

SUPPLEMENTAL TABLE

Supplement to:

Antifungal activity and functional components of cell-free supernatant from *Bacillus amyloliquefaciens* LZN01 inhibit *Fusarium oxysporum* f. sp. *niveum* growth

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Table S1 Compounds in the CFS from *B. amyloliquefaciens* LZN01 and LB medium.

72h-ck				12h-ck				12h-72h			
Metabolites	m/z	Retention time (min)	Fold change (72h/ck)	Metabolites	m/z	Retention time (min)	Fold change (12h/ck)	Metabolites	m/z	Retention time (min)	Fold change (72h/12h)
Asp-Pro-Lys	359	1.85	0.11	N-epsilon-Acetyl-L-lysine	189	1.80	0.05	S-Japonin	695	2.57	4.95
L-Arginine	173	0.73	0.02	L-isoleucyl-L-proline	229	2.25	0.21	L-Isoleucine	130	1.29	0.01
N-epsilon.-Acetyl-L-lysine	189	1.80	0.02	Glycyl-Isoleucine	189	2.02	0.07	3-Indolepropionic acid	377	1.29	0.00
Indecainide	655	2.84	0.08	L-Glutamic acid	146	0.81	0.05	6-Chloroapigenin	349	2.96	2.02
Quinapril	439	2.64	94.11	L-Arginine	173	0.73	0.30	Austalide C	592	2.65	0.08
S-Japonin	695	2.57	7.79	Asp-Pro-Lys	359	1.85	0.54	Indecainide	655	2.84	0.09
3-Indolepropionic acid	377	1.29	0.00	2-(3-hydroxyphytyl)-3-phytyl-sn-glycerol	670	3.38	9.46	3-O-alpha-L-rhamnopyranosyl-3-hydroxy decanoyl-3-hydroxydecanoic acid	543	3.00	0.02
L-Leucine	132	1.05	0.10	24, 24-difluoro-1alpha, 25-dihydroxy-26, 27-dimethyl-24a-homovitamin D3 / 24, 24-difluoro-1alpha, 25-dihydroxy-26, 27-dimethyl-24a-homocholecalciferol	539	2.93	393.11	Methyl (5E, 17E)-18-bromo-octadeca-5, 17-diene-15-ynoate	735	3.82	0.19
D-Ribulose 5-phosphate	211	0.97	0.14	Iodotyrosine	306	1.77	2.58	Isopentyl gentiobioside	430	2.42	0.07

Adenosine monophosphate	346	1.00	0.15	2'-Hydroxyfurano [2'', 3'':4', 3'] chalcone	309	0.73	0.18	Monepalin B	779	1.24	0.18
2'-Hydroxyfurano[2'',3'':4',3']chalcone	309	0.73	0.01	Stemonacetal	799	3.32	19.24	L-Leucine	132	1.05	0.16
L-Glutamic acid	146	0.81	0.15	Naringenin	317	2.21	0.01	Pro-Pro-Lys	363	2.47	0.03
Phaseolic acid	525	3.18	13.12	5-Oxo-ETE-d7	370	9.07	29.27	L-Arginine	173	0.73	0.05
Nitenin	355	9.04	3.17	Inosine	267	1.08	0.01	Adenosine monophosphate	346	1.00	0.30
Quinidine barbiturate	539	2.72	0.21	PI (17:2(9Z, 12Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))	913	0.65	16.32	Leukotriene E4	438	3.31	0.01
Irinotecan	587	3.25	0.04	Fluocinolone acetonide	470	1.33	0.06	S-Adenosylhomocysteine	383	1.29	0.16
2-(3-hydroxyphytanyl)-3-phytanyl-sn-glycerol	669	3.38	27.12	Isopentyl gentiobioside	430	2.42	2.79	D-Ribulose 5-phosphate	211	0.97	0.21
5-Methoxytryptamine	211	0.72	0.05	Prosafrinine	328	8.32	82.30	5-Methoxytryptamine	211	0.72	0.06
Malvidin 3-gentiobiside	654	2.90	0.25	Guanosine	282	1.05	0.19	Esprocarb	553	2.38	0.02
S-Adenosylhomocysteine	383	1.29	0.12	Flumethasone Pivalate	512	2.78	6.66	Liquiritigenin 7-apiofuranoside-4'-glucoside	571	2.73	0.16
3-O-alpha-L-rhamnopyranosyl-3-hydroxydecanoyl-3-hydroxydecanoic acid	543	3.00	0.03	Nitenin	355	9.04	2.10	Palmatine cation	705	2.98	0.03
L-Isoleucine	130	1.29	0.01	7-Hydroxy-2-methylisoflavone	503	0.85	0.32	(+)-Myristinin A	569	2.97	0.08
Morphiceptin	504	2.98	0.13	Phaseolic acid	525	3.18	15.41	Malvidin 3-gentiobiside	654	2.90	0.27
Stemonacetal	799	3.32	24.96	17a-Ethynylestradiol	341	8.29	1.65	Tyrosyl-Histidine	654	2.13	7.72
Tyrosyl-Histidine	654	2.13	32.16	9Z-Heptatriacontene	502	3.21	0.14	PI (20:3(8Z, 11Z, 14Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))	954	3.54	0.00
Naringenin	317	2.21	0.01	24-methylene-cholesterol sulphate	499	1.31	13.75	5, 8, 11, 14-Octadecatetraynoic acid	535	3.92	0.01
Fluocinolone Acetonide	470	1.33	0.01	Adenosine monophosphate	346	1.00	0.51	Brosimone H	485	1.17	0.02
L-Histidine	154	0.73	0.02	N-palmitoyl alanine	372	8.32	14942.5 0	5-O-Desmethyldonepezil	366	3.22	0.02
L-Tyrosine	180	1.05	2.06	L-Octanoylcarnitine	286	8.19	133.01	PI (13:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z))	835	3.17	0.03

7-Hydroxy-2-methylisoflavone	503	0.85	0.19	(6R)-6-methylvitamin D3 6, 19-sulphur dioxide adduct / (6R)-6-methylcholecalciferol 6, 19-sulphur dioxide adduct	483	1.47	35.41	Hirsutidin 3-O-(6-O-p-coumaroyl) glucoside	698	0.99	0.42
Inosine	267	1.08	0.01	Di-2-propenyl pentasulphide	502	3.21	0.13	Patuletin 7-(6"-isobutyrylglucoside)	545	2.82	0.03
Methyl (5E, 17E)-18-bromo-octadeca-5, 17-diene-15-ynoate	735	3.82	0.31	Myriocin	400	7.67	3003.47	Flumethasone Pivalate	512	2.78	0.19
9Z-Heptatriacontene	501	3.21	0.03	Micropine	286	3.59	0.00	Isoswertisin 6'''-O-feruloyl 2''-O-glucoside	765	0.90	0.46
1-Hexanol arabinosylglucoside	414	2.36	0.40	L-Histidine	154	0.73	0.25	4'-Methoxychalcone	259	3.09	0.07
Cytidine	264	0.94	7.23	Decanoylcarnitine	314	7.95	38.44	UDP-GlcNAc	652	1.07	0.43
Di-2-propenyl pentasulphide	501	3.21	0.02	Cer (d18:1/2:0)	386	8.35	48.94	(6R)-6-methylvitamin D3 6, 19-sulphur dioxide adduct / (6R)-6-methylcholecalciferol 6, 19-sulphur dioxide adduct	483	1.47	0.00
Gabapentin	216	4.26	#DIV/0!	Palmitine cation	705	2.98	3.62	Ouabain	605	3.71	0.20
Esprocarb	553	2.38	0.03	Predurmillone	401	0.85	0.38	thevetin A	893	3.22	0.14
Decanoylcarnitine	314	7.95	11.55	N-palmitoyl glycine	358	7.90	4685.16	Ombuin 3-rutinoside-5-glucoside	821	1.03	0.44
17a-Ethynylestradiol	341	8.29	2.10	L-Tyrosine	180	1.05	1.37	Gabapentin	216	4.26	6.84
Pyroterebic acid	227	6.18	#DIV/0!	Patuletin 7-(6"-isobutyrylglucoside)	545	2.82	5.48	Exiguaflavanone M	487	7.36	0.08
N-palmitoyl alanine	372	8.32	7826.64	PC (6:0/0:0)	376	3.97	20.92	5-Methoxytryptophol	236	4.97	0.03
UDP-GlcNAc	652	1.07	0.13	Methyl (5E, 17E)-18-bromo-octadeca-5, 17-diene-15-ynoate	735	3.82	1.63	7-Hydroxy-5-methoxy-6-methylflavan	315	0.81	0.19
Pantothenic acid	218	2.19	53.76	Gentiopiricin	377	0.81	0.18	2-Geranyl-3,4,2',4'-tetrahydroxydihydroc	819	1.56	0.03

halcone											
N-palmitoyl glycine	358	7.90	2640.2	Irinotecan	587	3.25	0.46	3, 4-Dihydrocoumarin	166	1.46	1.60
7											
Monepalin B	779	1.24	0.22	Sphingofungin E	416	6.29	#DIV/0!	10S, 11R-epoxy-punaglandin 3	557	0.90	0.40
Sphingofungin E	416	6.29	#DIV/0!	UDP-GlcNAc	652	1.07	0.31	PA (20:3(8Z, 11Z, 14Z)/0:0)	481	7.85	30.74
!											
6-Chloroapigenin	349	2.96	1.71	cis-5-Tetradecenoylcarnitine	414	7.80	306.22	14, 15-HxA3-C(11S)	642	3.62	0.06
Guanosine	282	1.05	0.26	Sphingofungin F	400	6.85	#DIV/0!	VD 2716	527	4.10	0.02
Acacetin 7-glucuronosyl-(1->2)-glucuronide	681	0.73	0.02	Hexanoylcarnitine	258	7.75	12.22	Gamma-Glutamylglutamine	256	1.17	0.10
Micropine	286	3.59	0.01	5-O-Desmethyldonepezil	366	3.22	3.17	PI (17:0/0:0)	585	5.15	0.00
Myriocin	400	7.67	2221.0	Pantothenic acid	218	2.19	10.74	PS (12:0/0:0)	422	4.63	#DIV/0!
3											
7-Hydroxy-5-methoxy-6-methylflavan	315	0.81	0.18	PG (14:0/0:0)	501	8.00	175.18	Wanepimedeside A	723	1.05	0.40
5-Hydroxylysine	161	0.72	2.25	17, 18-dehydro-clavulone I	887	4.12	9.53	6-hydroxy-7E, 9E-Octadecadiene-11, 13, 15, 17-tetraynoic acid	559	1.51	0.16
PI (13:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z))	835	3.17	0.04	Thymidine	241	1.57	0.11	Pantothenic acid	218	2.19	5.01
Liquiritigenin 7-apiofuranoside-4'-glucoside	571	2.73	0.14	N-oleoyl glycine	384	7.97	515.73	Scilliroside	585	3.85	0.09
PA (20:3(8Z, 11Z, 14Z)/0:0)	481	7.85	83.49	Brosimone H	485	1.17	3.47	17, 18-dehydro-clavulone I	887	4.12	0.07
3, 4-Dihydrocoumarin	166	1.46	1.67	2, 5-undecadienal	187	2.21	0.02	Linocide B	681	2.34	0.22
Sphingofungin F	400	6.85	#DIV/0!	3-Indolepropionic acid	377	1.29	0.60	Testosterone glucuronide	509	3.42	0.08
!											
5, 8, 11, 14-Octadecatetraynoic acid	535	3.92	0.01	Sphingofungin C	430	6.53	#DIV/0!	(-)-Jolkinol A	525	2.93	0.04
Okanin 4'-(6"-p-coumarylglucoside)	595	0.90	0.39	Morphiceptin	504	2.98	0.51	Butyl 3'-O-acetyl-2'-O-butanoyl-4, 6, 4'-tri-O-(2-methylpropanoyl)-neohesperidoside	749	1.84	0.00
Aminoacetone	145	0.72	1.87	4'-Chloroaurone	277	2.21	0.00	Coproporphyrin III	635	3.27	0.19
Gentiopiricin	377	0.81	0.20	O-Phosphoethanolamine	281	1.03	0.17	PGP (16:0/18:1(9Z))	809	5.71	0.00

O-Phosphoethanolamine	281	1.03	0.08	Acacetin	681	0.73	0.26	Methylimidazoleacetic acid	185	0.90	0.45
				7-glucuronosyl-(1->2)-glucuronide							
Thymidine	241	1.57	0.06	L-Leucine	132	1.05	0.63	Catechin 3-O-rutinoside	597	1.02	0.48
PI (20:3(8Z, 11Z, 14Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))	953	3.54	0.00	Gallocatechin 4'-methyl ether	341	1.28	0.13	7, 8, 7', 8'-Tetrahydroastaxanthin	613	1.63	0.00
PI (17:2(9Z, 12Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))	913	0.65	11.95	Thevetin A	893	3.22	2.98	3'-Geranyl-2', 4', 6'-trihydroxychalcone	783	1.35	0.07
Ouabain	605	3.71	0.23	Leukotriene C4	624	2.66	7.04	PS (22:2(13Z, 16Z)/0:0)	598	3.12	0.04
2, 5-undecadienal	187	2.21	0.00	7, 8, 7', 8'-Tetrahydroastaxanthin	613	1.63	7.69	12-oxo-5E, 8E, 10Z-dodecatricienoic acid	229	1.09	0.11
(+)-Myristinin A	569	2.97	0.08	Melatonin	277	2.25	0.06	Ikariside D	523	2.35	0.04
PGP (18:3(6Z, 9Z, 12Z)/18:3(6Z, 9Z, 12Z))	885	3.22	45.70	Caloxanthin sulphate	685	2.77	15.10	L-Tyrosine	180	1.05	1.50
PC (6:0/0:0)	376	3.97	228.60	Vicenin-1 6''-O-acetate	627	1.05	0.63	Gossypol	517	1.05	0.28
2, 4, 7-tridecatrienal	213	1.29	0.04	Epsilon-(gamma-Glutamyl)-lysine	274	2.80	0.00	17alpha-(N-Acetyl-D-glucosaminyl)-estra diol 3-D-glucuronide	632	3.79	0.12
3-Indoleacrylic acid	205	2.20	1.54	Scillaren A	673	0.63	4.57	6-Hydroxyluteolin	549	1.15	0.39
								7-(6''-malonylglucoside)			
Gallocatechin 4'-methyl ether	341	1.28	0.09	Isoauricularin	839	3.69	1.78	(25S)-11alpha, 20, 26-trihydroxyecdysone	557	3.89	0.04
3'-Deoxymaysin	541	0.81	0.60	D-Ribulose 5-phosphate	211	0.97	0.68	Leukotriene C4	624	2.66	0.05
Scilliroside	585	3.85	0.04	Tephrowatsin B	671	3.68	0.11	Catechin 5, 3'-di-O-beta-D-glucopyranoside	595	2.27	0.10
14, 15-HxA3-C(11S)	642	3.62	0.08	Eggregiachloride C	703	4.04	0.25	O-Desmethylanolensin	515	1.05	0.40
Melatonin	277	2.25	0.00	Isoswertisin 6'''-O-feruloyl 2''-O-glucoside	765	0.90	1.38	27-nor-campestan-3beta, 4beta, 5alpha, 6alpha, 7beta, 8beta, 14alpha, 15alpha, 24-nonol	537	4.26	0.01
4'-Methoxychalcone	259	3.09	0.07	Artomunoxanthentrione	465	1.03	0.55	5, 7, 3', 4'-Tetrahydroxyflavanone	581	2.28	0.11
								7-alpha-L-arabinofuranosyl-(1->6)-			

								glucoside			
Brosimone H	485	1.17	0.08	PI (18:4(6Z, 9Z, 12Z, 15Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))	923	2.55	0.05	29-demethylgeodisterol-O-sulphite	513	1.03	0.19
5-Methoxytryptophol	236	4.97	0.04	Quassin	775	3.04	3.75	Coproporphyrinogen I	641	3.12	0.13
Villinol	483	1.77	0.08	PI (22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/20:5(5Z, 8Z, 11Z, 14Z, 17Z))	974	4.07	0.09	Geodisterol-O-sulphite	527	3.28	0.11
27-nor-campestan-3beta, 4beta, 5alpha, 6alpha, 7beta, 8beta, 14alpha, 15alpha, 24-nonol	537	4.26	0.01	Cys-Arg-Arg	889	3.47	24.37	SQMG (16:1(9Z)/0:0)	575	3.47	0.17
Nicotinuric acid	225	1.03	12.53	PA (14:1(9Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))	711	5.08	45.36	Salicifolioside A	607	1.52	0.26
Patuletin 7-(6''-isobutyrylglucoside)	545	2.82	0.16	Okaniin 4'-(6''-p-coumarylglucoside)	595	0.90	0.59	PG (14:0/0:0)	501	8.00	0.06
Norepinephrine sulphate	294	1.84	1.19	Lithocholytaurine	528	4.66	0.03	Peonidin 3-(6''-p-coumarylglucoside)	654	1.52	0.43
PS (22:2(13Z, 16Z)/0:0)	598	3.12	0.06	1(3)-glyceryl-6-keto-PGF1alpha	489	4.59	0.07	Herbacetin 3-glucoside-8-xyloside	641	1.05	0.58
PI (17:0/0:0)	585	5.15	0.00	L-Isoleucine	130	1.29	0.62	Diuvaretin	483	1.07	0.36
(+)-Tephrosin A	425	2.24	0.01	Merodesmosine	385	3.21	0.41	Pelargonidin 3-lathyroside	586	2.08	0.08
Scillaren A	673	0.63	7.75	Leukotriene E4	438	3.31	1.73	Nostoxanthin sulphate	683	3.38	0.06
Gossypol	517	1.05	0.27	Cerotic acid (d3)	798	1.63	0.24	PS (19:1(9Z)/0:0)	558	4.31	0.11
2-O-(beta-D-galactopyranosyl-(1->6)-beta-D-galactopyranosyl) 2S-hydroxynonanoic acid	479	4.49	10.20	Salicifolioside A	607	1.52	2.26	2', 4', 6', 3, 4-Pentahydroxy-3'-geranyl-5-prenyldihydrochalcone	988	4.59	0.02
15-HETE-T	426	3.31	0.02	Villinol	483	1.77	0.34	Aminoacetone	145	0.72	1.66
6-Hydroxyluteolin 7-(6''-malonylglucoside)	549	1.15	0.31	Hirsutidin 3-O-(6-O-p-coumaroyl) glucoside	698	0.99	1.34	3-Indoleacrylic acid	205	2.20	1.40
Tephrosin B	671	3.68	0.02	3'-Deoxymaysin	541	0.81	0.76	Butyl 3'-O-butanoyl-4, 6, 4'-tri-O-(2-methylpropanoyl)-neohesperidoside	683	2.52	0.13

Exiguaflavanone M	487	7.36	0.06	6-bromo-heneicosa-5E,9Z-dienoic acid	399	2.67	0.22	Quassin	775	3.04	0.07
Ac-Ser-Asp-Lys-Pro-OH	488	2.23	1.45	GS 1500	541	4.35	0.21	Caloxanthin sulphate	685	2.77	0.01
Cerotic acid(d3)	797	1.63	0.03	Diuvaretin	483	1.07	1.75	Anhydroicaritin	883	1.48	0.36
								3-galactosyl-(1->3)-rhamnoside-7-glucoside			
PGP (16:0/18:1(9Z))	809	5.71	0.00	(6RS, 24R)-24, 25-dihydroxyvitamin D3 6, 19-sulphur dioxide adduct / (6RS, 24R)-24, 25-dihydroxycholecalciferol 6, 19-sulphur dioxide adduct	501	1.96	3.70	PI (12:0/14:1(9Z))	745	3.63	0.02
(25S)-11alpha,20,26-trihydroxyecdysone	557	3.89	0.04	Moralbanone	471	1.34	0.15	2', 3', 4', 6'-Tetramethoxychalcone	655	2.87	0.28
12-oxo-5E,8E,10Z-dodecatricenoic acid	229	1.09	0.13	7, 8, 4'-Trihydroxy-3', 5'-dimethoxyflavanone 4'-O-glucoside	539	0.81	0.69	PC (6:0/0:0)	376	3.97	10.93
VD 2716	527	4.10	0.02	1,25-Dihydroxy-20S-21-(3-hydroxy-3-methylbutyl)-23-yne-26, 27-hexafluorovitamin D3	587	1.63	3.77	2-O-(beta-D-galactopyranosyl-(1->6)-beta-D-galactopyranosyl) 2S-hydroxynonanoic acid	479	4.49	14.62
Testosterone glucuronide	509	3.42	0.09	3'-Geranyl-2',4',6'-trihydroxychalcone	783	1.35	2.25	Decanoylcarnitine	314	7.95	0.30
2-Geranyl-3, 4, 2', 4'-tetrahydroxydihydrochalcone	819	1.56	0.03	3, 5, 6-Trimethoxy-3', 4'-methylene-dioxyfurano[2, 3:7, 8]flavone	417	0.73	0.73	Ikariside F	631	1.19	0.29
Gamma-Glutamylglutamine	256	1.17	0.11	PA (12:0/14:1(9Z))	583	4.32	3.85	Peonanin	916	1.14	0.38
Epsilon-(gamma-Glutamyl)-lysine	274	2.81	0.05	Ustilagic acid	783	3.92	0.35	Triuvaretin	589	3.79	0.21
Ustilagic acid	783	3.92	0.05	Coproporphyrin III	635	3.27	1.82	PI (16:0/0:0)	617	4.63	0.13
PI (22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z)/20:5(5Z, 8Z, 11Z, 14Z, 17Z))	974	4.07	0.00	PI (13:0/20:5(5Z, 8Z, 11Z, 14Z, 17Z))	835	3.17	1.64	Brosimacutin C	683	1.54	0.17
(-)-Jolkinol A	525	2.93	0.04	Isoamoritin	487	3.12	0.29	Carpelastofuran	567	1.39	0.23
Piperaduncin A	489	1.05	0.12	Scilliroside	585	3.85	0.48	Piperaduncin A	489	1.05	0.18
Butyl 3'-O-acetyl-2'-O-butanoyl-4, 6,	749	1.84	0.01	Methyl jasmonate	245	1.07	0.34	2'-O-Methylcajanone	417	1.28	0.16

4'-tri-O-(2-methylpropanoyl)-neohesperido side												
10S, 11R-epoxy-punaglandin 3	557	0.90	0.48	2, 4, 7-tridecatrienal	213	1.29	0.54	Anhydroicaritin	659	1.59	0.20	
								3-rhamnosyl-(1->2)-rhamnoside				
GS 1500	541	4.35	0.00	29-demethylgeodisterol-O-sulphite	513	1.03	1.72	Tephrowatsin B	671	3.68	0.14	
PI (18:4(6Z, 9Z, 12Z, 15Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))	923	2.55	0.02	PI (12:0/14:1(9Z))	745	3.63	2.08	Nicotinuric acid	225	1.03	6.44	
Nostoxanthin sulphate	683	3.38	0.06	9, 12, 13-TriHOME	329	7.30	0.27	Leucadenone A	539	2.31	0.08	
SQMG (16:1(9Z)/0:0)	575	3.47	0.25	SQDG (22:5(5Z, 8Z, 11Z, 14Z, 17Z)/16:1(13Z))	861	4.70	2.40	SQDG (22:5(5Z, 8Z, 11Z, 14Z, 17Z)/16:1(13Z))	861	4.70	0.00	
7, 8, 4'-Trihydroxy-3', 5'-dimethoxyflavanone 4'-O-glucoside	539	0.81	0.61	Chenodeoxycholic acid 3-glucuronide	589	4.46	0.29	Leukotriene D4	495	2.60	0.01	
3'-Geranyl-2', 4', 6'-trihydroxychalcone	783	1.35	0.15	Butyl 3'-O-acetyl-2'-O-butanoyl-4, 6, 4'-tri-O-(2-methylpropanoyl)-neohesperidoside	749	1.84	1.82	(+)-Tephrocin A	425	2.24	0.02	
Coproporphyrinogen I	641	3.12	0.15	(+)-Tephrocin A	425	2.24	0.50	Epimedin C	803	1.84	0.26	
geodisterol-O-sulphite	527	3.28	0.13	Peonidin 3-(6''-p-coumarylglucoside)	654	1.52	1.33	18-acetoxy-PGF2alpha-11-acetate methyl ester	513	3.82	0.03	
Catechin 5, 3'-di-O-beta-D-glucopyranoside	595	2.27	0.09	Alpinumisoflavone dimethyl ether	727	3.02	1.34	rhodexin A	581	4.84	0.00	
5, 7, 3', 4'-Tetrahydroxyflavanone 7-alpha-L-arabinofuranosyl-(1->6)-glucoside	581	2.28	0.10	Citric acid	191	1.05	0.45	Taurochenodeoxycholic acid 3-sulphate	562	4.33	0.07	
Deoxyipyridinolone	457	3.50	0.20	Catechin 3-O-rutinoside	597	1.02	1.26	PA (12:0/14:1(9Z))	583	4.32	0.00	
Methylimidazoleacetic acid	185	0.90	0.54	Esprocarb	553	2.38	1.33	Alpinumisoflavone dimethyl ether	727	3.02	0.49	
6-hydroxy-7E, 9E-Octadecadiene-11, 13, 15, 17-tetraynoic acid	559	1.51	0.19	PS (18:3(6Z, 9Z, 12Z)/22:6(4Z, 7Z, 10Z, 13Z, 16Z, 19Z))	810	5.00	0.40	PI (20:5(5Z, 8Z, 11Z, 14Z, 17Z)/0:0)	617	3.59	0.25	
Isoamoritin	487	3.12	0.01	Epothilone B	488	4.64	0.46	26, 26, 26, 27, 27, 27-hexafluoro-1alpha,	499	4.07	0.13	

								25-dihydroxy-16, 17, 23, 23, 24, 24-hexadehydrovitamin D3 / 26, 26, 26, 27, 27, 27-hexafluoro-1alpha, 25-dihydroxy-16, 17, 23, 23, 24, 24-hexadehydrocholecalciferol			
Hirsutidin 3-O-(6-O-p-coumaroyl) glucoside	698	0.99	0.57	17alpha-(N-Acetyl-D-glucosaminy)- estradiol 3-D-glucuronide	632	3.79	0.56	Ustilagic acid	783	3.92	0.13
2', 4', 6', 3, 4-Pentahydroxy-3'-geranyl-5-prenyldihydro chalcone	988	4.59	0.01	14, 15-HxA3-C(11S)	642	3.62	1.46	Taurochenodeoxycholic acid 7-sulphate	578	4.10	0.25
O-Desmethylangolensin	515	1.05	0.44	UDP-2, 3-diacyl-GlcN	998	3.06	1.36	Moralbanone	471	1.34	0.13
6-bromo-heneicosa-5E, 9Z-dienoic acid	399	2.67	0.10	SQMG (16:1(9Z)/0:0)	575	3.47	1.42	Protoporphyrin IX	543	2.94	0.27
Ikariside F	631	1.19	0.33	Sempervirenoside B	895	2.67	1.40	Isosophoranone	875	1.84	0.06
Ombuin 3-rutinoside-5-glucoside	821	1.03	0.53	10S, 11R-epoxy-punaglandin 3	557	0.90	1.20	Cys-Arg-Arg	889	3.47	0.03
17alpha-(N-Acetyl-D-glucosaminy)- estradiol 3-D-glucuronide	632	3.79	0.07					epothilone D	512	1.56	0.02
PI (12:0/14:1(9Z))	745	3.63	0.05					Chaetoglobosin A	573	1.32	0.14
Vicenin-1 6"-O-acetate	627	1.05	0.63					Adonixanthin/ 4-Ketozeaxanthin	627	4.78	0.69
18-acetoxy-PGF2alpha-11-acetate methyl ester	513	3.82	0.03					PS (8:0/8:0)	556	4.49	0.11
Poriolide	611	0.90	0.61					2-O-(beta-D-galactopyranosyl-(1->6)-beta -D-galactopyranosyl) 2S-hydroxyundecanoic acid	547	2.00	0.08
Anhydroicaritin 3-rhamnosyl-(1->2)-rhamnoside	659	1.59	0.23					Brousoflavan A	851	4.78	0.18
Moralbanone	471	1.34	0.02					Euchrenone a14	517	2.90	0.16
Taurochenodeoxycholic acid 3-sulphate	562	4.33	0.08					2-O-(beta-D-galactopyranosyl-(1->6)-beta	575	2.77	0.15

				-D-galactopyranosyl)			
				2S-hydroxytridecanoic acid			
Pelargonidin 3-lathyroside	586	2.08	0.07	N-palmitoyl alanine	372	8.32	0.52
PS (19:1(9Z)/0:0)	558	4.31	0.08	Ac-Ser-Asp-Lys-Pro-OH	488	2.23	1.37
Rhodexin A	581	4.84	0.00	5-Hydroxy-6, 7, 3', 4', 5'-pentamethoxyflavanone 5-O-rhamnoside	581	1.39	0.50
7, 8, 7', 8'-Tetradehydroastaxanthin	613	1.63	0.04	thevetin B	903	4.28	0.40
PA (17:0/0:0)	445	3.51	0.01	Genistein 7-O-glucoside-6''-malonate	563	2.08	0.26
PA (18:4(6Z, 9Z, 12Z, 15Z)/0:0)	475	2.90	0.14	PGF2alpha-dihydroxypropanylamine	854	5.25	0.45
Triuvaretin	589	3.79	0.31	Sempervirenoside B	895	2.67	0.55
3-Methyl-2-oxovaleric acid	175	3.45	#DIV/0 !	N-palmitoyl glycine	358	7.90	0.56
Methyl jasmonate	245	1.07	0.14	11-Oxo-androsterone glucuronide	525	4.03	0.60
Carpelastofuran	567	1.39	0.29	3, 5, 6-Trimethoxy-3', 4'-methylene-dioxyfurano [2, 3:7, 8]flavone	417	0.73	1.32
Herbacetin 3-glucoside-8-xyloside	641	1.05	0.63	Neoglabrescin A	899	2.49	2.13
Epothilone B	488	4.64	0.00	UDP-2, 3-diacyl-GlcN	998	3.06	1.58
Chandalone	449	0.73	3.18	Porphobilinogen	225	2.03	1.38
2'-O-Methylcajanone	417	1.28	0.15	Nonoxynol-9	634	7.99	19.62
thevetin A	893	3.22	0.43				
Antiarone J	911	5.30	0.05				
Xanthine	151	0.99	0.55				
Brosimacutin C	683	1.54	0.24				
2', 3', 4', 6'-Tetramethoxychalcone	655	2.87	0.36				
Leucadenone A	539	2.31	0.08				

Butyl 3'-O-butanoyl-4, 6, 4'-tri-O-(2-methylpropanoyl)-neohesperido side	683	2.52	0.15
26, 26, 26, 27, 27, 27-hexafluoro-1alpha, 25-dihydroxy-16, 17, 23, 23, 24, 24-hexadehydrovitamin D3 / 26, 26, 26, 27, 27, 27-hexafluoro-1alpha, 25-dihydroxy-16, 17, 23, 23, 24, 24-hexadehydrocholecalciferol	499	4.07	0.12
PS (8:0/8:0)	556	4.49	0.09
Leukotriene D4	495	2.60	0.00
PI (20:5(5Z, 8Z, 11Z, 14Z, 17Z)/0:0)	617	3.59	0.29
PGF2alpha-dihydroxypropylamine	853	5.25	0.42
PS (18:3(6Z,9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19 Z))	810	4.50	0.00
UDP-2,3-diacyl-GlcN	998	3.06	2.14
PS (18:1(9Z)/0:0)	544	4.03	0.08
epothilone D	512	1.56	0.02
2-O-(beta-D-galactopyranosyl-(1->6)-beta-D -galactopyranosyl) 2S-hydroxyundecanoic acid	547	2.00	0.07
Anhydroicaritin 3-galactosyl-(1->3)-rhamnoside-7-glucoside	883	1.48	0.41
Linocide B	681	2.34	0.29
PI (16:0/0:0)	617	4.63	0.19
Neoglabrescin A	899	2.49	3.36

Protoporphyrin IX	543	2.94	0.32
Brousoflavan A	851	4.78	0.16
Chenodeoxycholic acid 3-glucuronide	589	4.46	0.05
Euchrenone a14	517	2.90	0.13
Chaetoglobosin A	573	1.32	0.14
Peonanin	916	1.14	0.47
Sulphamisterin	460	2.00	0.15
Catechin 3-O-rutinoside	597	1.02	0.61
Ptilosteroid A	445	3.15	0.26
Leukotriene C4	624	2.66	0.35
thevetin B	903	4.28	0.41
2-O-(beta-D-galactopyranosyl-(1->6)-beta-D -galactopyranosyl) 2S-hydroxytridecanoic acid	575	2.77	0.19
Genistein 7-O-glucoside-6''-malonate	563	2.08	0.26
5-Hydroxy-6, 7, 3', 4', 5'-pentamethoxyflavanone 5-O-rhamnoside	581	1.39	0.51
Alpinumisoflavone dimethyl ether	727	3.02	0.65
9, 12, 13-TriHOME	329	7.30	0.29
Porphobilinogen	225	2.03	1.54
17, 18-dehydro-clavulone I	887	4.12	0.64
11-Oxo-androsterone glucuronide	525	4.03	0.66