

Table S1 Identified metabolites in the fresh shoots of tea accessions

NO.	Name	Formula	Molecular Weight	RT (min)
aa-001	L-Arginine	C6H14N4O2	174.1117	0.83
aa-002	L-Alanine	C3H7NO2	89.0478	0.85
aa-003	L-Aspartic acid	C4H7NO4	133.0375	0.85
aa-004	L-Glutamic acid	C5H9NO4	147.0532	0.86
aa-005	Sucrose	C12H22O11	342.1167	0.89
aa-006	L-Proline	C5H9NO2	115.0634	0.91
aa-007	Betaine	C5H11NO2	117.0790	0.91
aa-008	DL-Tartaric acid	C4H6O6	150.0165	0.91
aa-009	D-Erythrose	C4H8O4	120.0424	0.92
aa-010	L-Theanine	C7H14N2O3	174.1004	0.97
aa-011	Malic Acid	C4H6O5	134.0216	0.98
aa-012	L-Isoleucine	C6H13NO2	131.0947	1.06
aa-013	L-Leucine	C6H13NO2	131.0947	1.21
aa-014	Citric acid	C6H8O7	192.0271	1.22
aa-015	Adenine	C5H5N5	135.0546	1.24
aa-016	Succinic acid	C4H6O4	118.0267	1.31
aa-017	Nicotinamide	C6H6N2O	122.0481	1.34
aa-018	GA-hexoside	C13H16O10	332.0747	1.48
aa-019	L-Phenylalanine	C9H11NO2	165.0791	1.56
aa-020	Xanthine	C5H4N4O2	152.0335	1.62
aa-021	Adenosine	C10H13N5O4	267.0967	1.69
aa-022	Gallic acid (GA)	C7H6O5	170.0216	1.92
aa-023	Pantothenic acid	C9H17NO5	219.1108	2.06
aa-024	Theogallin (Trihydroxybenzoic acid glycoside)	C14H16O10	344.0745	2.25
aa-025	7-Methylxanthine	C6H6N4O2	166.0491	2.59
aa-026	Gallocatechin (GC)	C15H14O7	306.0741	3.22
aa-027	Neochlorogenic acid (5-O-Caffeoylquinic acid)	C16H18O9	354.0954	3.61
aa-028	Theobromine	C7H8N4O2	180.0647	4.14
aa-029	Methyl gallate	C8H8O5	184.0372	4.40
aa-030	Epigallocatechin (EGC)	C15H14O7	306.0741	4.41
aa-031	3,4-Dihydroxybenzaldehyde	C7H6O3	138.0316	4.41
aa-032	1,3,7-Trimethyluric acid	C8H10N4O3	210.0754	4.83
aa-033	Procyanidin B3	C30H26O12	578.1427	4.95
aa-034	(+)Catechin (C)	C15H14O6	290.0793	4.96
aa-035	Strictinin	C27H22O18	634.0813	5.18
aa-036	Chlorogenic acid (3-O-Caffeoylquinic acid)	C16H18O9	354.0953	5.35
aa-037	Procyanidin B4	C30H26O12	578.1430	5.69
aa-038	Epicatechin (EC)	C15H14O6	290.0793	5.86
aa-039	4-Hydroxybenzaldehyde	C7H6O2	122.0364	5.86
aa-040	Caffeine	C8H10N4O2	194.0804	6.26
aa-041	(-)-Epigallocatechin 3-O-gallate(EGCG)	C22H18O11	458.0853	6.75

aa-042	TriGA-glucose	C27H24O18	636.0970	7.27
aa-043	Quercetin	C15H10O7	302.0424	7.78
aa-044	Schaftoside (Apigenin 6-C-arabinoside-8-C-glucoside)	C26H28O14	564.1485	7.49
aa-045	Myricetin 3-O-galactoside	C21H20O13	480.0907	7.49
aa-046	Rutin	C27H30O16	610.1539	8.16
aa-047	Isoquercetin	C21H20O12	464.0959	8.38
aa-048	Ellagic acid	C14H6O8	302.0065	8.51
aa-049	Kaempferitrin (kaempferol 3,7-dirhamnoside)	C27H30O14	578.1639	8.58
aa-050	EGCG4"Me	C23H20O11	472.1010	8.09
aa-051	Naringin (Naringenin 7-O-neohesperidoside)	C27H32O14	580.1801	8.64
aa-052	Quercetin 3-O-a-D-xylopyranoside	C20H18O11	434.0853	8.65
aa-053	Prunin (Naringenin 7-O-glucoside)	C21H22O10	434.1218	8.69
aa-054	Cynaroside	C21H20O11	448.1008	8.72
aa-055	2-Hydroxy cinnamic acid	C9H8O3	164.0474	8.72
aa-056	Myricetin	C15H10O8	318.0379	8.93
aa-057	Eriodictyol	C15H12O6	288.0637	8.96
aa-058	Kaempferin (Afzelin, Kaempferol 3-rhamnoside)	C21H20O10	432.1059	8.98
aa-059	Baicalin	C21H18O11	446.0856	9.02
aa-060	Tricetin (5,7,3',4',5'-Pentahydroxyflavone)	C15H10O7	302.0429	9.05
aa-061	Abscisic acid	C15H20O4	264.1363	9.28
aa-062	Naringenin	C15H12O5	272.0688	9.54
aa-063	Kaempferol	C15H10O6	286.0481	9.65
aa-064	Procyanidin B1	C30H26O12	578.1429	4.73
aa-065	Procyanidin C1	C30H26O12	578.1430	6.96
aa-066	Dihydromyricetin	C15H12O8	320.0535	6.23
aa-067	Vitexin-2"-o-rhamnoside	C27H30O14	578.1638	8.17
aa-068	Vitexin (Apigenin 8-C-glucoside)	C21H20O10	432.1058	8.37
aa-069	Epicatechin gallate (ECG)	C22H18O10	442.0904	8.23
aa-070	Catechin gallate (CG)	C22H18O10	442.0899	8.43
aa-071	Quercitrin	C21H20O11	448.1009	8.66
aa-072	Luteolin	C15H10O6	286.0481	9.38
aa-073	Phloretin	C15H14O5	274.0845	9.53
aa-074	Oxalic acid	C2H2O4	89.9954	0.91
aa-075	cis-Aconitic acid	C6H6O6	174.0165	1.02
aa-076	L-Glutathione oxidized	C20H32N6O12S2	612.1520	1.23
aa-077	Guanine	C5H5N5O	151.0495	1.23
aa-078	Xanthosine	C10H12N4O6	284.0759	1.96
aa-079	Esculin (6,7-Dihydroxycoumarin-6-glucoside)	C15H16O9	340.0797	4.73
aa-080	Baimaside (Quercetin-3-O-sophoroside)	C27H30O17	626.1490	7.27
aa-081	Shikimic acid	C7H10O5	174.0527	6.26
aa-082	Theacrine	C9H12N4O3	224.0908	5.63
aa-083	1,2-di-O-galloyl-HHDP-glucose(Dalichasu)	C34H26O22	786.0927	6.96
aa-084	GC-diGA	C29H22O15	610.0968	8.39

aa-085	GC-GCG	C37H30O18	762.1441	5.72
bb-001	trans-4-Hydroxy-L-proline	C5H9NO3	131.0583	1.27
bb-002	Glutaric acid	C5H8O4	132.0423	1.85
bb-003	2,5-Dihydroxy benzoic acid O-hexside	C13H16O9	316.0800	2.43
bb-004	Ellagic acid glucoside	C21H24O12	468.1272	2.59
bb-005	Protocatechuic acid O-glucoside	C13H16O9	316.0800	2.93
bb-006	4-(beta-D-Glucosyloxy)benzoic acid	C13H16O8	300.0848	3.36
bb-007	diGA-glucose	C20H20O14	484.0858	5.00
bb-008	3-O-p-Coumaroyl quinic acid	C16H18O8	338.1006	6.26
bb-009	Eriodictyol C-hexoside	C21H22O11	450.1168	6.27
bb-010	Cyanidin 3-O-rutinoside (Keracyanin)	C27H30O15	594.1590	8.59
bb-011	diGC-GA	C37H30O17	746.1492	6.49
bb-012	Nictoflorin	C27H30O15	594.1590	7.90
bb-013	4',7-Dihydroxyflavanone	C15H12O4	256.0734	8.80
cc-001	Agmatine	C5H14N4	130.1219	0.75
cc-002	Lactobionic acid	C12H22O12	358.1116	0.84
cc-003	Nitrilacarb	C9H15N3O2	197.1165	0.84
cc-004	1-Deoxy-D-alto-heptulose 7-phosphate	C7H15O9P	274.0458	0.86
cc-005	4-Amino-4-deoxypentopyranose	C5H11NO4	149.0688	0.86
cc-006	L-Pyroglutamic acid	C5H7NO3	129.0427	0.86
cc-007	Maleamic acid	C4H5NO3	115.0269	0.87
cc-008	(2S,4S)-4-Amino-2-hydroxy-2-methylpentanedioic acid	C6H11NO5	177.0637	0.87
cc-009	Glycerol 3-phosphate	C3H9O6P	172.0138	0.88
cc-010	Glycerophosphoglycerol	C6H15O8P	246.0506	0.88
cc-011	7-Hydroxy-6-methyl-8-(1-D-ribityl)lumazine	C12H16N4O7	328.1012	0.89
cc-012	3-Phosphoglyceric acid	C3H7O7P	185.9929	0.89
cc-013	3-Deoxy-D-manno-2-octulosonic acid	C8H14O8	238.0691	0.89
cc-014	Uridine 5'-diphosphogalactose	C15H24N2O17P2	566.0558	0.90
cc-015	2-Acetamido-2-deoxyglucose	C8H15NO6	221.0899	0.90
cc-016	Dihydrothymine	C5H8N2O2	128.0586	0.91
cc-017	Trimethadione	C6H9NO3	143.0583	0.91
cc-018	Oxaceprol	C7H11NO4	173.0688	0.91
cc-019	L-Threonic acid	C4H8O5	136.0373	0.92
cc-020	Hydroxycitric acid	C6H8O8	208.0221	0.93
cc-021	Gly-L-pro	C7H12N2O3	172.0849	0.93
cc-022	Ethanoic anhydride	C4H6O3	102.0317	0.93
cc-023	Dihydrolipoic acid	C8H16O2S2	208.0585	0.93
cc-024	alpha-Methyl D-mannoside	C7H14O6	194.0792	0.96
cc-025	4-Piperidinecarboxamide	C6H12N2O	128.0950	0.97
cc-026	Ethanal tetramer	C8H16O4	176.1040	0.98
cc-027	Uridine monophosphate (UMP)	C9H13N2O9P	324.0361	0.99
cc-028	2-Furoic acid	C5H4O3	112.0161	0.99
cc-029	5'-Xanthylic acid	C10H13N4O9P	364.0413	1.01

cc-030	N-Acetyl-L-glutamic acid	C7H11NO5	189.0638	1.07
cc-031	Malonic acid	C3H4O4	104.0110	1.08
cc-032	Streptamine 4-phosphate	C6H15N2O7P	258.0623	1.13
cc-033	2-Oxo-3-(5-oxofuran-2-ylidene)propanoic acid	C7H4O5	168.0062	1.15
cc-034	L-Lupinic acid	C13H18N6O3	306.1426	1.22
cc-035	Methyl 2-O-beta-L-arabinofuranosyl-beta-L-arabinofuranoside	C11H20O9	296.1110	1.23
cc-036	2-(Carboxymethyl)-5-oxo-2,5-dihydro-2-furoic acid	C7H6O6	186.0165	1.23
cc-037	Gly-Lys	C8H17N3O3	203.1272	1.23
cc-038	(+)-a(S)-Butyr-amido-r-butyrrolactone	C8H13NO3	171.0895	1.24
cc-039	Prolylleucine	C11H20N2O3	228.1474	1.24
cc-040	Guvacine	C6H9NO2	127.0634	1.29
cc-041	2-Methylcitric acid	C7H10O7	206.0427	1.30
cc-042	1,3,4-Trihydroxy-5-oxocyclohexanecarboxylic acid	C7H10O6	190.0479	1.32
cc-043	DL-Mevalonic acid	C6H12O4	148.0736	1.35
cc-044	Hymexazol O-glucoside	C10H15NO7	261.0850	1.39
cc-045	5'-O-beta-D-Glucosylpyridoxine	C14H21NO8	331.1272	1.41
cc-046	3-Hydroxy-3-methylglutaric acid	C6H10O5	162.0529	1.42
cc-047	N-Phenyl-beta-D-glucopyranosylamine	C12H17NO5	255.1106	1.49
cc-048	N-Acetyl-L-2-aminoadipic acid	C8H13NO5	203.0796	1.51
cc-049	alpha-Ketoadipic acid	C6H8O5	160.0372	1.60
cc-050	tert-Butyl 3-amino-1-methyl-2,3-dioxopropylcarbamate	C9H16N2O4	216.1111	1.68
cc-051	2-(3,4,5-Trihydroxyphenyl)-3,4,5,7-chromanetetrol	C15H14O8	322.0693	1.75
cc-052	(+/-)-2-Hydroxyglutaric acid	C5H8O5	148.0372	0.93
cc-053	Lamiide	C17H26O12	422.1432	1.92
cc-054	Riboflavin reduced	C15H16N4O6	348.1061	2.06
cc-055	Adenosine 5'-phosphoramidate	C10H15N6O6 P	346.0794	2.23
cc-056	(Hydroxyethyl)methacrylate	C6H10O3	130.0631	2.44
cc-057	trans-3-Indoleacrylic acid	C11H9NO2	187.0634	2.48
cc-058	3,5-Dihydroxy-4-[(6-O-sulfo-beta-D-glucopyranosyl)oxy]benzoic acid	C13H16O13S	412.0317	2.53
cc-059	Diacetin	C7H12O5	176.0685	2.83
cc-060	2,3-Dihydroxypropyl 3,4,5-trihydroxybenzoate	C10H12O7	244.0585	3.15
cc-061	3-[(1-Carboxyvinyl)oxy]benzoic acid	C10H8O5	208.0372	3.19
cc-062	Malonylglycitin	C25H24O13	532.1223	3.20
cc-063	Histidylglycine	C8H12N4O3	212.0910	3.32
cc-064	5-[(E)-2-Carboxyvinyl]-2-hydroxyphenyl beta-D-glucopyranosiduronic acid	C15H16O10	356.0747	3.37
cc-065	Diphenol glucuronide	C12H14O8	286.0691	3.59
cc-066	Sulfanilic acid	C6H7NO3S	173.0146	3.68
cc-067	Succinylacetone	C7H10O4	158.0579	3.69
cc-068	Nifurquinazol	C16H16N4O5	344.1111	4.03
cc-069	beta-D-glucose pentaacetate	C16H22O11	390.1169	4.07
cc-070	5-(2-Carboxyethyl)-2-hydroxyphenyl beta-D-glucopyranosiduronic acid	C15H18O10	358.0904	4.09
cc-071	5'-S-Methyl-5'-thioadenosine	C11H15N5O3 S	297.0895	4.12
cc-072	1,5-Diphenylcarbazine	C13H14N4O	242.1157	4.12

cc-073	1,6-Bis-O-(3,4,5-trihydroxybenzoyl)hexopyranose	C20H20O14	484.0858	4.12
cc-074	Zizybeoside I	C19H28O11	432.1638	4.15
cc-075	(1S)-1,5-Anhydro-1-[2,4,6-trihydroxy-3-(4-hydroxybenzoyl)phenyl]-D-glucitol	C19H20O10	408.1063	4.22
cc-076	(-)-L-Chicoric acid	C22H18O12	474.0802	4.25
cc-077	N-Acetyl-D-alloisoleucine	C8H15NO3	173.1054	4.29
cc-078	Melilotoside	C15H18O8	326.1006	4.30
cc-079	Phenylacetaldehyde	C8H8O	120.0574	4.31
cc-080	4-(2-Carboxyethyl)-2-methoxyphenyl beta-D-glucopyranosiduronic acid	C16H20O10	372.1060	4.34
cc-081	5-Hydroxy-6-methoxy-3-(4-methoxyphenyl)-4-oxo-4H-chromen-7-yl beta-D-glucopyranosiduronic acid	C23H22O12	490.1118	4.41
cc-082	Aspirin	C9H8O4	180.0423	4.42
cc-083	Propentofylline	C15H22N4O3	306.1690	4.61
cc-084	1-O-vanilloyl-beta-D-glucose	C14H18O9	330.0955	4.72
cc-085	Benzyl 6-O-beta-D-xylopyranosyl-beta-D-glucopyranoside	C18H26O10	402.1531	4.73
cc-086	1,3-Propane sultone	C3H6O3S	122.0038	4.75
cc-087	7-Ethoxycoumarin	C11H10O3	190.0630	4.77
cc-088	Sinapaldehyde glucoside	C17H22O9	370.1269	4.77
cc-089	Kynurenic acid	C10H7NO3	189.0426	4.79
cc-090	Caffeoylmalic acid	C13H12O8	296.0530	4.94
cc-091	2,4-Diacetylphloroglucinol	C10H10O5	210.0529	5.24
cc-092	1-Naphthyl glucuronide	C16H16O7	320.0897	5.29
cc-093	5-Nitro-2-propoxyaniline	C9H12N2O3	196.0845	6.26
cc-094	5-(3,4-diacetoxybut-1-ynyl)-2,2'-bithiophene	C16H14O4S2	334.0331	6.32
cc-095	3-(5'-methylthio)pentylmalic acid	C10H18O5S	250.0877	6.32
cc-096	Gentiopiricin	C16H20O9	356.1108	6.40
cc-097	1,5-Anhydro-1-[3-(3,4-dihydroxybenzoyl)-2,4,6-trihydroxyphenyl]hexitol	C19H20O11	424.0988	6.45
cc-098	Sweroside	C16H22O9	358.1270	6.45
cc-099	4,7,8-Trihydroxy-3-(4-hydroxyphenyl)dibenzo[b,d]furan-1,2-diyl diacetate	C22H16O9	424.0793	6.95
cc-100	N-Acetyl-DL-tryptophan	C13H14N2O3	246.1006	6.97
cc-101	1-(β-D-Glucopyranosyloxy)-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[c]pyran-4-carboxylic acid	C16H24O9	360.1426	7.04
cc-102	1,6-bis-O-galloyl-beta-D-glucose	C20H20O14	484.0854	7.27
cc-103	8-Demethyl-8-(alpha-L-rhamnosyl)tetracenomycin C	C28H28O15	604.1438	7.41
cc-104	iso-Quercitrin 6"-acetate	C23H22O13	506.1068	7.62
cc-105	4-Carboxy nevirapine	C15H12N4O3	296.0898	7.68
cc-106	Mascaroside	C26H36O11	524.2264	7.79
cc-107	Glucosylgalactosyl hydroxylysine	C18H34N2O13	486.2077	7.79
cc-108	beta-D-Fructofuranosyl 2,4-bis-O-(3-methylbutanoyl)-alpha-D-glucopyranoside	C22H38O13	510.2317	7.79
cc-109	Eugenyl Glucoside	C16H22O7	326.1365	7.81
cc-110	beta-Syringin	C17H24O9	372.1424	7.82
cc-111	Astilbin	C21H22O11	450.1169	7.90
cc-112	Malonylgenistin	C24H22O13	518.1071	8.09
cc-113	11-O-Demethyl-7-methoxypradinone II	C25H18O11	494.0832	8.10
cc-114	Gallocatechin-(4alpha->8)-epigallocatechin	C30H26O14	610.1320	8.30

cc-115	N-Adenylylanthranilic acid	C17H19N6O8 P	466.1018	8.38
cc-116	Eupatoriochromene	C13H14O3	218.0943	8.49
cc-117	Tiliroside	C30H26O13	594.1375	8.53
cc-118	Olsalazine	C14H10N2O6	302.0538	8.64
cc-119	(2Z)-3-[4,5-Dihydroxy-2-(2-hydroxy-2-propanyl)-2,3-dihydro-1-benzofuran-7-yl]acrylic acid	C14H16O6	280.0949	8.72
cc-120	Cynarine	C25H24O12	516.1273	8.77
cc-121	(2R,3R)-5,7-Dihydroxy-2-(4-hydroxyphenyl)-3,4-dihydro-2H-chromen-3-yl 3,4,5-trihydroxybenzoate	C22H18O9	426.0956	8.80
cc-122	Azelaic acid	C9H16O4	188.1049	8.83
cc-123	Swertianolin	C20H20O11	436.1010	8.84
cc-124	Salvianolic acid D	C20H18O10	418.0904	8.85
cc-125	Luteolin 7-O-(6-O-malonyl-beta-D-glucoside)	C24H22O14	534.1014	8.87
cc-126	Picrotin	C15H18O7	310.1056	8.88
cc-127	(-)-Caryophyllene oxide	C15H24O	220.1828	8.89
cc-128	Naringin dihydrochalcone	C27H34O14	582.1959	9.01
cc-129	Amarogentin	C29H30O13	586.1696	9.20
cc-130	Silandrin	C25H22O9	466.1260	9.24
cc-131	Lappaol	C30H34O10	554.2162	9.32
cc-132	Kolaflavanone	C31H24O12	588.1278	9.34
cc-133	Atrovirone	C25H28O8	456.1792	9.36
cc-134	Lamifiban	C24H28N4O6	468.1999	9.39
cc-135	Chitobiose	C16H28N2O1 I	424.1707	9.41
cc-136	2-Amino-1,3,4-octadecanetriol	C18H39NO3	317.2929	9.55
cc-137	Methyl 3,4,5-trimethoxycinnamate	C13H16O5	252.1000	9.60
cc-138	Traumatic acid	C12H20O4	228.1364	9.61
cc-139	Propofol	C12H18O	178.1358	9.69
cc-140	7-Dehydrocholesterol benzoate	C34H48O2	488.3660	9.78
cc-141	Demethylphyloquinone	C30H44O2	436.3342	9.82
cc-142	1,4-Anhydro-6-O-dodecanoyl-2,3-bis-O-(2-hydroxyethyl)-D-glucitol	C22H42O8	434.2883	10.01
cc-143	Embelin	C17H26O4	294.1835	10.08
cc-144	2-Linoleoyl-sn-glycero-3-phosphoethanolamine	C23H44NO7P	477.2859	10.20
cc-145	Matricin	C17H22O5	306.1470	10.23
cc-146	Mucronine A	C29H38N4O4	506.2888	10.38
cc-147	1-Oleoyl-sn-glycero-3-phosphoethanolamine	C23H46NO7P	479.3016	10.38
cc-148	1-Linoleoyl-sn-glycero-3-phosphocholine	C26H50NO7P	519.3326	10.47
cc-149	Lauramide	C12H25NO	199.1936	10.70
cc-150	Allylcyclohexane	C9H16	124.1253	11.97
cc-151	xi-p-Menth-3-ene	C10H18	138.1409	11.97
cc-152	4,5-Dihydroxy-4-(2,3,4-trihydroxytetrahydro-2-furanyl)-3,4-dihydro-2H-pyrrole-2-carboxylic acid	C9H13NO8	263.0643	0.92
cc-153	beta-D-Ethyl glucuronide	C8H14O7	222.0743	0.92
cc-154	7-Hydroxycoumarin	C9H6O3	162.0317	5.19
a0-001	gamma-Aminobutyric acid	C4H9NO2	103.0634	0.85
a0-002	L-Serine	C3H7NO3	105.0426	0.86

a0-003	L-Threonine	C4H9NO3	119.0583	0.86
a0-004	D-Glucose 6-Phosphate	C6H13O9P	260.0299	0.86
a0-005	D(+)-Glucuronic Acid	C6H10O7	194.0427	0.88
a0-006	D(-)-Quinic acid	C7H12O6	192.0635	0.93
a0-007	D-Glucono-1,5-lactone	C6H10O6	178.0479	0.95
a0-008	alpha-Oxoglutarate	C5H6O5	146.0216	1.08
a0-009	Thymine	C5H6N2O2	126.0429	1.57
a0-010	Inosine	C10H12N4O5	268.0809	1.59
a0-011	Guanosine	C10H13N5O5	283.0917	1.59
a0-012	L-Tryptophan	C11H12N2O2	204.0897	2.46
a0-013	3-Methylxanthine	C6H6N4O2	166.0491	2.90
a0-014	2,5-Dihydroxybenzoic acid	C7H6O4	154.0267	3.50
a0-015	beta-Resorecylic acid	C7H6O4	154.0267	4.76
a0-016	2-Hydroxybenzoic acid	C7H6O3	138.0317	6.97
a0-017	(-)-Gallocatechin 3-O-gallate(GCG)	C22H18O11	458.0854	7.32
0a-001	D-Fructose-6-phosphate	C6H13O9P	260.0296	0.84
0a-002	L-Homoserine	C4H9NO3	119.0582	0.84
0a-003	Gluconic acid	C6H12O7	196.0584	0.85
0a-004	D-(+)-Xylose	C5H10O5	150.0528	0.90
0a-005	L-Glutathione (reduced)	C10H17N3O6 S	307.0840	1.10
0a-006	L-Tyrosine	C9H11NO3	181.0738	1.24
0a-007	Aconitic acid	C6H6O6	174.0166	1.41
0a-008	1-O-Galloyl-β-D-glucose	C13H16O10	332.0746	1.45
0a-009	Gallotanin 1,2,6-tri-O-galloyl-β-d-glucopyranose	C27H24O18	636.0976	6.94
0a-010	Rhoifolin (Apigenin 7-O-neohesperidoside)	C27H30O14	578.1649	8.73
0a-011	ECG4"Me	C23H20O10	456.1057	8.78
0a-012	Sinapinaldehyde	C11H12O4	176.0472	8.89
0a-013	Apigenin (5,7,4'-trihydroxyflavone)	C15H10O5	270.0527	9.65
0a-014	Hypoxanthin	C5H4N4O	136.0386	1.55
0a-015	D(-)-Fructose	C6H12O6	180.0636	0.95
b0-001	Tricatechins1	C45H38O18	866.2070	6.37
b0-002	Chlorogenic acid methyl ester	C17H20O9	368.1110	6.84
b0-003	Tricatechins2	C45H38O18	866.2069	6.93
b0-004	Tricatechins3	C45H38O18	866.2073	8.02
0b-001	1,2,4,6-Tetra-O-galloyl-β-D-glucose	C34H28O22	788.1091	8.37
c0-001	1-Aminocyclohexanecarboxylic acid	C7H13NO2	143.0947	0.97
c0-002	Adenosine 5'-monophosphate	C10H14N5O7 P	347.0631	1.22
c0-003	Inosine-5'-monophosphate (IMP)	C10H13N4O8 P	348.0474	1.24
c0-004	S-Adenosyl homocysteine	C14H20N6O5 S	384.1218	1.41
c0-005	Fumaric acid	C4H4O4	116.0110	1.45
c0-006	Neosaxitoxin	C10H17N7O5	315.1294	1.58
c0-007	Ethylmalonic acid	C5H8O4	132.0424	1.89
c0-008	Pyrogallol	C6H6O3	126.0318	1.92

c0-009	(-)-Fustin	C15H12O6	288.0633	2.62
c0-010	Citral	C10H16O	152.1202	4.57
c0-011	Methyl cinnamate	C10H10O2	162.0681	4.75
c0-012	Phthaldialdehyde	C8H6O2	134.0368	5.18
c0-013	(-)-Corey lactone	C8H12O4	172.0737	5.46
c0-014	Eriocitrin	C27H32O15	596.1751	5.52
c0-015	{{(1R,2R)-2-[(2Z)-5-(Hexopyranosyloxy)-2-penten-1-yl]-3-oxocyclopentyl }acetic acid	C18H28O9	388.1739	5.75
c0-016	Bioside	C20H30O12	462.1745	5.80
c0-017	2-Amino-1,3-octadecanediol	C18H39NO2	301.2979	9.81
c0-018	8'-Apo-beta-carotenol	C30H42O	418.3235	9.88
c0-019	1-Methyl-4-phenyl-1,2,3,6-tetrahydropyridine	C12H15N	173.1205	9.91
c0-020	3-O-(2-Methylbutanoyl)-beta-D-fructofuranosyl 3-O-dodecanoyl-4-O-(3-methylbutanoyl)-alpha-D-glucopyranoside	C34H60O14	692.3997	10.01
c0-021	(+)-Eudesmin	C22H26O6	386.1730	10.06
c0-022	3-(2-Acetamidoethyl)-1-hexopyranuronosyl-5-methoxy-1H-indole	C19H24N2O8	408.1548	10.06
c0-023	Bis(4-ethylbenzylidene)sorbitol	C24H30O6	414.2041	10.33
c0-024	Lysophosphatidylinositol	C25H49O12P	572.2970	10.40
c0-025	Dodecyl sulfate	C12H26O4S	266.1554	10.67
c0-026	1-Linolenoyl-sn-glycero-3-phosphate	C21H37O7P	432.2280	10.69
c0-027	1-Linoleyl-sn-glycerol 3-phosphate	C21H39O7P	434.2437	10.91
c0-028	Yiamoloside B	C43H68O15	824.4549	11.06
c0-029	1-Palmitoyl lysophosphatidic acid	C19H39O7P	410.2439	11.09
c0-030	Etretinate	C23H30O3	354.2200	11.18
c0-031	Oleoyl-L- $\alpha$ -lysophosphatidic acid	C21H41O7P	436.2595	11.21
c0-032	Linoleamide	C18H33NO	279.2561	11.37
c0-033	Hexadecanamide	C16H33NO	255.2562	11.53
c0-034	Astaxanthin	C40H52O4	596.3864	11.58
c0-035	Oleamide	C18H35NO	281.2718	11.60
c0-036	Butylated hydroxyanisole	C11H16O2	180.1149	11.66
c0-037	Stearamide	C18H37NO	283.2874	11.91
c0-038	Oleoyl ethylamide	C20H39NO	309.3030	11.96
c0-039	1,7-Dimethyluric acid	C7H8N4O3	196.0596	2.72
c0-040	Fraxetin	C10H8O5	208.0372	4.08
c0-041	(E)-p-coumaric acid	C9H8O3	164.0473	9.63
0c-001	L-Histidine	C6H9N3O2	155.0695	0.78
0c-002	L(+)-2-Aminobutyric acid	C4H9NO2	103.0634	0.83
0c-003	$\beta$ -D-Glucopyranuronic acid	C6H10O7	194.0427	0.86
0c-004	Kanosamine	C6H13NO5	161.0689	0.88
0c-005	DL-Lactic Acid	C3H6O3	90.0318	0.90
0c-006	D(-)-Glutamine	C5H10N2O3	146.0692	0.92
0c-007	Ethyl- $\beta$ -D-glucuronide	C8H14O7	222.0741	0.94
0c-008	4-Guanidinobutyric acid	C5H11N3O2	145.0851	0.94
0c-009	Pyruvic acid	C3H4O3	88.0161	0.96
0c-010	$\alpha$ -Lactose	C12H22O11	388.1220	1.13



0c-011	Citraconic acid	C5H6O4	130.0267	1.19
0c-012	$\delta$ -Ribono-1,4-lactone	C5H8O5	148.0373	1.22
0c-013	Uric acid	C5H4N4O3	168.0284	1.26
0c-014	Uridine	C9H12N2O6	244.0696	1.28
0c-015	Cymoxanil	C7H10N4O3	198.0753	1.32
0c-016	N-Acetyl-DL-glutamic acid	C7H11NO5	189.0639	1.35
0c-017	Itaconic acid	C5H6O4	130.0268	1.37
0c-018	7-Methylguanine	C6H7N5O	165.0651	1.42
0c-019	Aminorex	C9H10N2O	162.0794	1.88
0c-020	8-Hydroxyquinoline	C9H7NO	145.0528	2.48
0c-021	N-Acetylvaline	C7H13NO3	159.0896	2.51
0c-022	2,3-Dihydroxybenzoic acid	C7H6O4	154.0267	2.60
0c-023	3,7-Dimethyluric acid	C7H8N4O3	196.0597	2.70
0c-024	2-Isopropylmalic acid	C7H12O5	176.0686	2.79
0c-025	2,3-Dihydro-1,4-benzodioxine-5-carboxylic acid	C9H8O4	180.0424	3.16
0c-026	4-Hydroxybenzoic acid	C7H6O3	138.0316	3.20
0c-027	Caffeic acid	C9H8O4	180.0422	3.60
0c-028	2,3-Dihydro-1-benzofuran-2-carboxylic acid	C9H8O3	164.0473	3.75
0c-029	Phenylacetic acid	C8H8O2	136.0526	4.01
0c-030	Artemisinin	C15H22O5	264.1359	4.38
0c-031	Xanthurenic acid	C10H7NO4	205.0374	4.59
0c-032	2,4-Dihydroxybenzoic acid	C7H6O4	154.0267	4.63
0c-033	Quercetin-3 $\beta$ -D-glucoside	C21H20O12	464.0943	4.82
0c-034	Eugenol	C10H12O2	164.0837	5.43
0c-035	3,4-Dihydroxyphenylpropionic acid	C9H10O4	164.0474	5.90
0c-036	4-Coumaric acid	C9H8O3	164.0474	6.55
0c-037	2,5-Dihydroxybenzaldehyde	C7H6O3	138.0317	6.56
0c-038	Resorcinol monoacetate	C8H8O3	152.0472	6.56
0c-039	3-Coumaric acid	C9H8O3	164.0475	7.75
0c-040	3,22-Dihydroxy-28-oxoolean-12-en-16-yl acetate	C32H50O5	514.3656	8.88
0c-041	Ursolic acid	C30H48O3	456.3593	9.28
0c-042	Isophorone	C9H14O	138.1045	9.32
0c-043	3-Acetyl-11-keto- $\beta$ -boswellic acid	C32H48O5	512.3498	9.69
0c-044	3-Phenylpropionitrile	C9H9N	131.0735	9.80