

Lipid A Pathway Intermediates	Fatty acid chain length	Product of	Charge	QQQ precursor ion (m/z)	QQQ tret experimental (min)	QQQ tret standard (min)	QTOF m/z theoretical	QTOF m/z experimental	QTOF experimental mass error (ppm)	QTOF m/z standard	QTOF standard mass error (ppm)	QTOF tret experimental (min)	QTOF tret standard (min)
UDP-3-O-(R)-3-OH-C ₁₂ -GlcNAc	1 acyl group 12:0(3-OH)	LpxA	1-	804.3	2.8	-	804.2362	804.2361	0.1	-	-	3.1	-
UDP-3-O-(R)-3-OH-C ₁₄ -GlcNAc	1 acyl group 14:0(3-OH)	LpxA	1-	832.3	3.0	3.0	832.2675	832.2632	5.2	832.2701	-3.1	3.3	3.3
UDP-3-O-(R)-3-OH-C ₁₂ -GlcN	1 acyl group 12:0(3-OH)	LpxC	1-	762.3	2.7	2.9	762.2257	762.2243	1.8	-	-	3.2	-
UDP-3-O-(R)-3-OH-C ₁₄ -GlcN	1 acyl group 14:0(3-OH)	LpxC	1-	790.3	2.9	3.1	790.2570	790.2556	1.8	790.2576	-0.8	3.4	3.4
UDP-2,3-diacyl-GlcN	2 acyl groups, 12:0(3-OH)	LpxD	1-	960.5	3.3	3.3	960.3877	960.3889	-1.2	960.3853	2.5	3.8	3.6
UDP-2,3-diacyl-GlcN	1 acyl group 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxD	1-	988.5	3.4	3.4	988.4190	988.4196	-0.6	988.4188	0.2	3.8	3.7
UDP-2,3-diacyl-GlcN	2 acyl groups, 14:0(3-OH)	LpxD	1-	1016.5	3.5	3.5	1,016.4503	-	-	1,016.4517	-1.4	-	3.8
Lipid X	1 acyl group 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxH	1-	682.4	3.7	3.6	682.3937	682.3915	3.2	682.3932	0.7	4.1	3.9
Lipid X	2 acyl groups, 14:0(3-OH)	LpxH	1-	710.4	3.8	3.7	710.4250	-	-	710.4262	-1.7	-	4.0
DSMP (Disaccharide-1-P)	3 acyl groups 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxB	1-	1239.9	4.1	-	1,239.7864	1,239.7831	2.7	-	-	4.4	-
DSMP (Disaccharide-1-P)	2 acyl groups 12:0(3-OH), 2 acyl group 14:0(3-OH)	LpxB	1-	1267.9	4.1	4.1	1,267.8177	1,267.8147	2.4	-	-	4.4	-
DSMP (Disaccharide-1-P)	4 acyl group 14:0(3-OH)	LpxB	1-	1323.9	-	4.2	1,323.8803	-	-	1,323.8808	-0.4	-	4.4
Lipid IV _A	3 acyl groups 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxK	1-	1319.9	4.2	4.2	1,319.7528	-	-	-	-	-	-
Lipid IV _A	3 acyl groups 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxK	2-	659.45	4.2	4.2	659.3728	-	-	-	-	-	-
Lipid IV _A	2 acyl groups 12:0(3-OH), 2 acyl groups 14:0(3-OH)	LpxK	1-	1347.9	4.2	4.2	1,347.7841	-	-	-	-	-	-
Lipid IV _A	2 acyl groups 12:0(3-OH), 2 acyl groups 14:0(3-OH)	LpxK	2-	673.45	4.2	4.2	673.3884	-	-	-	-	-	-
Lipid IV _A	4 acyl groups 14:0(3-OH)	LpxK	1-	1403.9	-	4.1	1,403.8467	-	-	1,403.8464	0.2	-	4.3
Lipid IV _A	4 acyl groups 14:0(3-OH)	LpxK	2-	701.4	-	4.1	701.4197	-	-	701.4211	-2.0	-	4.3