	Guanine	$C_5H_5N_5O$	73-40-5	91.03	152.06	POS
46	p-Aminobenzoic acid	$C_7H_7NO_2$	150-13-0	94.99	138.05	POS
47	Phenylacetic acid	$C_8H_8O_2$	103-82-2	95.66	135.05	NEG
48	Quinic acid	$C_7H_{12}O_6$	77-95-2	99.6	191.06	NEG
49	Uridine	$C_9H_{12}N_2O_6$	58-96-8	110.55	243.06	NEG
50	Galactinol	$C_7H_{12}O_6$	3687-64-7	112.88	401.12	NEG

51	Citraconic acid	C ₅ H ₆ O ₄	498-23-7	115.22	129.02	NEG
52	Nor-psi-tropine	C ₉ H ₁₅ NO	501-33-7	133.91	128.11	POS
53	2,3-Dihydroxybenzoic acid	C ₇ H ₆ O ₄	303-38-8	136.79	153.02	NEG
54	Succinic acid	C ₄ H ₆ O ₄	110-15-6	139.04	119.03	POS
55	Pyridoxine	C ₈ H ₁₁ NO ₃	65-23-6	140.62	170.08	POS
56	L-Ascorbic acid	C ₆ H ₈ O ₆	50-81-7	141.91	175.02	NEG
57	L-Isoleucine	C ₆ H ₁₃ NO ₂	73-32-5	146.05	132.1	POS
58	4-Aminophenol	C ₆ H ₇ NO	123-30-8	153.95	110.06	POS
59	Dehydroascorbic acid	C ₆ H ₆ O ₆	490-83-5	154.15	173.01	NEG
60	3-Hydroxyphenylacetic acid	C ₈ H ₈ O ₃	621-37-4	156.53	151.04	NEG
61	Methylmalonic acid	C ₅ H ₈ O ₄	516-05-2	158.42	117.02	NEG
62	Piperidine	C ₅ H ₁₁ N	110-89-4	158.69	86.1	POS
63	Cyclohexylamine	C ₆ H ₁₃ N	108-91-8	167.36	100.11	POS
64	Oleoside dimethyl ester	C ₂₀ H ₃₀ O ₁₀	30164-95-5	170.46	419.15	POS
65	L-Phenylalanine	C ₉ H ₁₁ NO ₂	63-91-2	170.57	166.09	POS
66	N-Ethylacetamide	C ₄ H ₉ NO	625-50-3	170.74	88.08	POS
67	5,7-Dihydroxy-6-methoxyflavone 5-rhamnoside	C ₂₇ H ₃₂ O ₁₆	163350-29-6	171.63	431.13	POS
68	Pyrrole-2-carboxylic acid	C ₅ H ₅ NO ₂	634-97-9	172.28	110.02	NEG
69	Phloretic acid	C ₉ H ₁₀ O ₃	501-97-3	175.01	165.06	NEG
70	(2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal	C ₁₀ H ₁₀ O ₃	20649-42-7	176.08	179.07	POS
71	1-Methylguanine	C ₆ H ₇ N ₅ O	938-85-2	180.1	164.06	NEG
72	2-Pyrrolidinone	C ₄ H ₇ NO	616-45-5	180.89	86.06	POS
73	Glyoxylic acid	C ₂ H ₂ O ₃	298-12-4	180.91	72.99	NEG
74	2-Hydroxycinnamic acid	C ₉ H ₈ O ₃	583-17-5	186.73	209.05	NEG
75	Hydroxyphenylacetyl glycine	C ₁₀ H ₁₁ NO ₄	28116-23-6	187.49	210.07	POS
76	Nicotinamide	C ₆ H ₆ N ₂ O	98-92-0	188.34	123.06	POS

77	Vanillin	C ₈ H ₈ O ₃	121-33-5	190.36	151.04	NEG
78	Vanillic acid	C ₈ H ₈ O ₅	121-34-6	190.75	167.03	NEG
79	DL-Dopa	C ₉ H ₁₁ NO ₄	63-84-3	193.47	196.06	NEG
80	7-Hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-carboxylic acid 7-glucoside	C ₁₅ H ₁₈ O ₉	127615-74-1	196.81	383.09	POS
81	D-Pantothenic acid	C ₉ H ₁₇ NO ₅	79-83-4	196.89	220.12	POS
82	2-Pyrrolidineacetic acid	C ₇ H ₁₁ NO ₃	56879-46-0	198.77	130.09	POS
83	Sarmentosin	C ₇ H ₈ O ₄	71933-54-5	199.3	276.11	POS
84	Methylgallate	C ₈ H ₈ O ₅	99-24-1	210.02	183.03	NEG
85	4-Acetylbutyrate	C ₆ H ₈ O ₄	3128/6/1	210.4	131.07	POS
86	Adenosine	C ₁₀ H ₁₃ N ₅ O ₄	58-61-7	211.31	266.09	NEG
87	Salicylic acid beta-D-glucoside	C ₇ H ₈ O ₆	10366-91-3	211.6	301.09	POS
88	trans-Zeatin-riboside	C ₁₀ H ₁₄ N ₅ O ₅	6025-53-2	211.6	352.16	POS
89	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	327-97-9	211.71	353.09	NEG
90	4-Hydroxybenzoic acid	C ₇ H ₆ O ₃	99-96-7	212.74	137.02	NEG
91	Syringic acid	C ₉ H ₁₀ O ₅	530-57-4	213.8	197.04	NEG
92	Maltol	C ₆ H ₈ O ₃	118-71-8	214.65	127.04	POS
93	2-Methyltetrahydrofuran-3-one	C ₆ H ₈ O ₂	3188-00-9	215.16	101.06	POS
94	Asparaginylnl-Tryptophan	C ₁₂ H ₁₄ N ₂ O ₃	74105-03-6	216.14	319.14	POS
95	3,4-Dihydroxyphenylglycol	C ₈ H ₁₁ NO ₃	28822-73-3	219.63	169.05	NEG
96	N-(3-Methylbut-2-EN-1-YL)-9H-purin-6-amine	C ₁₀ H ₁₂ N ₆	2365-40-4	220.28	202.11	NEG
97	1,4-Dimethyl-7-ethylazulene	C ₁₅ H ₁₈	529-05-5	225.53	185.13	POS
98	Glucotropaeolin	C ₁₄ H ₁₉ NO ₉ S ₂	499-26-3	225.65	408.04	NEG
99	DL-Tryptophan	C ₁₁ H ₁₂ N ₂ O ₂	1954/12/6	225.72	205.1	POS
100	L-Tryptophan	C ₁₁ H ₁₂ N ₂ O ₂	73-22-3	226.38	203.08	NEG
101	Caffeic acid	C ₉ H ₈ O ₄	331-39-5	229.07	179.03	NEG

102	p-Toluenesulfonic acid	C ₇ H ₈ O ₃ S	104-15-4	231.49	171.01	NEG
103	N-Methylcalystegine Cl	C ₁₆ H ₂₃ NO ₆	197449-07-3	232.52	206.1	POS
104	p-Octopamine	C ₈ H ₁₁ NO ₂	104-14-3	232.63	154.09	POS
105	4-Coumaroyl-2-hydroxyputrescine	C ₁₃ H ₁₈ N ₂ O ₃	24177-22-8	232.68	251.14	POS
106	2-Acetyl-3,6-dimethylpyrazine	C ₈ H ₁₀ N ₂ O	54300-09-3	232.69	151.09	POS
107	Xanthurenic acid	C ₁₃ H ₁₀ N ₂ O ₄	59-00-7	232.75	206.05	POS
108	Niacinamide	C ₆ H ₆ N ₂ O	98-92-0	236.92	123.06	POS
109	Methionyl-Arginine	C ₁₃ H ₂₂ N ₄ O ₃	60461-10-1	239.72	306.15	POS
110	Salsolinol	C ₁₀ H ₁₃ NO ₂	27740-96-1	240.24	178.09	NEG
111	L-Malic acid	C ₄ H ₆ O ₅	97-67-6	240.33	133.01	NEG
112	Phenyllactic acid	C ₉ H ₁₀ O ₃	828-01-3	241.95	165.06	NEG
113	Isoquinoline	C ₉ H ₇ N	119-65-3	243.07	130.07	POS
114	Isovanillic acid	C ₈ H ₈ O ₄	645-08-9	243.34	167.03	NEG
115	Phenylethylamine	C ₈ H ₁₁ N	64-04-0	243.5	122.1	POS
116	3-Hydroxycinnamic acid	C ₉ H ₈ O ₃	588-30-7	244.52	163.04	NEG
117	Paeonoside	C ₂₃ H ₂₈ O ₁₁	25615-14-9	244.83	327.11	NEG
118	Cadalene	C ₁₅ H ₂₄	483-78-3	245.55	199.14	POS
119	(-)-Gallocatechin	C ₁₅ H ₁₄ O ₇	3371-27-5	247.26	305.07	NEG
120	N-Acetyl-L-phenylalanine	C ₁₁ H ₁₃ NO ₃	2018-61-3	248.63	206.08	NEG
121	Sweroside	C ₁₆ H ₂₂ O ₉	14215-86-2	253.42	357.12	NEG
122	Palmitone	C ₁₆ H ₃₂ O	502-73-8	254.56	352.14	POS
123	Cyanidin 3-gentiobioside	C ₂₇ H ₃₁ O ₁₅ Cl	58285-26-0	255.28	611.16	POS
124	6-Hydroxy-1H-indole-3-acetamide	C ₁₀ H ₁₀ N ₂ O ₂	192184-73-9	255.96	191.08	POS
125	3-O-Feruloylquinic acid	C ₁₇ H ₂₀ O ₈	62929-69-5	255.97	367.1	NEG
126	Glyceraldehyde	C ₃ H ₆ O ₃	56-82-6	259.43	89.02	NEG
127	4-Methylbenzoic acid	C ₈ H ₈ O ₂	99-94-5	259.76	135.05	NEG

128	3,4-Dihydroxybenzaldehyde	C ₇ H ₆ O ₃	139-85-5	259.98	137.02	NEG
129	4-Hydroxy-3-methylbenzoic acid	C ₈ H ₈ O ₃	499-76-3	260.17	151.04	NEG
130	Aucubin	C ₁₅ H ₂₂ O ₉	479-98-1	260.53	405.14	NEG
131	5'-Methylthioadenosine	C ₁₁ H ₁₅ N ₅ O ₃ S	2457-80-9	260.55	296.08	NEG
132	Adenine	C ₅ H ₅ N ₅	73-24-5	260.55	134.05	NEG
133	4,5-Di-O-caffeoylquinic acid	C ₂₅ H ₂₄ O ₁₂	57378-72-0	260.55	515.12	NEG
134	Tropic acid	C ₉ H ₁₀ O ₃	529-64-6	262.43	165.06	NEG
135	Scoparone	C ₁₁ H ₁₀ O ₄	120-08-1	266.41	207.07	POS
136	trans-Ferulic acid	C ₁₀ H ₁₀ O ₄	537-98-4	266.41	195.07	POS
137	Sinapic acid	C ₉ H ₁₀ O ₂	530-59-6	268.24	223.06	NEG
138	2-Methoxy-4-vinylphenol	C ₁₀ H ₁₀ O ₄	7786-61-0	268.81	149.06	NEG
139	Isoferulic acid	C ₁₂ H ₁₃ NO ₂	537-73-5	269.17	193.05	NEG
140	Indole-3-butyric acid	C ₂₅ H ₃₀ O ₁₃	133-32-4	270.5	248.09	NEG
141	Citroside A	C ₁₀ H ₉ NO ₃	120330-44-1	271.55	387.2	POS
142	5-Hydroxyindoleacetate	C ₄ H ₄ O ₃	54-16-0	272.55	190.05	NEG
143	Succinic anhydride	C ₆ H ₁₀ O ₆	108-30-5	272.87	99.01	NEG
144	L-Gulonolactone	C ₉ H ₆ O ₄	1128-23-0	273.12	177.04	NEG
145	ESCULETIN	C ₄ H ₄ O ₄	305-01-1	274.09	177.02	NEG
146	Maleic acid	C ₂₇ H ₃₀ O ₁₇	110-16-7	274.21	115	NEG
147	Quercetin-3-O-sophoroside	C ₅ H ₇ NOS	18609-17-1	274.53	625.14	NEG
148	5-Methoxy-2-methylthiazole	C ₁₁ H ₁₁ NO ₃	38205-64-0	274.59	130.03	POS
149	Indolelactic acid	C ₉ H ₈ O ₃	1821-52-9	275.4	206.09	POS
150	4-Hydroxycinnamic acid	C ₁₃ H ₁₄ N ₂ O ₄	7400-08-0	277.02	163.04	NEG
151	Acetyl-N-formyl-5-methoxykynurenamine	C ₂₅ H ₂₄ O ₁₂	52450-38-1	277.26	265.12	POS
152	3,4-Dicaffeoylquinic acid	C ₂₇ H ₃₀ O ₁₆	14534-61-3	280.1	515.12	NEG
153	Kaempferol 3-O-beta-sophoroside	C ₁₉ H ₂₈ O ₁₁	19895-95-5	284.6	609.15	NEG

154	Phenylethyl primeveroside	C ₁₅ H ₁₂ O ₅	129932-48-5	285.34	434.2	POS
155	(2R,3R)-3,4',7-Trihydroxyflavanone	C ₈ H ₁₆ O ₃	111915-65-2	289.39	273.07	POS
156	Hydroxyoctanoic acid	C ₉ H ₁₀ O ₂	617-73-2	290.08	159.1	NEG
157	Hydrocinnamic acid	C ₆ H ₁₂ O ₆	501-52-0	292.18	149.06	NEG
158	D-Galactose	C ₇ H ₆ O ₂	59-23-4	293.2	179.06	NEG
159	Benzoic acid	C ₉ H ₇ NO ₂	65-85-0	294.56	121.03	NEG
160	2-Indolecarboxylic acid	C ₉ H ₇ NO	1477-50-5	295.69	160.04	NEG
161	Indole-3-carboxaldehyde	C ₂₁ H ₂₀ O ₁₁	487-89-8	297.93	146.06	POS
162	Hyperoside	C ₁₆ H ₁₈ O ₉	482-36-0	298.57	463.09	NEG
163	Laccarin	C ₁₅ H ₂₀ O ₄	175669-28-0	302	195.12	POS
164	(S)-Absciscic acid	C ₉ H ₁₆ O ₄	21293-29-8	305.17	263.13	NEG
165	Azelaic acid	C ₁₀ H ₁₆ S ₂ O	123-99-9	305.9	187.1	NEG
166	(R)-(E)-Sulforaphene	C ₈ H ₈ O ₂	2404-46-8	307.17	174	NEG
167	2-Methylbenzoic acid	C ₈ H ₈ O ₃	118-90-1	307.34	135.05	NEG
168	p-Anisic acid	C ₁₀ H ₉ NO ₂	100-09-4	309.96	151.04	NEG
169	Indole-3-acetic acid	C ₁₅ H ₁₂ O ₄	87-51-4	313.79	174.06	NEG
170	Pinobanksin	C ₈ H ₈ O ₄	548-82-3	313.85	273.07	POS
171	Syringaldehyde	C ₁₈ H ₂₀ O ₅	134-96-3	314.21	181.05	NEG
172	p-Hydroxyphenethyl trans-ferulate	C ₄ H ₇ NOS	84873-15-4	316.71	315.12	POS
173	Sulforaphane	C ₈ H ₈	4478-93-7	317.79	178.04	POS
174	Styrene	C ₉ H ₁₀ O ₄	100-42-5	318.98	105.07	POS
175	3,4-Dihydroxyhydrocinnamic acid	C ₁₀ H ₁₀ O ₃	1078-61-1	321.11	227.06	NEG
176	Coniferaldehyde	C ₈ H ₁₀ O ₂	458-36-6	321.23	179.07	POS
177	Syringol	C ₁₁ H ₁₄ O ₃	1991/10/1	329.57	172.1	POS
178	Sinapyl alcohol	C ₁₀ H ₁₀ O ₂	537-33-7	331.03	193.09	POS
179	1-Methoxy-1H-indole-3-carboxaldehyde	C ₈ H ₇ N	67282-55-7	331.75	176.07	POS

180	trans-Cinnamic acid	C ₉ H ₈ O ₂	140-10-3	336.45	147.04	NEG
181	1H-Indole-3-carboxaldehyde	C ₉ H ₇ N	487-89-8	337.43	146.06	POS
182	Diethyl phthalic acid	C ₁₂ H ₁₄ O ₄	84-66-2	338.08	221.08	NEG
183	Pisumionoside	C ₂₄ H ₃₄ O ₁₁	371113-06-3	338.49	405.2	POS
184	Alantolactone	C ₁₅ H ₂₀ O ₂	546-43-0	340.73	233.15	POS
185	Absciscic acid	C ₁₅ H ₂₀ O ₄	7773-56-0	340.89	263.13	NEG
186	gamma-Carboxyglutamic acid	C ₆ H ₈ O ₄	53445-96-8	343.3	192.05	POS
187	5-Isothiocyanato-1-pentene	C ₆ H ₁₁ NS	18060-79-2	348.42	128.05	POS
188	2',4'-Dihydroxyacetophenone	C ₈ H ₈ O ₃	89-84-9	350.42	151.04	NEG
189	3-Phenylpropionic acid	C ₉ H ₁₀ O ₂	501-52-0	352.1	149.06	NEG
190	N-a-Acetyl-L-arginine	C ₈ H ₁₄ N ₄ O ₂	155-84-0	352.14	217.13	POS
191	Acetovanillone	C ₉ H ₁₀ O ₃	498-02-2	354.6	165.06	NEG
192	5,7-Dimethoxyflavone	C ₁₇ H ₁₆ O ₄	21392-57-4	356.4	281.08	NEG
193	1-(2-Furanyl)-1-butanone	C ₈ H ₁₀ O ₂	4208-57-5	357.03	139.08	POS
194	Melatonin	C ₁₃ H ₁₆ N ₂ O ₂	73-31-4	358.33	233.13	POS
195	Medicarpin	C ₁₆ H ₁₂ O ₄	32383-76-9	358.69	269.08	NEG
196	Indoleacetaldehyde	C ₁₀ H ₉ NO	2591-98-2	359.22	160.08	POS
197	3-Indoleacrylic acid	C ₁₁ H ₉ NO ₂	1204-06-4	360.47	186.06	NEG
198	Precocene II	C ₁₈ H ₁₆ O ₄	644-06-4	363.76	221.12	POS
199	Ecgonine methyl ester	C ₉ H ₁₅ NO ₃	1915211	374.27	200.13	POS
200	alpha-Corocalene	C ₁₅ H ₁₈	20129-39-9	379.79	201.16	POS
201	Ethyl caffeate	C ₁₁ H ₁₂ O ₄	102-37-4	380.41	207.07	NEG
202	Asparaginy-Lysine	C ₁₀ H ₁₉ N ₃ O ₃	22677-58-3	383.97	261.16	POS
203	Pterosin P	C ₁₅ H ₂₂ O ₂	56374-22-2	387.44	235.14	POS
204	Dihydrojasmonic acid	C ₁₂ H ₁₈ O ₃	98674-52-3	388.16	211.13	NEG
205	p-Mentha-1,8-dien-7-ol	C ₁₀ H ₁₆ O	536-59-4	388.42	135.12	POS

206	1-Isothiocyanato-6-(methylsulfinyl)hexane	C ₇ H ₁₃ NS ₂	4430-35-7	392.04	206.07	POS
207	(-)-Parthenolide	C ₁₅ H ₂₀ O ₃	20554-84-1	393.77	249.15	POS
208	LysoPC(10:0)	C ₂₅ H ₅₂ NO ₇ P	22248-63-1	394.34	412.25	POS
209	Traumatic acid	C ₁₂ H ₁₆ O ₃	6402-36-4	395.6	227.13	NEG
210	Isorhamnetin	C ₁₆ H ₁₂ O ₇	480-19-3	400.76	315.05	NEG
211	Indoleacetic acid	C ₁₀ H ₉ NO ₂	87-51-4	401.82	174.06	NEG
212	Indole-3-propionic acid	C ₁₁ H ₁₁ NO ₂	830-96-6	406.02	188.07	NEG
213	5-Acetylamino-6-formylamino-3-methyluracil	C ₈ H ₉ N ₃ O ₄	85438-96-6	406.14	227.08	POS
214	Dodecanedioic acid	C ₁₂ H ₂₂ O ₄	693-23-2	406.34	229.14	NEG
215	Cucurbic acid	C ₁₀ H ₁₂ O ₃	58240-50-9	408.21	213.15	POS
216	Isoalantolactone	C ₁₅ H ₂₀ O ₂	470-17-7	408.83	233.15	POS
217	Andrographolide	C ₂₀ H ₃₀ O ₅	5508-58-7	409.28	395.21	NEG
218	Harmine	C ₁₃ H ₁₂ N ₂ O	442-51-3	411.33	257.09	NEG
219	Bate-sitosterol	C ₂₉ H ₅₀ O	83-46-5	414.7	415.72	NEG
220	Edulisin II	C ₂₁ H ₂₈ O ₈	96608-83-2	414.87	427.18	POS
221	3-Hydroxydecanoic acid	C ₁₀ H ₂₀ O ₃	14292-26-3	424.47	187.13	NEG
222	8-hydroxy-7-methoxy-3-(2-methylbut-3-en-2-yl)- 2H-chromen-2-one	C ₁₅ H ₁₄ O ₄	61899-42-1	426.41	278.14	POS
223	3,6-Dimethyl-2(3H)-benzofuranone	C ₁₀ H ₁₀ O ₂	65817-24-5	438.33	163.08	POS
224	Tetradecanedioic acid	C ₁₄ H ₂₆ O ₄	821-38-5	444.2	257.18	NEG
225	4-Methylumbelliferone	C ₁₀ H ₈ O ₃	90-33-5	452.43	177.05	POS
226	Nobiletin	C ₂₁ H ₂₂ O ₈	478-01-3	456.75	403.14	POS
227	Indole-3-carboxylic acid	C ₉ H ₇ NO ₂	771-50-6	478.43	254.14	POS
228	Scolymoside	C ₂₈ H ₃₂ O ₁₄	25694-72-8	482.25	371.2	POS
229	(9S,10E,12Z,15Z)-9-Hydroxy-10,12,15- octadecatrienoic acid	C ₁₈ H ₂₈ O ₃	89886-42-0	511.65	277.22	POS

230	Fasciculic acid C	C ₂₅ H ₄₄ O ₃	126882-56-2	514.66	692.45	POS
231	LysoPC(18:2(9Z,12Z))	C ₂₂ H ₄₆ NO ₇ P	22252-07-9	517.53	520.34	POS
232	Norcorydine	C ₁₉ H ₂₁ NO ₄	26931-78-2	519.69	328.15	POS
233	16-Hydroxy hexadecanoic acid	C ₁₆ H ₃₂ O ₃	506-13-8	539.25	271.23	NEG
234	MG(0:0/18:1(9Z)/0:0)	C ₂₁ H ₄₂ O ₄	3443-84-3	544.34	357.3	POS
235	L-Proline	C ₅ H ₉ NO ₂	147-85-3	546.78	116.07	POS
236	Phytosphingosine	C ₁₈ H ₃₉ NO ₃	554-62-1	556.13	318.3	POS
237	N-Phenyl-2-naphthylamine	C ₁₆ H ₁₃ N	135-88-6	557.46	220.11	POS
238	Monoisobutyl phthalic acid	C ₁₂ H ₁₄ O ₄	30833-53-5	582.9	223.1	POS
239	Anofinic acid	C ₁₀ H ₁₂ O ₂	34818-56-9	585.05	205.09	POS
240	all-trans-Retinoic acid	C ₁₈ H ₂₆ O ₂	302-79-4	595.57	299.2	NEG
241	Stearidonic acid	C ₁₈ H ₃₂ O ₂	20290-75-9	603.36	275.2	NEG
242	Macrocarpal B	C ₂₆ H ₃₄ O ₇	142698-60-0	605.47	471.28	NEG
243	Palmitoylethanolamide	C ₁₈ H ₃₅ NO ₂	544-31-0	621.64	300.29	POS
244	Sciadonic acid	C ₂₀ H ₃₂ O ₂	7019-85-4	635.42	307.26	POS
245	alpha-Linolenic acid	C ₁₈ H ₃₀ O ₂	463-40-1	645.06	277.22	NEG
246	Linoleic acid	C ₁₈ H ₃₂ O ₂	60-33-3	646.3	279.23	NEG
247	Oleamide	C ₁₈ H ₃₅ NO	301-02-0	650.36	282.28	POS
248	1-Butylamine	C ₄ H ₉ N	109-73-9	654.51	74.1	POS
249	Palmitic amide	C ₁₆ H ₃₃ NO	629-54-9	669.48	256.26	POS
250	N-Hexadecanoylpyrrolidine	C ₁₆ H ₃₁ NO	70974-48-0	693.09	310.31	POS
251	alpha-Amyrone	C ₁₅ H ₂₄ O	638-96-0	703.75	425.38	POS
252	D8'-Merulinic acid A	C ₂₀ H ₂₈ O ₁₂	69506-65-6	722.65	391.28	POS
253	Beta-Aminopropionitrile	C ₃ H ₆ N ₂	151-18-8	738.83	71.06	POS
254	Betaine aldehyde	C ₅ H ₁₁ NO	7418-61-3	781.51	102.09	POS
255	cis,cis-Muconic acid	C ₆ H ₆ O ₄	1119-72-8	783.12	141.02	NEG

256	trans-Resveratrol 3,4'-disulfate	$C_{14}H_{10}O_{10}S_2$	858187-20-9	800.22	389	POS
257	3-Phosphoglyceric acid	$C_3H_7O_6P$	820-11-1	802.67	187	POS
258	Methyl 2-(methylthio)acetate	$C_5H_{10}O_2S$	16630-66-3	818.65	107.02	POS
259	(R)-lipoic acid	$C_8H_{14}O_2S$	1200-22-2	897.95	223.02	NEG
