Lipid A Pathway Intermediates	Fatty acid chain length	Product of	Charge	QQQ precursor ion (m/z)	QTOF m/z theoretical	Spectra																		
UDP-3-*O*-[(*R*)-3-OH-C_{12}]-GlcNAc	1 acyl group 12:0(3-OH)	LpxA	1-	804.3	-	Exoerimental	403.7	*385.5*	343.9	322.8	*272.7*	177.0	*159.5*	97.0	79.2									
UDP-3-*O*-[(*R*)-3-OH-C_{14}]-GlcNAc	1 acyl group 14:0(3-OH)	LpxA	1-	832.3	-	Standard	403.6	*384.7*	344.0	322.1	*272.7*	177.0	*158.8*	97.6	78.9									
UDP-3-*O*-[(*R*)-3-OH-C_{14}]-GlcNAc	1 acyl group 14:0(3-OH)	LpxA	1-	-	832.2675	Standard	402.9941	*384.9845*	343.9935	-	*272.9566*	176.9536	*158.9255*	96.9695	78.9590									
				-	-	Theoretical	402.9949	384.9844	-	-	-	176.9359	158.9254	96.9696	78.9590									
UDP-3-*O*-[(*R*)-3-OH-C_{12}]-GlcN	1 acyl group 12:0(3-OH)	LpxC	1-	762.3	-	Exoerimental	-	-	-	**456.4**	403.1	*385.3*	323.1	*273.7*	-	*159.0*	-	-						
UDP-3-*O*-[(*R*)-3-OH-C_{14}]-GlcN	1 acyl group 14:0(3-OH)	LpxC	1-	790.3	-	Experimental	*546.4*	**484.0**	-	-	402.8	*385.2*	-	*273.4*	-	*159.3*	-	-						
UDP-3-*O*-[(*R*)-3-OH-C_{14}]-GlcN	1 acyl group 14:0(3-OH)	LpxC	1-	790.3	-	Standard	*546.5*	**484.9**	**466.7**	-	403.7	*385.3*	323.4	*273.3*	*240.5*	*159.1*	96.7	79.3						
UDP-3-*O*-[(*R*)-3-OH-C_{14}]-GlcN	1 acyl group 14:0(3-OH)	LpxC	1-	790.3	790.2570	Standard	*546.1873*	-	-	-	402.9947	*384.9849*	323.0288	*272.9574*	240.0276	*158.9255*	96.9699	78.9591						
				-	-	Theoretical	-	484.2317	466.2211	456.2004	402.9949	384.9844	323.0286		240.0279	158.9254	96.9696	78.9590						
UDP-2,3-diacyl-GlcN	2 acyl groups, 12:0(3-OH)	LpxD	1-	960.5		Exoerimental	-	-	-	-	**655.0**	**637.4**	-	403.1	*385.3*	323.4	*273.6*	215.2	177.4	*159.5*	111.0	-	-	
UDP-2,3-diacyl-GlcN	1 acyl group 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxD	1-	988.5		Experimental	-	-	**683.4**	**665.1**	-	-	466.8	403.5	*385.4*	323.6	*273.5*	215.8	177.4	-	-	-	-	
UDP-2,3-diacyl-GlcN	1 acyl group 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxD	1-		988.4190	Experimental	-	-	**682.3943**	**664.3839**	-	-	466.2216	402.9954	*384.9852*	323.0286	*272.9574*	-	176.9357	*158.9253*	-	96.9697	78.9590	
UDP-2,3-diacyl-GlcN	1 acyl group 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxD	1-	988.5		Standard	-	-	-	-	-	-		403.8	*385.8*	323.6	*273.0*	-	177.6	*159.0*	-			
UDP-2,3-diacyl-GlcN	1 acyl group 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxD	1-	988.4190		Standard	-	-	**682.4**	**664.4**	-	-	466.2	403.0	*385.0*	323.0	*273.0*	-	176.9	*158.9*	-	97.0	79.0	
UDP-2,3-diacyl-GlcN	2 acyl groups, 14:0(3-OH)	LpxD	1-	1016.5		Experimental	**711.5**	**693.3**	-	-	-	-		403.5	*385.8*	-		-	-	-	-	79.4	-	
UDP-2,3-diacyl-GlcN	2 acyl groups, 14:0(3-OH)	LpxD	1-	1016.5		Standard	**711.3**	**692.9**	-	-	-	-	467.0	403.2	*385.7*	322.9	*273.4*	-	-	*159.1*	-	-	-	
UDP-2,3-diacyl-GlcN	2 acyl groups, 14:0(3-OH)	LpxD	1-		1,016.4503	Standard	**710.4220**	**692.4111**	-	-	-	-	466.2194	402.9933	*384.9832*	323.0276	*272.9594*	-	176.9249	*158.9249*	-	96.9698	78.9589	
				-	-	Theoretical	710.4250	692.4144	682.3937	664.3831	654.3624	636.3518	466.2211	402.9949	384.9844	323.0286		215.1652	176.9359	158.9254	111.0200	96.9696	78.9590	
Lipid X	1 acyl group 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxH	1-	682.4		Exoerimental	**466.8**	-	*240.1*	96.9	79.1													
Lipid X	1 acyl group 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxH	1-		682.3937	Standard	**466.2204**	***438.1895***	*240.0272*	96.9682	78.9589													
Lipid X	2 acyl groups, 14:0(3-OH)	LpxH	1-	710.4		Standard	**466.8**	-	*239.8*	96.9	79.3													
Lipid X	2 acyl groups, 14:0(3-OH)	LpxH	1-		710.4250	Standard	**466.2216**	-	*240.0279*	96.9696	78.9590													
				-	-	Theoretical	466.2211	438.1898	240.0279	96.9696	79.9663													
DSMP (Disaccharide-1-P)	3 acyl groups 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxB	1-	1239.9		Experimental	-	-	-	***1,024.9***	-	-	***808.7***	-	-	-	652.6	-	-	448.5	-	97.0	-	
DSMP (Disaccharide-1-P)	2 acyl groups 12:0(3-OH), 2 acyl group 14:0(3-OH)	LpxB	1-	1267.9		Experimental	-	-	***1,052.6***	-	-	***836.2***	-	-	-	**725.1**	651.9	-	-	448.3	-	-	-	
DSMP (Disaccharide-1-P)	4 acyl group 14:0(3-OH)	LpxB	1-	1323.9		Standard	**1,099.1**	**1,080.8**	-	-	854.7	836.3	-	795.5	**753.7**	-	652.2	593.0	467.0	449.1	-	-	79.8	
DSMP (Disaccharide-1-P)	4 acyl group 14:0(3-OH)	LpxB	1-	1323.9	1,323.8803	Standard	1,097.6830	1,079.6783	-	-	853.4816	835.4713		794.4439	752.4343	-	-	592.2521		448.2095	242.2126	96.9699	78.9590	
						Theoretical	1,097.6871	1,079.6765	1,051.6452	1,023.5927	853.4832	835.4726	807.4410						466.2211		243.1965	96.9696	79.9663	
Lipid IVa	3 acyl groups 12:0(3-OH), 1 acyl group 14:0(3-OH)	LpxK	1-	1319.9		Experimental	-	-	-	-	-	-	-	-	-	-	-	-	**381.2**	363.9	-	-	253.7	227.2	211.5	153.2	-	-
Lipid IVa	2 acyl groups 12:0(3-OH), 2 acyl groups 14:0(3-OH)	LpxK	1-	1347.9		Exoerimental	-	-	-	-	-	646.1	-	-	**409.9**	-	392.0	364.0	-	-	281.5	268.2	256.0	227.6	211.6	153.4	-	*79.5*
Lipid IVa	2 acyl groups 12:0(3-OH), 2 acyl groups 14:0(3-OH)	LpxK	1-	1347.9		Standard	-	-	-	-	-	646.3	-	466.7	**409.9**	-	392.2	363.3	-	-	-	267.8	255.8	227.3	211.3	153.9	-	*79.8*
Lipid IVa	4 acyl groups 14:0(3-OH)	LpxK	1-	1403.9		Standard	-	-	-	688.8	-	646.5	-	-	**409.9**	403.9	392.1	-	-	-	281.9	-	256.0	-	-	153.7	97.1	-
Lipid IVa	4 acyl groups 14:0(3-OH)	LpxK	1-		1,403.8467	Standard	1,305.8671	1,159.6406	1,061.6656	687.4963	659.4605	-	483.2002	-	-	403.2239	391.2232	-	-	-	281.2471	267.3340	255.2321	-	211.0637	152.9954	-	-
						Ref*/Theo.	1305.92*	1159.67*	1061.75*					466.2211												96.9696	79.9663