

E. faecalis S613 and R712

Putative ID	Ret. Time (min)	Adduct	<i>m/z</i>	Accuracy (ppm)	CCS _{cal} ^a (Å ²)	RSD (%)	CCS _{ref} (Å ²)	ΔCCS (% diff)
DGDG 28:1	1.14	[M+Na] ⁺	857.526	2.0	289.5	0.09		
DGDG 30:2	1.09	[M+NH ₄] ⁺	878.585	1.5	295.4	0.01		
DGDG 30:1	1.10	[M+NH ₄] ⁺	880.603	3.5	298.4	0.02		
DGDG 30:0	1.09	[M+NH ₄] ⁺	882.614	-1.2	302.4	0.02		
DGDG 30:2	1.12	[M+Na] ⁺	883.537	-2.6	291.7	0.05		
DGDG 30:1	1.11	[M+Na] ⁺	885.557	1.8	295.5	0.02		
DGDG 30:0	1.12	[M+Na] ⁺	887.569	-1.8	299.6	0.10		
DGDG 30:1	1.12	[M+K] ⁺	901.532	2.7	298.1	0.02		
DGDG 32:2	1.06	[M+NH ₄] ⁺	906.619	4.3	302.2	0.04		
DGDG 32:1	1.07	[M+NH ₄] ⁺	908.637	6.1	305.4	0.04		
DGDG 32:0	1.06	[M+NH ₄] ⁺	910.642	-5.1	307.4	0.03		
DGDG 32:2	1.10	[M+Na] ⁺	911.573	2.6	298.0	0.04		
DGDG 32:1	1.10	[M+Na] ⁺	913.587	1.0	302.5	0.02		
DGDG 32:0	1.11	[M+Na] ⁺	915.597	-6.0	304.7	0.05		
DGDG 32:1	1.12	[M+K] ⁺	929.563	3.1	305.1	0.01		
DGDG 34:3	1.03	[M+NH ₄] ⁺	932.631	0.1	305.8	0.07	305.3 ^c	0.2
DGDG 34:2	1.03	[M+NH ₄] ⁺	934.653	6.5	309.0	0.06	307.5 ^c	0.5
DGDG 34:1	1.03	[M+NH ₄] ⁺	936.667	5.0	311.6	0.06		
DGDG 34:2	1.02	[M+Na] ⁺	939.606	4.0	305.2	0.03	306.5 ^c	-0.4
DGDG 34:1	1.02	[M+Na] ⁺	941.618	0.6	309.0	0.06		
DGDG 34:1	1.18	[M+K] ⁺	957.604	12.4	311.3	0.03		
DGDG 35:2	1.03	M+NH ₄ ⁺	948.664	2.4	315.0	0.08		
DGDG 35:2	1.02	[M+Na] ⁺	953.620	2.6	311.5	0.06		
DGDG 35:1	1.04	M+NH ₄ ⁺	950.675	-2.4	317.4	0.12		
DGDG 36:2	1.01	[M+NH ₄] ⁺	962.682	4.4	315.2	0.07		
DGDG 36:2	0.99	[M+Na] ⁺	967.635	1.9	312.4	0.08		
DGDG 36:2	0.99	[M+K] ⁺	983.610	2.5	315.3	0.11		
PG p31:2	1.40	[M-H] ⁻	687.461	-0.6	256.8	0.02		
PG p33:2	1.37	[M-H] ⁻	715.493	2.7	263.4	0.01		
PG p34:3	1.35	[M-H] ⁻	727.492	1.4	264.8	0.02		
PG p34:2	1.37	[M-H] ⁻	729.508	1.4	266.6	0.00		
PG 28:1	2.42	[M-H] ⁻	663.424	-1.1	251.2	0.13		
PG 28:0	2.43	[M-H] ⁻	665.438	-2.9	253.1	0.15		
PG 30:2	2.37	[M-H] ⁻	689.440	-0.1	255.0	0.10		
PG 30:1	2.40	[M-H] ⁻	691.457	2.3	257.1	0.03		
PG 30:0	2.40	[M-H] ⁻	693.470	-2.0	258.9	0.03		
PG 31:2	2.28	[M-H] ⁻	703.456	0.0	257.9	0.07		
PG 31:1	2.38	[M-H] ⁻	705.471	-0.4	260.2	0.04		
PG 32:2	2.30	[M-H] ⁻	717.473	2.4	261.4	0.06	261.0 ^b	0.1
PG 32:1	2.32	[M-H] ⁻	719.489	2.8	263.3	0.04	262.5 ^b	0.3
PG 32:0	2.32	[M-H] ⁻	721.501	-2.5	264.9	0.08	263.5 ^b	0.5
PG 33:2	2.29	[M-H] ⁻	731.487	0.4	264.5	0.02		
PG 33:1	2.31	[M-H] ⁻	733.503	1.2	267.0	0.06		
PG 34:2	2.25	[M-H] ⁻	745.503	0.3	268.1	0.03	267.4 ^b	0.2

PG 34:1	2.27	[M-H] ⁻	747.518	0.0	269.9	0.03	268.9 ^b	0.4
PG 34:0	2.26	[M-H] ⁻	749.529	-6.4	270.8	0.08	269.0 ^b	0.7
PG 35:2	2.23	[M-H] ⁻	759.519	1.6	271.4	0.03		
PG 35:1	2.26	[M-H] ⁻	761.535	1.2	273.2	0.07		
PG 36:2	2.19	[M-H] ⁻	773.533	-0.5	274.9	0.07	274.3 ^b	0.2
PG 36:1	2.19	[M-H] ⁻	775.544	-7.6	275.7	0.07	275.7 ^b	0.0
PG 37:1	2.18	[M-H] ⁻	787.549	-1.3	278.0	0.05		
LysylPG 30:1	7.73	[M-H] ⁻	821.569	-4.7	287.0	0.01		
LysylPG 30:0	7.75	[M+H] ⁺	823.584	-4.2	290.4	0.02		
LysylPG 32:2	7.68	[M+H] ⁺	847.589	-9.6	290.8	0.04		
LysylPG 32:1	7.70	[M+H] ⁺	849.601	-5.2	293.5	0.03		
LysylPG 34:2	7.63	[M+H] ⁺	875.625	-15.3	298.4	0.09		
LysylPG 34:1	7.66	[M+H] ⁺	877.632	-4.9	299.6	0.03		
LysylPG 35:2	7.63	[M+H] ⁺	889.632	-4.8	300.8	0.02		
LysylPG 35:1	7.66	[M+H] ⁺	891.647	-4.0	303.5	0.01		
LysylPG 36:2	7.61	[M+H] ⁺	903.647	-3.7	302.8	0.00		

***S. aureus* N315 and N315-D8**

Putative ID	Ret. Time (min)	Adduct	<i>m/z</i>	Accuracy (ppm)	CCS _{cal} ^a (Å ²)	RSD (%)	CCS _{ref} (Å ²)	ΔCCS (% diff)
DGDG 29:0	1.17	[M+NH ₄] ⁺	868.600	0.6	298.3	0.03		
DGDG 30:0	1.17	[M+NH ₄] ⁺	882.621	6.3	301.8	0.04		
DGDG 30:0	1.17	[M+Na] ⁺	887.573	2.0	299.6	0.03		
DGDG 31:0	1.15	[M+NH ₄] ⁺	896.633	2.3	305.4	0.05		
DGDG 31:0	1.15	[M+Na] ⁺	901.587	0.2	303.4	0.05		
DGDG 32:0	1.14	[M+NH ₄] ⁺	910.652	5.7	308.5	0.08		
DGDG 32:0	1.14	[M+Na] ⁺	915.603	1.3	306.7	0.07		
DGDG 33:0	1.11	[M+NH ₄] ⁺	924.665	2.7	311.5	0.06		
DGDG 33:0	1.11	[M+Na] ⁺	929.618	0.4	309.0	0.07		
DGDG 34:0	1.10	[M+NH ₄] ⁺	938.680	2.2	314.2	0.08		
DGDG 34:0	1.09	[M+Na] ⁺	943.634	0.1	311.8	0.08		
DGDG 35:0	1.07	[M+NH ₄] ⁺	952.695	1.5	317.1	0.06		
DGDG 35:0	1.07	[M+Na] ⁺	957.650	0.4	314.2	0.07		
DGDG 36:0	1.05	[M+NH ₄] ⁺	966.709	-0.1	326.8	0.01		
PG p29:1	1.59	[M-H] ⁻	661.445	1.4	252.2	0.04		
PG p30:1	1.55	[M-H] ⁻	675.461	1.5	255.3	0.04		
PG p31:1	1.53	[M-H] ⁻	689.477	2.3	258.5	0.03		
PG p32:1	1.50	[M-H] ⁻	703.492	1.3	262.1	0.07		
PG p33:1	1.49	[M-H] ⁻	717.508	1.4	265.1	0.07		
PG p34:1	1.45	[M-H] ⁻	731.523	0.8	268.6	0.03		
PG 29:0	2.41	[M-H] ⁻	679.457	2.2	255.2	0.02		
PG 30:0	2.39	[M-H] ⁻	693.480	13.1	258.7	0.05		
PG 31:0	2.33	[M-H] ⁻	707.492	7.3	262.0	0.07		
PG 32:0	2.30	[M-H] ⁻	721.512	13.6	265.1	0.08	263.5 ^b	0.6
PG 33:0	2.25	[M-H] ⁻	735.524	7.5	268.6	0.07		
PG 34:0	2.21	[M-H] ⁻	749.538	5.6	271.6	0.05	269.0 ^b	1.0
PG 35:0	2.16	[M-H] ⁻	763.552	2.6	275.0	0.04		
PG 36:0	2.13	[M-H] ⁻	777.565	-0.1	277.9	0.06		

PA 30:0	6.46	[M-H] ⁻	619.434	0.5	244.9	0.01		
PA 31:0	6.45	[M-H] ⁻	633.450	0.0	248.2	0.03		
PA 32:0	6.44	[M-H] ⁻	647.467	-1.7	251.1	0.01		
PA 33:0	6.42	[M-H] ⁻	661.481	0.6	254.5	0.02		
PA 34:0	6.43	[M-H] ⁻	675.499	-2.2	257.6	0.01		
PA 35:0	6.43	[M-H] ⁻	689.513	-0.9	261.0	0.02		
PA 36:0	6.42	[M-H] ⁻	703.529	-0.3	264.1	0.01		
LysylPG 28:0	7.70	[M+H] ⁺	795.550	1.3	284.7	0.04		
LysylPG 29:0	7.66	[M+H] ⁺	809.566	0.7	287.8	0.03		
LysylPG 30:0	7.64	[M+H] ⁺	823.582	1.9	290.9	0.01		
LysylPG 31:0	7.60	[M+H] ⁺	837.598	2.0	293.9	0.03		
LysylPG 32:0	7.57	[M+H] ⁺	851.613	0.9	296.8	0.02	297.0 ^c	-0.1
LysylPG 33:0	7.54	[M+H] ⁺	865.629	1.0	299.8	0.03		
LysylPG 34:0	7.52	[M+H] ⁺	879.644	0.8	302.5	0.02		
LysylPG 35:0	7.49	[M+H] ⁺	893.661	1.7	305.4	0.04		
LysylPG 36:0	7.59	[M+H] ⁺	907.677	-9.2	308.7	0.02		

***C. striatum* W40308 and W49297**

Putative ID	Ret. Time (min)	Adduct	<i>m/z</i>	Accuracy (ppm)	CCS _{cal} ^a (Å ²)	RSD (%)	CCS _{ref} (Å ²)	ΔCCS (% diff)
1.36_834.5291n	1.45	[M+Na] ⁺	857.523		292.8	0.01		
1.36_834.5291n	1.53	[M+K] ⁺	873.497		294.1	0.02		
GlcADG 16:0-18:1	2.25	[M+NH ₄] ⁺	788.596	-10.4	290.1	0.07		
GlcADG 16:0-18:1	2.27	[M+Na] ⁺	793.551	-9.6	288.1	0.07		
GlcADG 16:0-16:0	2.33	[M+NH ₄] ⁺	762.578	-6.6	286.0	0.07		
GlcADG 16:0-16:0	2.35	[M+Na] ⁺	767.532	-5.6	282.6	0.03		
PI 16:0-18:1	3.74	[M+Na] ⁺	859.540	-11.1	295.4	0.06		
PI 16:0-16:0	3.82	[M+Na] ⁺	833.521	-7.3	289.5	0.03		
AlaPG 34:1	4.51	[M+H] ⁺	820.581	-13.5	291.7	0.07		
AlaPG 34:1	4.50	[M+Na] ⁺	842.560	-9.9	294.3	0.10		
AlaPG 34:1	4.49	[M+K] ⁺	858.530	-4.9	293.6	0.11		
0.90_934.7546m/z	0.97	[M-H] ⁻	934.759		318.2	0.02		
1.36_834.5291n	1.35	[M-H] ⁻	833.527		282.8	0.02		
PG 16:0-18:1	2.06	[M-H] ⁻	747.521	-4.0	269.2	0.03	268.9 ^b	0.1
PG 16:0-16:0	2.15	[M-H] ⁻	721.505	-3.0	264.5	0.01	263.5 ^b	0.4
GlcADG 16:0-18:1	2.29	[M-H] ⁻	769.554	-8.4	272.7	0.03		
GlcADG 16:0-16:0	2.38	[M-H] ⁻	743.530	2.4	267.9	0.02		
PI 16:0-18:1	3.71	[M-H] ⁻	835.541	-7.7	285.5	0.02	283.7 ^b	0.6
PI 16:0-16:0	3.75	[M-H] ⁻	809.523	-5.3	280.9	0.05		
PA 16:0-18:1	6.28	[M-H] ⁻	673.484	-3.9	256.3	0.01	254.7 ^b	0.6
PA 16:0-16:0	6.49	[M-H] ⁻	647.469	-5.7	251.4	0.00		