Table S1. List and characteristics of the 164 "core" metabolites (including 72 identified) in isolates SG-S, SG-R and SG-rev.

							Abundance			Standard Deviation			Standard Error			p (SG-R versus SG-S)		(SG-R versus SG-S)	p (SG-R versus SG-rev)	
Name	**Formula**	**Mass**	**RT[a]**	**Mode[b]**	**FbF/MFE[c]**	**MM/Stnd[d]**	**SG-S**	**SG-R**	**SG-rev**	**SG-S**	**SG-R**	**SG-Rev**	**SG-S**	**SG-R**	**SG-rev**	**Univariate[e]**	**Bivariate[f]**	**SAM**	**Univariate[e]**	**Bivariate[f]**
Acetylaminobutanal	C6H11NO2	130.0863	7.5	POS	FbF	MM	1	0.923484	1.074218	0.154937	0.143972	0.352788	0.044726	0.041561	0.101841					
Acetyllysine	**C8H16N2O3**	**189.1234**	**1.3**	**POS**	**FbF**	**MM**	**1**	**1.469279**	**1.038538**	**0.347116**	**0.463426**	**0.57961**	**0.100204**	**0.13378**	**0.167319**	**< 0.01**	**< 0.01**	*	**0.06**	**NS**
Acetylneuraminate	C11H19NO9	310.1133	2.5	POS	FbF	MM	1	0.98896	0.959795	0.156273	0.316849	0.284569	0.045112	0.091467	0.082148					
Acetylornithine	C7H14N2O3	175.1077	6	POS	FbF	MM	1	0.778985	0.876928	0.096294	0.069078	0.129621	0.027798	0.019941	0.037418			*		
Adenine	C5H5N5	136.0618	6.7	POS	FbF	MM	1	1.06411	0.966932	0.170441	0.218758	0.227917	0.049202	0.06315	0.065794					
Adenosine	C10H13N5O4	268.104	5.2	POS	FbF	MM	1	0.771609	0.777375	0.065643	0.069024	0.111362	0.018949	0.019925	0.032147			*		
Alanine	C3H7NO2	90.055	7.3	POS	FbF	standard	1	0.909987	0.856267	0.091726	0.112367	0.156532	0.026479	0.032438	0.045187					
Alpha-ketoglutarate	C5H6O5	145.0143	1	NEG	FbF	standard	1	0.839598	1.514367	0.231428	0.117305	0.358671	0.066807	0.033863	0.103539			*		
Aminoacrylate	C3H5NO2	88.0393	6	POS	FbF	MM	1	0.613919	0.844481	0.229383	0.136932	0.347323	0.066217	0.039529	0.100264			*		
Aminoadipate	C6H11NO4	162.0761	6	POS	FbF	MM	1	0.631352	0.820226	0.295345	1.497671	0.631546	0.085259	0.43234	0.182312	< 0.01	< 0.01		< 0.01	< 0.05
Aminobutyraldehyde	C4H9NO	88.07569	2	POS	FbF	MM	1	0.8463	1.022939	0.174853	0.191438	0.340486	0.050476	0.055263	0.09829					
Aminocyanobutanoic acid	C5H8N2O2	129.0659	7	POS	FbF	MM	1	0.645552	0.963332	0.168478	0.117299	0.221023	0.048635	0.033861	0.063804			*		
Aminocyclopropane carboxylic acid	C4H7NO2	102.055	6	POS	FbF	MM	1	0.740458	0.918946	0.195426	0.118032	0.303059	0.056415	0.034073	0.087486			*		
Aminobutanoate	**C4H9NO2**	**104.0706**	**6**	**POS**	**FbF***	**standard**	**1**	**0.217881**	**0.854082**	**0.147029**	**0.193553**	**0.117456**	**0.042443**	**0.055874**	**0.033907**	**< 0.01**	**< 0.01**	*	**< 0.01**	**< 0.05**
Amino-oxopimelate	C7H11NO5	190.071	2.5	POS	FbF	MM	1	1.052571	1.000646	0.210538	0.232846	0.206761	0.060777	0.067217	0.059687					
Anthranilate	C7H7NO2	138.055	7.5	POS	FbF	MM	1	0.721654	0.83092	0.16143	0.229098	0.203264	0.046601	0.066135	0.058677					
Arginine	C6H14N4O2	175.119	13	POS	FbF	standard	1	0.925981	0.805117	0.052677	0.071807	0.156392	0.015207	0.020729	0.045147					
Aspargine	C4H8N2O3	133.0608	8	POS	FbF	standard	1	0.95353	0.83681	0.196112	0.167226	0.348611	0.056613	0.048274	0.100635					
Aspartate	C4H7NO4	134.0448	5.5	POS	FbF	standard	1	0.600656	0.782556	0.226349	0.135593	0.376746	0.065341	0.039142	0.108757			*		
Aspartate semialdehyde	C4H7NO3	118.0499	1.3	POS	FbF	MM	1	1.839666	2.487206	0.137784	0.480358	0.980309	0.039775	0.138668	0.282991	< 0.01	< 0.01	*	NS	NS
Carbamoyl aspartate	C5H8N2O5	177.0506	1.3	POS	FbF	MM	1	0.787375	0.980157	0.308004	0.175922	0.518533	0.088913	0.050784	0.149688					
Cis-aconitate	C6H6O6	173.0092	1	NEG	FbF	MM	1	1.056753	1.473807	0.122092	0.169239	0.356544	0.035245	0.048855	0.102926					
Citrate	C6H8O7	191.0197	1.4	NEG	FbF	standard	1	1.111278	1.265103	0.065977	0.133414	0.081643	0.019046	0.038513	0.023568					
Citrulline	**C6H13N3O3**	**176.103**	**9**	**POS**	**FbF**	**standard**	**1**	**1.633528**	**1.019183**	**0.194893**	**0.314853**	**0.203843**	**0.056261**	**0.09089**	**0.058844**	**< 0.01**	**< 0.01**	*	**< 0.01**	**< 0.05**
d-ala-dala	C6H12N2O3	161.0921	7	POS	FbF	MM	1	0.865998	0.697402	0.266306	0.224254	0.237289	0.076876	0.064736	0.068499					
Deoxyadenosine	C10H13N5O3	252.1091	11	POS	FbF	MM	1	0.397526	0.411628	0.062861	0.314536	0.276458	0.018147	0.090799	0.079807					
Fumarate	C4H4O4	115.0037	1.2	NEG	FbF	standard	1	0.893414	1.273897	0.208019	0.142593	0.310989	0.06005	0.041163	0.089775					
Galactonate	C6H12O7	195.051	2.4	NEG	FbF	MM	1	0.864626	1.241979	0.203403	0.185369	0.205166	0.058717	0.053511	0.059226					
Glucose	C6H12O6	179.0561	2.2	NEG	FbF	standard	1	1.295632	1.42341	0.133169	0.137177	0.281805	0.038443	0.039599	0.08135	< 0.01	< 0.01	*	NS	NS
Glutamate	C5H9NO4	146.0459	6.4	NEG	FbF	standard	1	0.95128	1.332839	0.222281	0.166498	0.398066	0.064167	0.048064	0.114912					
Glutamine	C5H10N2O3	145.0619	8	NEG	FbF	standard	1	1.133111	1.586426	0.370147	0.559771	0.878739	0.106852	0.161592	0.25367					
Glycerate	C3H6O4	105.0193	2.3	NEG	FbF	MM	1	1.381826	1.906643	0.320244	0.259625	0.699394	0.092447	0.074947	0.201898	< 0.01	< 0.01	*	< 0.01	< 0.05
Glycine	C2H5NO2	76.0393	7	POS	FbF	standard	1	1.085894	0.815468	0.056524	0.152026	0.143558	0.016317	0.043886	0.041442					
Guanidonobutanoate	C5H11N3O2	130.0975	6.2	POS	FbF	MM	1	0.944683	0.749528	0.204608	0.220282	0.224656	0.059065	0.06359	0.064853					
Guanidinobutanal	C5H11N3O	146.0924	6	POS	FbF	MM	1	0.858653	0.917739	0.047039	0.239627	0.166736	0.013579	0.069174	0.048133					
Guanine	C5H5N5O	152.0567	6	POS	FbF	MM	1	0.915869	0.906286	0.116692	0.154992	0.155817	0.033686	0.044742	0.044981					
Guanosine	C10H13N5O5	284.099	3	POS	FbF	MM	1	0.652825	0.761439	0.088464	0.07925	0.109693	0.025537	0.022878	0.031666			*		
Hexose phosphate	C6H13O9P	259.0224	5.0-6.0	NEG	FbF	standard	1	0.465002	1.193006	0.153405	0.222532	0.322405	0.044284	0.06424	0.09307			*		
Histidine	C6H9N3O2	156.0768	12	POS	FbF	standard	1	1.026585	0.777617	0.245842	0.164832	0.265679	0.070969	0.047583	0.076695					
Homovanillin	C9H10O3	165.0557	1	NEG	FbF	MM	1	1.263675	1.057825	0.377098	0.356348	0.303722	0.108859	0.102869	0.087677					
Homovanillinate	**C9H10O4**	**181.0506**	**1.3**	**NEG**	**FbF**	**MM**	**1**	**0.670138**	**1.070788**	**0.250429**	**0.109402**	**0.423357**	**0.072293**	**0.031582**	**0.122213**	**< 0.05**	**NS**	*	**0.06**	**NS**
Hypoxanthine	C5H4N4O	137.0458	2.5	POS	FbF	MM	1	1.073516	0.941069	0.130912	0.203771	0.181739	0.037791	0.058824	0.052464					
Lactaldehyde	C3H6O2	73.0295	1.3	NEG	FbF	MM	1	0.687728	1.311898	0.254423	0.096284	0.457926	0.073446	0.027795	0.132192			*		
Lactate	C3H6O3	89.02442	2.5	NEG	FbF	standard	1	1.242906	1.296777	0.143625	0.154184	0.287386	0.041461	0.044509	0.082961	<0.01	<0.01	*	NS	NS
Leucine	C6H13NO2	132.1019	6	POS	FbF	standard	1	0.924841	1.059153	0.115536	0.090431	0.102209	0.033352	0.026105	0.029505					
Lysine	C6H14N2O2	147.1128	12	POS	FbF	standard	1	0.770636	0.895513	0.29421	0.204277	0.166971	0.084931	0.05897	0.0482					
Malate	C4H6O5	133.0143	1.3	NEG	FbF	standard	1	0.98519	1.310312	0.177941	0.116564	0.39376	0.051367	0.033649	0.113669					
Methionine	C5H11NO2S	150.0583	5.6	POS	FbF	MM	1	0.773346	0.875352	0.087942	0.090049	0.111999	0.025387	0.025995	0.032331			*		
Methionine oxide	C5H11NO3S	166.0532	9.4	POS	FbF	MM	1	1.072472	0.968337	0.049095	0.099481	0.088942	0.014173	0.028718	0.025675					
Methylglyoxal	C3H4O2	71.01385	1.3	NEG	FbF	MM	1	0.343742	0.881903	0.262406	0.499159	0.340359	0.07575	0.144095	0.098253					
Methylthioadenosine	C11H15N5O3S	298.0968	4.5	POS	FbF	MM	1	1.087744	0.805887	0.061811	0.167935	0.149906	0.017843	0.048479	0.043274					
Methymalate	**C5H8O5**	**147.0299**	**1.3**	**NEG**	**FbF**	**MM**	**1**	**0.485834**	**1.565936**	**0.300271**	**0.17356**	**0.419497**	**0.086681**	**0.050102**	**0.121098**	**<0.01**	**<0.01**	*	**<0.01**	**<0.01**
Ornithine	C5H12N2O2	133.0972	12	POS	FbF	standard	1	1.163482	0.796735	0.328578	0.300087	0.295385	0.094852	0.086628	0.08527					
Oxoisocapriopoic acid	C6H10O3	129.0557	6	NEG	FbF	MM	1	1.166124	1.706392	0.246722	0.161477	0.334154	0.071223	0.046614	0.096462					
Oxoproline	C5H7NO3	130.0499	1.5	POS	FbF	MM	1	0.786362	0.657382	0.539843	0.504622	0.798848	0.155839	0.145672	0.230607					
Pentose phosphate	**C5H11O8P**	**229.0119**	**4.3**	**NEG**	**FbF**	**MM**	**1**	**0.356736**	**1.37736**	**0.288669**	**0.219981**	**0.572849**	**0.083332**	**0.063503**	**0.165367**	**<0.01**	**<0.01**	*	**<0.01**	**<0.01**
Phenylalanine	C9H11NO2	166.0863	5.5	POS	FbF	standard	1	0.867046	1.076365	0.151568	0.088381	0.155846	0.043754	0.025513	0.044989					
Phenylpyruvate	C9H8O3	163.0401	1.2	NEG	FbF	MM	1	0.701159	1.459753	0.262198	0.15677	0.370934	0.07569	0.045256	0.107079					
Proline	C5H9NO2	116.0706	8	POS	FbF	standard	1	0.801802	0.995126	0.168488	0.107576	0.209467	0.048638	0.031054	0.060468			*		
Propanoyl phosphate	C3H7O5P	152.9958	2.7	NEG	FbF	MM	1	0.644955	0.989407	0.117933	0.125353	0.214964	0.034044	0.036186	0.062055			*		
Propynoate	C3H2O2	68.9982	0.5	NEG	FbF	MM	1	0.905836	1.318814	0.213036	0.232603	0.271331	0.061498	0.067147	0.078327					
Pyruvate	C3H4O3	87.00877	1.5	NEG	FbF	standard	1	1.261675	1.397717	0.149393	0.1444	0.197326	0.043126	0.041685	0.056963	< 0.01	< 0.01	*	NS	NS
Serine	C3H7NO3	106.0499	7	POS	FbF	MM	1	1.031986	0.86434	0.044747	0.164958	0.130794	0.012917	0.047619	0.037757					
Succinate semialdehyde	C4H6O3	101.0244	1.3	NEG	FbF	MM	1	1.078008	1.810041	0.207965	0.206952	0.43375	0.060034	0.059742	0.125213					

Succinic acid	C4H6O4	117.0193	1	NEG	FbF	standard	1	0.664867	1.333608	0.263923	0.102556	0.513289	0.076188	0.029605	0.148174			*		
Succinylarginine	C10H18N4O5	275.135	9	POS	FbF	MM	1	0.809202	0.828366	0.166337	0.106764	0.288891	0.048017	0.03082	0.083396					
Tartronate semialdehyde	C3H4O4	103.0037	1.2	NEG	FbF	MM	1	1.027123	1.387024	0.134233	0.244037	0.429901	0.03875	0.070447	0.124102					
Threonine	C4H9NO3	120.0655	6.7	POS	FbF	MM	1	1.181481	0.886601	0.189266	0.156777	0.201309	0.054636	0.045258	0.058113					
Tryptophan	C11H12N2O2	205.0972	5	POS	FbF	standard	1	0.824303	0.866012	0.041526	0.114634	0.096432	0.011988	0.033092	0.027837					
Tyramine	C8H11NO	138.0913	5.7	POS	FbF	MM	1	0.75862	0.887078	0.062517	0.259008	0.12814	0.018047	0.074769	0.036991					
Tyrosine	C9H11NO3	182.0812	5.5	POS	FbF	standard	1	0.680746	0.911988	0.137991	0.107538	0.143568	0.039834	0.031044	0.041444			*		
Valine	C5H11NO2	118.0863	6	POS	FbF	standard	1	0.880527	1.100558	0.159041	0.11347	0.231039	0.045911	0.032756	0.066695					
1		66.0152	12.725	POS	MFE	NA	1	0.892013	0.977816	0.171358	0.223051	0.244133	0.049467	0.064389	0.070475					
2		71.0744	6.663	POS	MFE	NA	1	0.851316	0.902271	0.203098	0.06992	0.222442	0.058629	0.020184	0.064213					
3		83.0377	6.434	POS	MFE	NA	1	0.735646	0.918944	0.187495	0.227299	0.214732	0.054125	0.065616	0.061988	< 0.01	<0.05		< 0.01	NS
4		83.0738	12.352	POS	MFE	NA	1	0.804947	0.901519	0.082864	0.076274	0.149151	0.023921	0.022018	0.043056					
5		85.0529	2.094	POS	MFE	NA	1	0.975789	0.95405	0.118569	0.151995	0.157035	0.034228	0.043877	0.045332					
6		85.0896	6.106	POS	MFE	NA	1	0.873986	0.938447	0.22579	0.208135	0.192755	0.06518	0.060083	0.055644					
7		89.048	7.364	POS	MFE	NA	1	0.912598	0.860174	0.089802	0.105581	0.158416	0.025924	0.030479	0.045731					
8		99.0683	2.27	POS	MFE	NA	1	0.940628	0.914287	0.07085	0.092803	0.123708	0.020453	0.02679	0.035711					
9		103.063	7.752	POS	MFE	NA	1	0.069318	0.042194	0.152675	0.239174	0.466065	0.044074	0.069044	0.134541	< 0.01	<0.01		< 0.01	<0.01
10		113.0584	8.008	POS	MFE	NA	1	0.851477	0.888303	0.154883	0.12515	0.147738	0.044711	0.036128	0.042648					
11		119.0728	5.777	POS	MFE	NA	1	0.907157	0.917748	0.061804	0.087924	0.092363	0.017841	0.025382	0.026663					
12		131.0612	7.415	POS	MFE	NA	1	1.173877	1.852636	0.29309	0.194469	0.431541	0.084608	0.056138	0.124575					
13		196.1218	1.689	POS	MFE	NA	1	0.801772	0.845062	0.061674	0.104379	0.066485	0.017804	0.030132	0.019193					
14		197.0351	2.597	POS	MFE	NA	1	0.663496	0.845054	0.18351	0.132501	0.263977	0.052975	0.03825	0.076204	< 0.01	NS		NS	NS
15		211.0949	2.723	POS	MFE	NA	1	0.990226	0.843131	0.081467	0.102704	0.107159	0.023518	0.029648	0.030934					
16		226.1213	1.165	POS	MFE	NA	1	0.835555	0.861482	0.067988	0.135534	0.091036	0.019626	0.039125	0.02628					
17		228.0889	1.659	POS	MFE	NA	1	0.829954	0.873634	0.055243	0.102778	0.058403	0.015947	0.02967	0.01686					
18		244.1223	1.586	POS	MFE	NA	1	0.819177	0.841755	0.051348	0.103415	0.073989	0.014823	0.029853	0.021359					
19		256.1419	9.229	POS	MFE	NA	1	0.972181	1.113492	0.322666	0.338237	0.616173	0.093146	0.097641	0.177874					
20		260.1184	1.613	POS	MFE	NA	1	0.812918	0.883862	0.084753	0.104356	0.091939	0.024466	0.030125	0.02654					
21		264.078	5.869	POS	MFE	NA	1	0.613774	0.805991	0.230708	0.160606	0.37801	0.0666	0.046363	0.109122	< 0.01	NS		< 0.05	NS
22		311.1806	1.658	POS	MFE	NA	1	0.956538	0.835644	0.180611	0.176806	0.153903	0.052138	0.051039	0.044428					
23		314.1688	1.243	POS	MFE	NA	1	0.737119	0.897641	0.129674	0.103877	0.201229	0.037434	0.029987	0.05809					
24		338.2473	1.162	POS	MFE	NA	1	0.952889	0.854139	0.071061	0.125627	0.106662	0.020514	0.036265	0.030791					
25		355.2752	1.159	POS	MFE	NA	1	0.725559	0.753115	0.162895	0.134057	0.110058	0.047024	0.038699	0.031771	< 0.05	NS		NS	NS
26		382.2741	1.185	POS	MFE	NA	1	0.933194	0.846041	0.082697	0.122682	0.132448	0.023872	0.035415	0.038235					
27		384.2392	7.234	POS	MFE	NA	1	1.041311	0.830726	0.089804	0.13383	0.112521	0.025924	0.038633	0.032482					
28		389.1935	9.263	POS	MFE	NA	1	0.695412	0.653872	0.165334	0.142572	0.356578	0.047728	0.041157	0.102935					
29		397.2809	1.144	POS	MFE	NA	1	0.855459	0.89576	0.083766	0.190855	0.23276	0.024181	0.055095	0.067192					
30		399.3012	1.178	POS	MFE	NA	1	0.74911	0.779743	0.134055	0.107813	0.115326	0.038698	0.031123	0.033292	< 0.05	NS		NS	NS
31		411.2693	1.855	POS	MFE	NA	1	0.983063	0.833168	0.618923	0.263316	0.276262	0.178668	0.076013	0.07975					
32		411.7716	1.851	POS	MFE	NA	1	0.963284	0.842071	0.113259	0.129709	0.126854	0.032695	0.037444	0.03662					
33		420.2272	1.163	POS	MFE	NA	1	0.757303	0.854127	0.293119	0.147745	0.281789	0.084616	0.04265	0.081345					
34		426.2965	1.197	POS	MFE	NA	1	0.910413	0.98383	0.105173	0.130527	0.107329	0.030361	0.03768	0.030983					
35		433.2844	1.983	POS	MFE	NA	1	1.00631	0.770418	0.147525	0.156978	0.178088	0.042587	0.045316	0.05141					
36		433.7792	1.978	POS	MFE	NA	1	0.964028	0.867782	0.135806	0.152558	0.14158	0.039204	0.04404	0.040871					
37		441.2096	13.419	POS	MFE	NA	1	1.024973	0.787284	0.071967	0.059656	0.115815	0.020775	0.017221	0.033433					
38		443.3232	1.193	POS	MFE	NA	1	0.751712	0.799471	0.147414	0.117901	0.126139	0.042555	0.034035	0.036413	< 0.05	NS		NS	NS
39		455.2826	2.121	POS	MFE	NA	1	1.241114	0.85358	0.094031	0.206361	0.167124	0.027145	0.059571	0.048244					
40		460.281	12.611	POS	MFE	NA	1	1.002274	0.870182	0.047015	0.103697	0.081391	0.013572	0.029935	0.023495					
41		474.2182	6.361	POS	MFE	NA	1	1.000998	0.899475	0.051675	0.127973	0.081146	0.014917	0.036943	0.023425					
42		485.3104	2.148	POS	MFE	NA	1	0.379258	0.837661	0.170313	0.295155	0.156189	0.049165	0.085204	0.045088	< 0.01	< 0.01		< 0.01	NS
43		485.8201	2.347	POS	MFE	NA	1	0.890059	0.797215	0.092132	0.099993	0.07567	0.026596	0.028865	0.021844					
44		486.3167	2.335	POS	MFE	NA	1	1.016202	0.797592	0.083896	0.115909	0.113949	0.024219	0.03346	0.032894					
45		487.354	1.239	POS	MFE	NA	1	0.735629	0.793954	0.176735	0.114204	0.168831	0.051019	0.032968	0.048737	< 0.05	NS		NS	NS
46		524.261	3.601	POS	MFE	NA	1	1.319172	1.147413	0.097385	0.172231	0.211971	0.028113	0.049719	0.061191					
47		525.8088	12.552	POS	MFE	NA	1	1.024177	0.817408	0.08566	0.092469	0.090084	0.024728	0.026693	0.026005					
48		529.8452	2.776	POS	MFE	NA	1	1.042416	0.762934	0.138597	0.133327	0.140015	0.040009	0.038488	0.040419					
49		531.3806	1.456	POS	MFE	NA	1	0.719812	0.81806	0.172723	0.148957	0.170714	0.049861	0.043	0.049281	< 0.05	NS		NS	NS
50		543.3401	3.0852	POS	MFE	NA	1	1.150858	0.986496	0.15969	0.175499	0.230144	0.046099	0.050662	0.066437					
51		551.8591	3.076	POS	MFE	NA	1	1.064367	0.76996	0.129711	0.263385	0.244075	0.037444	0.076033	0.070458					
52		561.814	7.62	POS	MFE	NA	1	1.04878	0.752023	0.135454	0.130177	0.122694	0.039102	0.037579	0.035419					
53		567.834	12.674	POS	MFE	NA	1	0.962908	0.726865	0.086944	0.099617	0.120728	0.025099	0.028757	0.034851					
54		575.407	1.324	POS	MFE	NA	1	0.718877	0.843331	0.18102	0.116685	0.182791	0.052256	0.033684	0.052767	< 0.05	NS		NS	NS
55		614.2758	10.058	POS	MFE	NA	1	1.026208	0.80901	0.090932	0.09461	0.102749	0.02625	0.027312	0.029661					
56		619.4338	1.368	POS	MFE	NA	1	0.745046	0.860752	0.181584	0.119625	0.166853	0.052419	0.034533	0.048166	< 0.05	NS		NS	NS
57		707.482	1.375	POS	MFE	NA	1	0.866596	0.872807	0.112931	0.087009	0.097555	0.0326	0.025117	0.028162					
58		728.4138	1.615	POS	MFE	NA	1	0.781489	0.870372	0.183426	0.14586	0.178789	0.052951	0.042106	0.051612					
59		820.4329	2.365	POS	MFE	NA	1	1.00274	0.865155	0.068974	0.102395	0.096002	0.019911	0.029559	0.027714					
60		839.5653	1.861	POS	MFE	NA	1	0.807551	0.814501	0.090856	0.083813	0.094544	0.026228	0.024195	0.027293					
61		90.0335	1.38	NEG	MFE	NA	1	1.021514	0.722897	0.147867	0.14654	0.265336	0.042686	0.042302	0.076596					

62	146.1082	12.327	NEG	MFE	NA	1	0.973864	1.448123	0.148837	0.122407	0.425901	0.042966	0.035336	0.122947				
63	163.0868	9.343	NEG	MFE	NA	1	1.101436	1.504103	0.248591	0.208865	0.336754	0.071762	0.060294	0.097213				
64	165.0792	5.752	NEG	MFE	NA	1	1.08872	1.401074	0.146028	0.129362	0.226143	0.042155	0.037344	0.065282				
65	174.1149	12.335	NEG	MFE	NA	1	1.153918	1.240428	0.076583	0.074692	0.162966	0.022108	0.021562	0.047044				
66	192.031	1.365	NEG	MFE	NA	1	1.141617	1.267752	0.070298	0.085552	0.071118	0.020293	0.024697	0.02053				
67	197.0388	2.593	NEG	MFE	NA	1	0.962157	1.373168	0.203393	0.136055	0.355784	0.058714	0.039276	0.102706				
68	200.0846	1.907	NEG	MFE	NA	1	1.051335	1.53068	0.170978	0.155582	0.223493	0.049357	0.044913	0.064517				
69	216.0402	2.665	NEG	MFE	NA	1	1.364897	1.524521	0.115818	0.155733	0.124763	0.033434	0.044956	0.036016	< 0.05	NS	NS	NS
70	226.0719	2.655	NEG	MFE	NA	1	1.295424	1.467279	0.128604	0.144155	0.180562	0.037125	0.041614	0.052124	< 0.05	NS	NS	NS
71	264.0829	5.858	NEG	MFE	NA	1	0.95	1.332495	0.199118	0.131588	0.410739	0.05748	0.037986	0.11857				
72	270.1329	0.984	NEG	MFE	NA	1	1.139882	1.438837	0.134992	0.072963	0.164726	0.038969	0.021062	0.047552				
73	278.0441	2.661	NEG	MFE	NA	1	1.447829	1.373572	0.08563	0.218562	0.149046	0.024719	0.063093	0.043026	< 0.01	NS	NS	NS
74	284.1486	0.987	NEG	MFE	NA	1	1.221824	1.444242	0.140058	0.083269	0.163413	0.040431	0.024038	0.047173				
75	298.1643	1.002	NEG	MFE	NA	1	1.210572	1.51102	0.170307	0.070378	0.191157	0.049163	0.020317	0.055182				
76	310.1623	1.024	NEG	MFE	NA	1	1.063061	1.375598	0.120753	0.095173	0.141494	0.034859	0.027474	0.040846				
77	312.1804	1.021	NEG	MFE	NA	1	1.143124	1.47922	0.152346	0.083013	0.165476	0.043978	0.023964	0.047769				
78	316.1292	1.261	NEG	MFE	NA	1	1.339512	1.443942	0.107464	0.12642	0.169813	0.031022	0.036494	0.049021	< 0.05	NS	NS	NS
79	324.1785	1.035	NEG	MFE	NA	1	1.143219	1.50892	0.13453	0.098907	0.173499	0.038835	0.028552	0.050085				
80	326.1967	1.032	NEG	MFE	NA	1	1.14074	1.545177	0.162492	0.104781	0.191662	0.046907	0.030248	0.055328				
81	340.2113	1.062	NEG	MFE	NA	1	1.08631	1.52628	0.196915	0.135167	0.214707	0.056845	0.039019	0.061981				
82	354.227	1.08	NEG	MFE	NA	1	1.105397	1.603331	0.182278	0.16275	0.234156	0.052619	0.046982	0.067595				
83	368.246	1.109	NEG	MFE	NA	1	1.120895	1.566269	0.171344	0.119813	0.212066	0.049463	0.034587	0.061218				
84	388.1328	4.38	NEG	MFE	NA	1	1.262715	1.356738	0.111865	0.217586	0.257565	0.032293	0.062812	0.074353				
85	417.1481	1.382	NEG	MFE	NA	1	1.13402	1.386612	0.069585	0.09826	0.19569	0.020088	0.028365	0.056491				
86	454.2199	2.032	NEG	MFE	NA	1	1.22595	1.536416	0.145209	0.190304	0.21128	0.041918	0.054936	0.060991				
87	474.3011	1.306	NEG	MFE	NA	1	0.738427	1.521059	0.315137	0.223022	0.577598	0.090972	0.064381	0.166738				
88	552.1982	2.053	NEG	MFE	NA	1	1.083186	1.346662	0.091516	0.076091	0.128447	0.026418	0.021966	0.037079				
89	575.3608	12.597	NEG	MFE	NA	1	1.406711	1.411404	0.097683	0.093743	0.12505	0.028199	0.027061	0.036099	<0.05	NS	NS	NS
90	726.4559	1.627	NEG	MFE	NA	1	1.342339	1.38584	0.147084	0.158124	0.215305	0.04246	0.045647	0.062153	< 0.05	NS	NS	NS
91	775.3619	1.901	NEG	MFE	NA	1	1.049325	1.456682	0.166437	0.097756	0.21319	0.048046	0.02822	0.061543				
92	814.5114	1.759	NEG	MFE	NA	1	1.457814	1.286446	0.150377	0.149674	0.189839	0.04341	0.043207	0.054802	< 0.05	NS	NS	NS

[a] Retention Time (RT)

[b] Positive Mode (POS) versus Negative Mode (NEG)

[c] Molecular Feature Extraction (MFE) extracts chromatographic peaks by molecular features versus Find by Formula (FBF) which extracts peaks by chemical formula.

[d] denotes metabolites confirmed by chemical standard (stnd). All other identifications are provisional identifications made by matching against a database of accurate mass-retention time pairs (mass-matching, MM).

[e] Univariate statististical analysis of changes (> 0.25-fold) in mean intracellular abundance by heirarchical modeling, adjusted by Benjamini-Hochberg procedure.

[f] Bivariate analysis of changes in intracellular abundance and variance by heirarchical modeling, adjusted by Benjamini-Hochberg procedure

Significance Analysis of Microarrays (SAM) analysis of changes in intracellular abundance (> 0.25-fold, FDR < 1%), significant metabolites denoted by an asterix (*)

Bold font is used to indicate those metabolites whose abundance was altered in a similar fashion in the VISA isolate from both series (SG-R and JH2) and subsequently reversed in the revertant, SG-rev, as shown in Figure 4.