Unsaturation Elements and other Modifications of Phospholipids in Bacteria: New Insight from UVPD Mass Spectrometry

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Supporting Information

Table of Contents

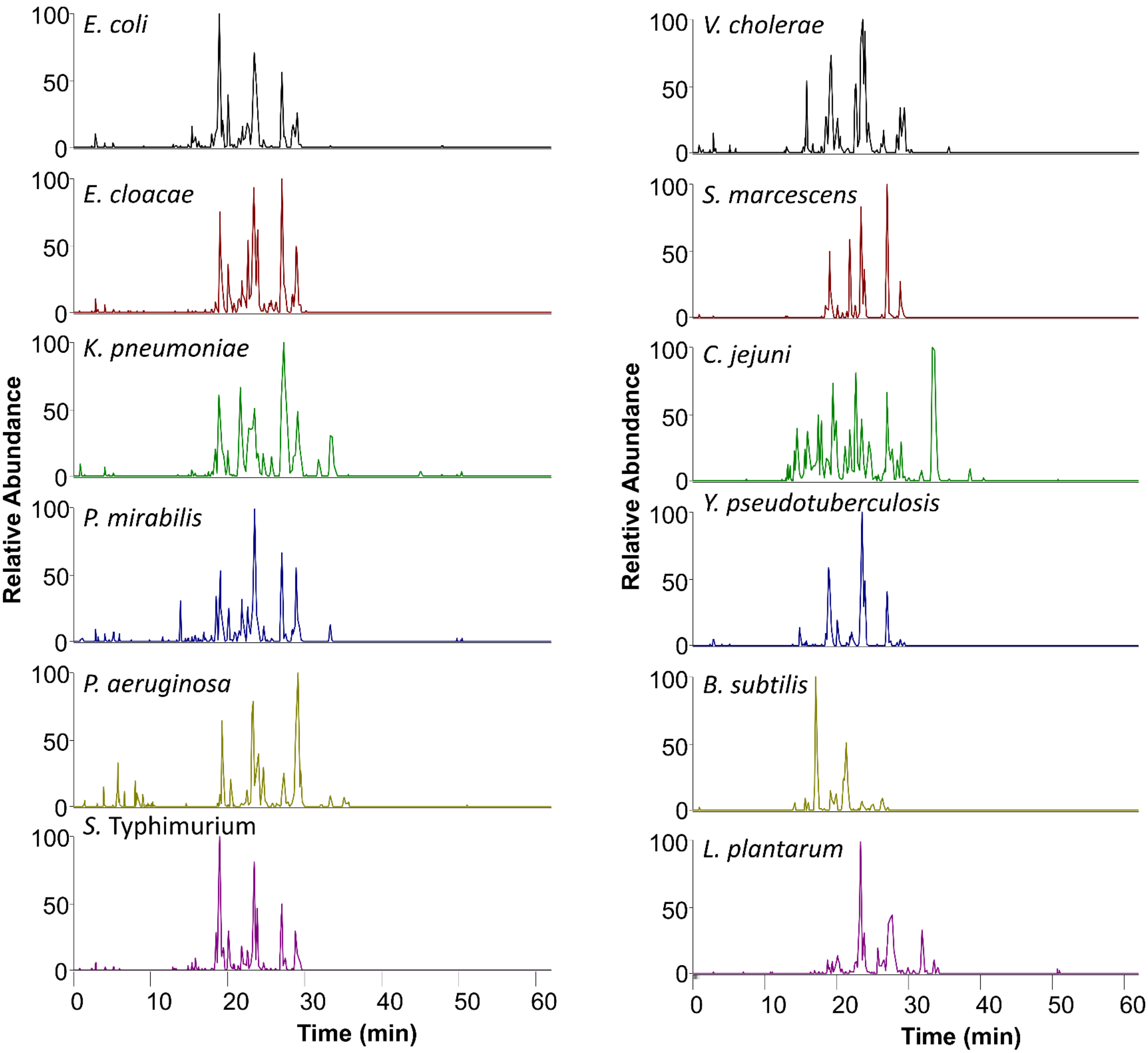
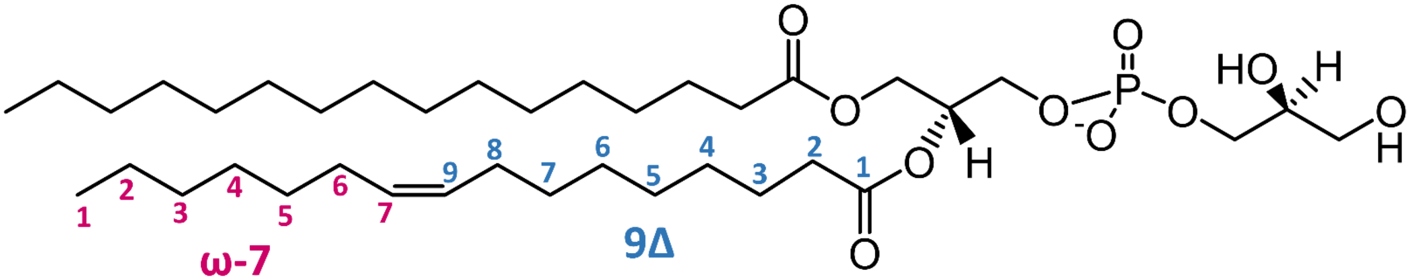


Figure S1. Base peak LC-MS traces of all 12 investigated bacterial lipid extracts.

PG 16:0/16:1(9Z)
PG 16:0/16:1(*cis* ω-7)



PG 16:0/18:1(11Z)
PG 16:0/18:1(*cis* ω-7)

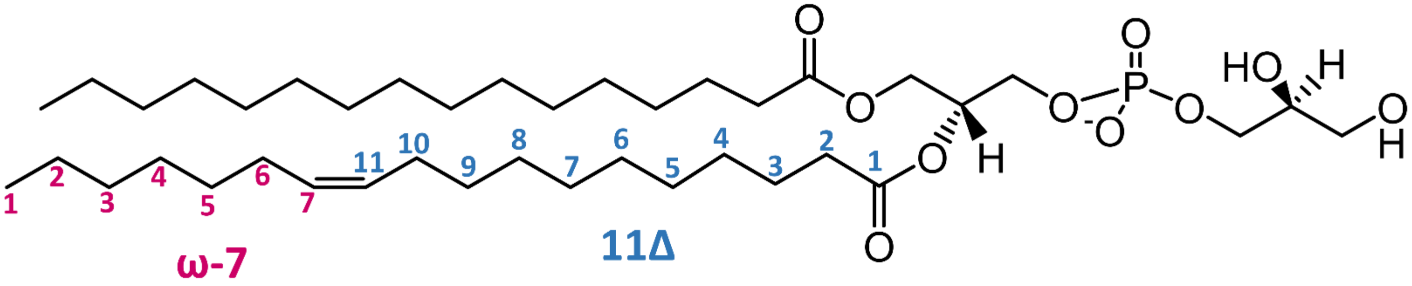


Figure S2. The omega nomenclature (ω-7) in pink font allows simple recognition of unsaturation elements which are found at the same position from the terminal acyl chain carbon end despite having different numbers of carbon atoms within the acyl chains. The contrasting delta nomenclature is shown in blue font.

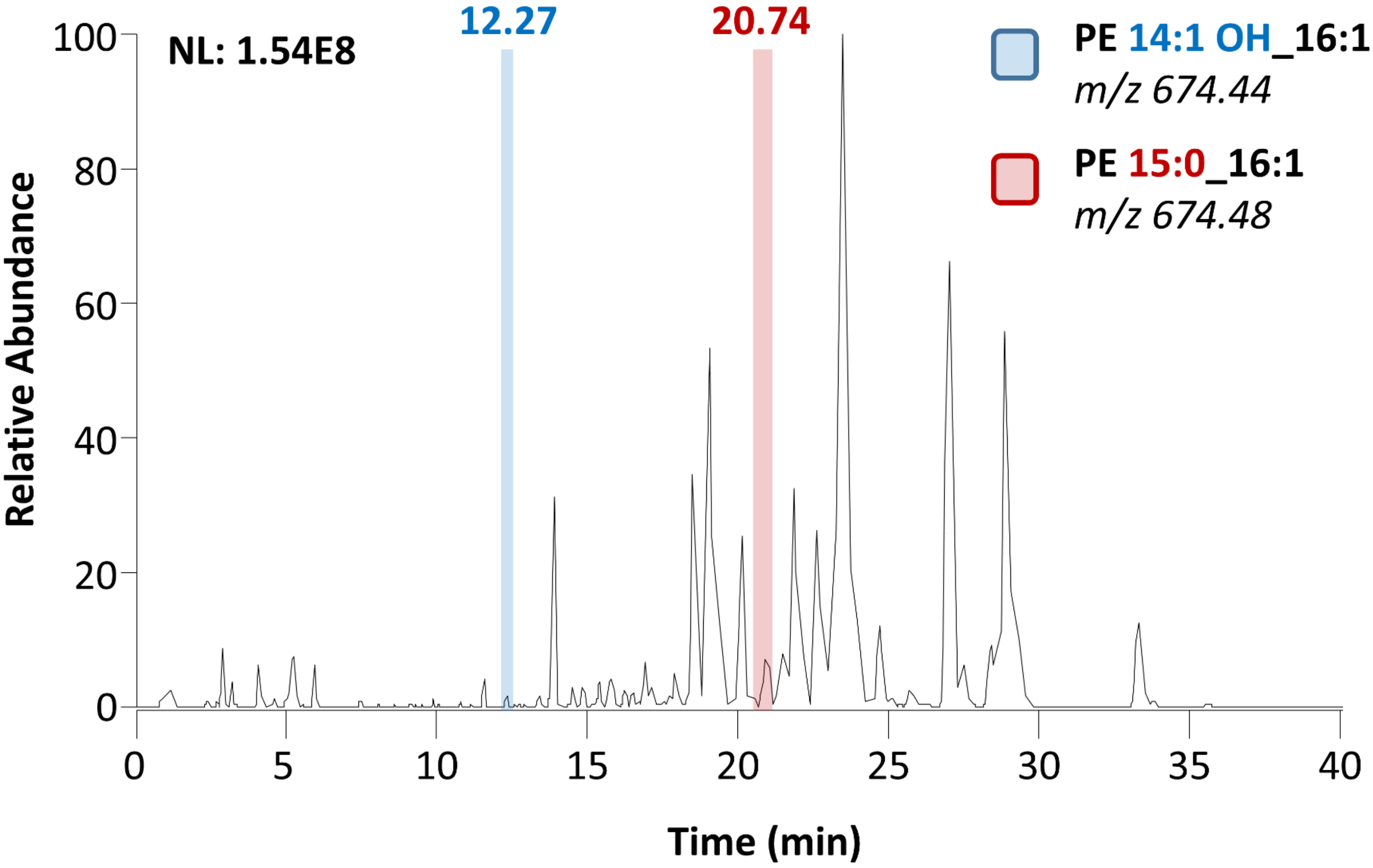
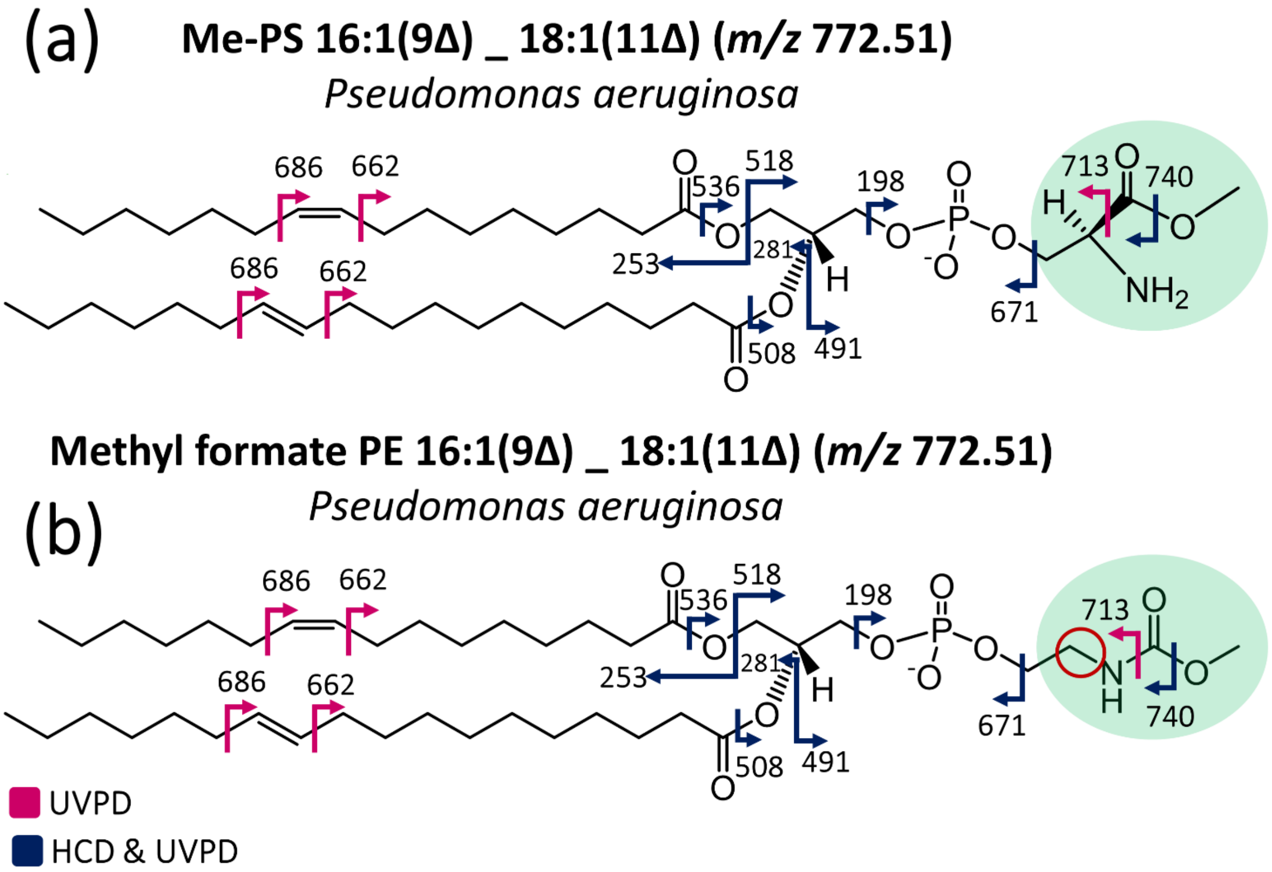


Figure S3. Example of marked differences in retention time of two lipids - one containing an unsaturated hydroxyl acyl chain (PE 14:1 OH_16:1 of *m/z* 674.44) and its non-hydroxyl lipid counterpart (PE 15:0_16:1 of *m/z* 674.48) from *P. mirabilis* lipid extract. With lack of high-resolution instrumentation, differences in retention time enable differentiation (albeit not complete characterization) of hydroxyl lipids and their isobaric non-hydroxyl counterparts with a mass difference of 0.04 Da.



(a) **Me-PS 16:1(9Δ) _ 18:1(11Δ) (*m/z* 772.51)**

Pseudomonas aeruginosa

Methyl formate PE 16:1(9Δ) _ 18:1(11Δ) (*m/z* 772.51)

(b) *Pseudomonas aeruginosa*

Figure S4. Two possible structures for the observed unique headgroup as shown for a lipid of *m/z* 772.51 from *P. aeruginosa* lipid extract; (**a**) Me-PS type lipid and **(b)** modified PE headgroup with methyl formate. Both structural possibilities align with the measured intact mass and fragmentation patterns. Hypothetical cleavage of the C-N bond circled in red in **(b)** (theoretical *m/z* 698) could unambiguously identify the correct structure for this headgroup, but is not observed, making **(a)** the more likely structure.

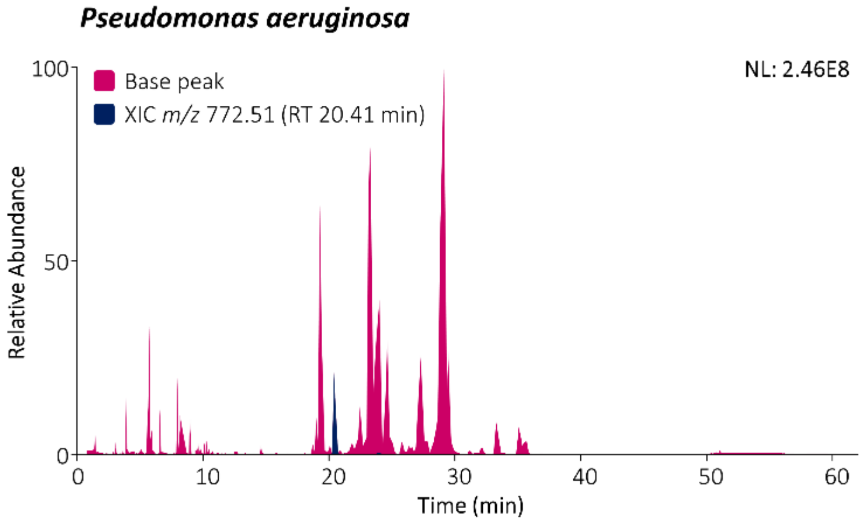


Figure S5. Base peak LC-MS trace of *Pseudomonas aeruginosa* lipid extract with XIC of *m/z* 772.51 identified as Me-PS 16:1(9Δ) _ 18:1(11Δ) highlighted.

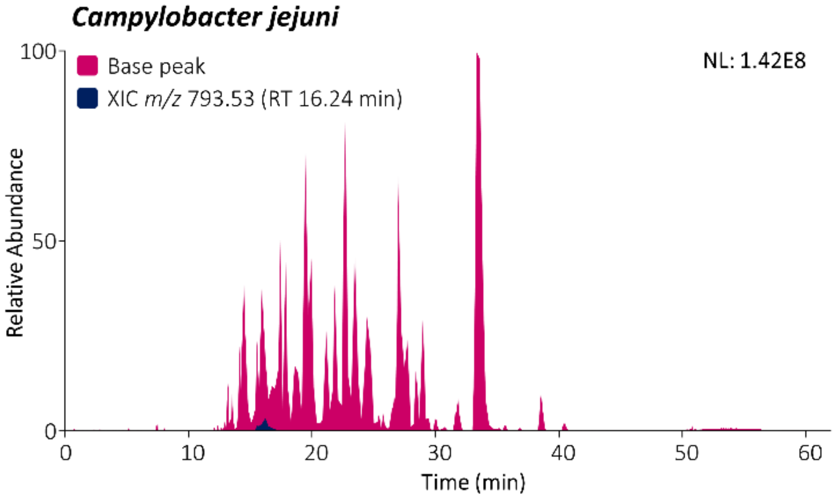


Figure S6. Base peak LC-MS trace of *Campylobacter jejuni* lipid extract with XIC of *m/z* 793.53 identified as Lysyl-PG 13:0_15:0 highlighted.

	Species	Strain
Gram(-)	*Escherichia coli*	W3110
	Enterobacter cloacae	R/S-WT
	Klebsiella pneumoniae	MKP103
	Proteus mirabilis	NR0250
	Pseudomonas aeruginosa	PA14
	Salmonella enterica serovar Typhimurium	LT2
	Vibrio cholerae	C6706
	Serratia marcescens	NR0342
	Campylobacter jejuni	81176
	Yersinia pseudotuberculosis	pB1+
Gram(+)	*Bacillus subtilis*	168
	Lactobacillus plantarum	WCFS1

Table S1. List of investigated bacterial lipid extracts including 10 Gram-negative and 2 Gram-positive species.

E. coli

Precursor m/z	Precursor m/z (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	m/z	m/z (theo)	ppm error	acyl chain 2	m/z	m/z (theo)	ppm error	Unsat Ion 1 m/z	Unsat Ion 1 m/z (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 m/z	Unsat Ion 2 m/z (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
691.4562	691.4556	0.9	15.48	PG	14:0	227.2018	227.2017	0.4	16:1	253.2175	253.2173	0.8	581.3485	581.346	4.3	605.3403	605.346	-9.4	23.99	9Δ	ω-7
646.4453	646.4453	0.0	17.02	PE	12:0	199.1703	199.1704	-0.5	17:1	267.2329	267.2330	-0.4	534.3184	534.3201	-3.2	548.3322	548.3358	-6.6	14.01	9Δ	ω-7
705.4713	705.4712	0.1	17.56	PG	14:0	227.2017	227.2017	0.0	17:1	267.2330	267.2330	0.0	593.3423	593.346	-6.2	607.3586	607.3617	-5.1	14.02	9Δ	ω-7
674.4738	674.4766	-4.2	20.86	PE	15:0	241.2176	241.2173	1.2	16:1	253.2176	253.2173	1.2	564.3688	564.3671	3.0	588.3705	588.3671	5.8	24.00	9Δ	ω-7
674.4781		2.2	21.33		14:0	227.202	227.2017	1.3	17:1	267.2334	267.2330	1.5	562.3510	562.3514	-0.7	576.3656	576.3671	-2.6	14.01		
733.504	733.5025	2.0	21.63	PG	16:0	255.2329	255.2330	-0.4	17:1	267.2328	267.2330	-0.7	621.3748	621.3773	-4.0	635.3902	635.393	-4.4	14.02	9Δ	ω-7
688.4968	688.4923	6.5	23.29	PE	16:1	253.219	253.2173	6.7	16:0	255.2333	255.2330	1.2	578.3784	578.3827	-7.4	602.382	602.3827	-1.2	24.00	9Δ	ω-7
688.4935		1.7	24.15	PE	15:0	241.2176	241.2173	1.2	17:1	267.2332	267.2330	0.7	576.3669	576.3671	-0.3	590.3782	590.3827	-7.6	14.01	9Δ	ω-7
773.5356	773.5338	2.3	24.00	PG	18:1	281.2488	281.2486	0.7	18:1	281.2488	281.2486	0.7	663.4229	663.4243	-2.1	687.4188	687.4243	-8.0	24.00	11Δ	ω-7
714.5084	714.5079	0.7	24.59	PE	17:1	267.2329	267.2330	-0.4	17:1	267.2329	267.2330	-0.4	602.3824	602.3827	-0.5	616.3964	616.3984	-3.2	14.01	9Δ	ω-7
702.5106	702.5079	3.8	26.82	PE	16:0	255.2335	255.2330	2.0	17:1	267.2336	267.2330	2.2	590.3806	590.3827	-3.6	604.3992	604.3984	1.3	14.02	9Δ	ω-7
716.5267	716.5236	4.3	29.02	PE	16:0	255.2337	255.2330	2.7	18:1	281.2495	281.2486	3.2	606.418	606.414	6.6	630.4118	630.414	-3.5	23.99	11Δ	ω-7
742.5407	742.5392	2.0	29.47	PE	18:1	281.2491	281.2486	1.8	18:1	281.2491	281.2486	1.8	632.4254	632.4297	-6.8	656.429	656.4297	-1.1	24.00	11Δ	ω-7
730.5395	730.5392	0.4	33.15	PE	16:0	255.233	255.2330	0.0	19:1	295.2643	295.2639	1.4	618.4097	618.414	-7.0	632.4281	632.4297	-2.5	14.02	11Δ	ω-7
730.5394		0.3	33.62		17:1	267.2329	267.233	-0.4	18:0	283.2643	283.2643	0.0	618.4081		-9.5	632.426		-5.9	14.02	9Δ	ω-7

Table S2. List of all identified unsaturated lipids in *E. coli* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

E. cloacae

Precursor m/z	Precursor m/z (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	m/z	m/z (theo)	ppm error	acyl chain 2	m/z	m/z (theo)	ppm error	Unsat Ion 1 m/z	Unsat Ion 1 m/z (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 m/z	Unsat Ion 2 m/z (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
632.4302	632.4297	0.8	14.79	PE	12:0	199.1704	199.1704	0.0	16:1	253.2174	253.2173	0.4	522.3250	522.3201	9.4	546.3161	546.3201	-7.3	23.99	9Δ	ω-7
691.4559	691.4556	0.4	15.33	PG	14:0	227.2018	227.2017	0.4	16:1	253.2174	253.2173	0.4	581.3483	581.346	4.0	605.3417	605.346	-7.1	23.99	9Δ	ω-7
646.4458	646.4453	0.8	17.11	PE	12:0	199.1705	199.1704	0.5	17:1	267.2331	267.2330	0.4	534.319	534.3201	-2.1	548.3337	548.3358	-3.8	14.01	9Δ	ω-7
705.4714	705.4712	0.3	17.57	PG	14:0	227.2017	227.2017	0.0	17:1	267.2330	267.2330	0.0	593.3426	593.346	-5.7	607.3588	607.3617	-4.8	14.02	9Δ	ω-7
719.4877	719.4869	1.1	19.09	PG	16:0	255.2329	255.2330	-0.4	16:1	253.2176	253.2173	1.2	609.3812	609.3773	6.4	633.3773	633.3773	0.0	24.00	9Δ	ω-7
686.4773	686.4766	1.0	19.25	PE	16:1	253.2174	253.2173	0.4	16:1	253.2174	253.2173	0.4	576.3707	576.3671	6.2	600.3616	600.3671	-9.2	23.99	9Δ	ω-7
674.4785	674.4766	2.8	20.82	PE	15:0	241.2177	241.2173	1.7	16:1	253.2178	253.2173	2.0	564.3664	564.3671	-1.2	588.3699	588.3671	4.8	24.00	9Δ	ω-7
674.4791		3.7	21.37		14:0	227.2022	227.2017	2.2	17:1	267.2336	267.2330	2.2	562.3516	562.3514	0.4	576.366	576.3671	-1.9	14.01	9Δ	ω-7
733.5064	733.5025	5.3	21.88	PG	16:0	255.2338	255.2330	3.1	17:1	267.2339	267.2330	3.4	621.3762	621.3773	-1.8	635.3918	635.393	-1.9	14.02	9Δ	ω-7
688.4983	688.4923	8.7	23.39	PE	16:1	253.2195	253.2173	8.7	16:0	255.2334	255.2330	1.6	578.379	578.3827	-6.4	602.3827	602.3827	0.0	24.00	9Δ	ω-7
688.4945		3.2	24.21		15:0	241.2178	241.2173	2.1	17:1	267.2336	267.2330	2.2	576.3666	576.3671	-0.9	590.3792	590.3827	-5.9	14.01	9Δ	ω-7
714.5082	714.5079	0.4	24.66	PE	16:1	253.2174	253.2173	0.4	18:1	281.2502	281.2486	5.7	604.3972	604.3984	-2.0	628.3955	628.3984	-4.6	24.00	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
					17:1	267.2331	267.2330	0.4	17:1	267.2331	267.2330	0.4	602.3776	602.3827	-8.5	616.3969	616.3984	-2.4	14.02	9Δ, 9Δ	ω-7, ω-7
702.5103	702.5079	3.4	26.28	PE	16:1	253.2178	253.2173	2.0	17:0	269.2492	269.2486	2.2	592.3999	592.3984	2.5	616.3953	616.3984	-5.0	24.00	9Δ	ω-7
702.5106		3.8	26.81		16:0	255.2335	255.2330	2.0	17:1	267.2336	267.2330	2.2	590.3806	590.3827	-3.6	604.3992	604.3984	1.3	14.02	9Δ	ω-7
728.5271	728.5236	4.8	27.49	PE	17:1	267.2337	267.2330	2.6	18:1	281.2495	281.2486	3.2	618.4108	618.414	-5.2	642.4083	642.414	-8.9	24.00	9Δ(17:1), 11Δ(18:1)	ω-7
													616.3972	616.3984	-1.9	630.4114	630.414	-4.1	14.01		
716.5265	716.5236	4.0	28.86	PE	16:0	255.2337	255.2330	2.7	18:1	281.2494	281.2486	2.8	606.4182	606.414	6.9	630.412	630.414	-3.2	23.99	11Δ	ω-7
716.5243		1.0	30.14		17:1	267.2332	267.2330	0.7	17:0	269.2486	269.2486	0.0	604.3951	604.3984	-5.5	618.412	618.414	-3.2	14.02	9Δ	ω-7
730.5397	730.5392	0.7	33.48	PE	16:0	255.233	255.2330	0.0	19:1	295.2643	295.2639	1.4	618.41	618.414	-6.5	632.4272	632.4297	-4.0	14.02	9Δ(17:1), 11Δ(19:1)	ω-7, ω-7
					17:1	267.2330	267.2330	0.0	18:0	283.2644	283.2643	0.4									

Table S3. List of all identified unsaturated lipids in *E. cloacae* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

K. pneumoniae

Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
717.4713	717.4712	0.1	15.72	PG	16:1	253.2173	253.2173	0.0	16:1	253.2173	253.2173	0.0	607.3639	607.3617	3.6	631.3564	631.3617	-8.4	23.99	9Δ	ω-7
646.4460	646.4453	1.1	17.06	PE	12:0	199.1705	199.1704	0.5	17:1	267.2332	267.2330	0.7	534.3186	534.3201	-2.8	548.3332	548.3358	-4.7	14.01	9Δ	ω-7
705.4719	705.4712	1.0	17.45	PG	14:0	227.2018	227.2017	0.4	17:1	267.2332	267.2330	0.7	593.3433	593.346	-4.6	607.3599	607.3617	-3.0	14.02	9Δ	ω-7
705.4713		0.1	17.75		15:1	239.2016	239.2017	-0.4	16:0	255.2330	255.2330	0.0	593.3425	593.346	-5.9	607.3587	607.3617	-4.9	14.02	7Δ	ω-7
719.4877	719.4869	1.1	19.03	PG	16:0	255.2329	255.2330	-0.4	16:1	253.2176	253.2173	1.2	609.3813	609.3773	6.6	633.3832	633.3773	9.3	24.00	9Δ	ω-7
719.4874		0.7	19.52		15:0	241.2174	241.2173	0.4	17:1	267.2331	267.2330	0.4	607.3596	607.3617	-3.5	621.3796	621.3773	3.7	14.02	9Δ	ω-7
745.5029	745.5025	0.5	20.91	PG	17:1	267.2329	267.2330	-0.4	17:1	267.2329	267.2330	-0.4	633.3743	633.3773	-4.7	647.3898	647.393	-4.9	14.02	9Δ, 9Δ	ω-7, ω-7
674.4789	674.4766	3.4	21.36	PE	14:0	227.2022	227.2017	2.2	17:1	267.2336	267.2330	2.2	562.3518	562.3514	0.7	576.3665	576.3671	-1.0	14.01	9Δ	ω-7
733.5034	733.5025	1.2	21.87	PG	16:0	255.2332	255.2330	0.8	17:1	267.2332	267.2330	0.7	621.3751	621.3773	-3.5	635.3906	635.393	-3.8	14.02	9Δ	ω-7
688.4933	688.4923	1.5	24.25	PE	15:0	241.2175	241.2173	0.8	17:1	267.2332	267.2330	0.7	576.3668	576.3671	-0.5	590.3782	590.3827	-7.6	14.01	9Δ	ω-7
747.5187	747.5182	0.7	23.75	PG	16:1	253.2174	253.2173	0.4	18:0	283.2644	283.2643	0.4	637.4102	637.4086	2.5	661.4063	661.4086	-3.5	24.00	9Δ	ω-7
					16:0	255.2330	255.2330	0.0	18:1	281.2487	281.2486	0.4								11Δ	ω-7
714.5103	714.5079	3.4	24.06	PE	16:1	253.2178	253.2173	2.0	18:1	281.2493	281.2486	2.5	604.3991	604.3984	1.2	628.4047	628.3984	10.0	24.01	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
714.5083		0.6	24.54		17:1	267.2329	267.2330	-0.4	17:1	267.2329	267.2330	-0.4	602.3795	602.3827	-5.3	616.397	616.3984	-2.3	14.02	9Δ, 9Δ	ω-7, ω-7
702.5085	702.5079	0.9	26.70	PE	16:0	255.2330	255.2330	0.0	17:1	267.2331	267.2330	0.4	590.3792	590.3827	-5.9	604.3984	604.3984	0.0	14.02	9Δ	ω-7
761.5354	761.5338	2.1	27.45	PG	16:0	255.2334	255.2330	1.6	19:1	295.2647	295.2639	2.7	649.4069	649.4086	-2.6	663.4225	663.4243	-2.7	14.02	11Δ	ω-7
728.5267	728.5236	4.3	27.92	PE	17:1	267.2337	267.2330	2.6	18:1	281.2495	281.2486	3.2	618.4108	618.414	-5.2	642.4086	642.414	-8.4	24.00	9Δ(17:1), 11Δ(18:1)	ω-7
													616.3976	616.3984	-1.3	630.4116	630.414	-3.8	14.01		
716.5273	716.5236	5.2	29.07	PE	16:0	255.2339	255.2330	3.5	18:1	281.2496	281.2486	3.6	606.4194	606.414	8.9	630.4113	630.414	-4.3	23.99	11Δ	ω-7
716.5239		0.4	29.57		16:1	253.2174	253.2173	0.4	18:0	283.2643	283.2643	0.0	606.4146	606.414	1.0	630.4111	630.414	-4.6	24.00	9Δ	ω-7
716.5239		0.4	29.89		15:0	241.2174	241.2173	0.4	19:1	295.2643	295.2639	1.4	604.3932	604.3984	-8.6	618.413	618.414	-1.6	14.02	11Δ	ω-7
742.5415	742.5392	3.1	31.53	PE	17:1	267.233	267.2330	0.0	19:1	295.2643	295.2639	1.4	630.4122	630.414	-2.9	644.4269	644.4297	-4.3	14.01	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
730.5399	730.5392	1.0	33.02	PE	16:0	255.2331	255.2330	0.4	19:1	295.2644	295.2639	1.7	618.4104	618.414	-5.8	632.429	632.4297	-1.1	14.02	11Δ	ω-7
730.5396		0.5	33.84		17:1	267.2330	267.2330	0.0	18:0	283.2644	283.2643	0.4	618.4097	618.414	-7.0	632.4281	632.4297	-2.5	14.02	9Δ	ω-7
756.5578	756.5549	3.8	33.95	PE	18:1	281.2494	281.2486	2.8	19:1	295.2650	295.2639	3.7	646.445	646.4453	-0.5	670.4503	670.4453	7.5	24.01	11Δ, 11Δ	ω-7, ω-7
													644.4269	644.4297	-4.3	658.4447	658.4453	-0.9	14.02		
744.5557	744.5549	1.1	35.58	PE	18:1	281.2489	281.2486	1.1	18:0	283.2643	283.2643	0.0	634.4459	634.4453	0.9	658.4434	658.4453	-2.9	24.00	11Δ	ω-7
770.5709	770.5705	0.5	38.40	PE	19:1	295.2643	295.2639	1.4	19:1	295.2643	295.2639	1.4	658.4431	658.4453	-3.3	672.4579	672.461	-4.6	14.01	11Δ, 11Δ	ω-7, ω-7

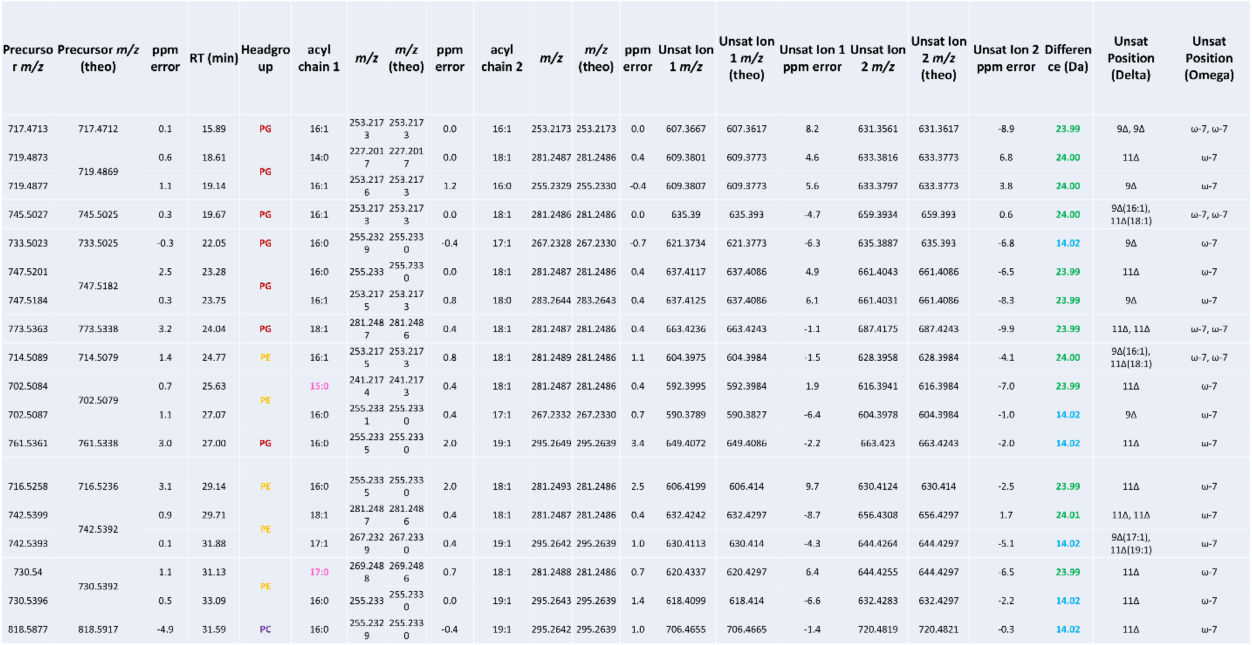
Table S4. List of all identified unsaturated lipids in *K. pneumonia* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

P. mirabilis

Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
648.4255	648.4246	1.4	11.51	PE	12:0 OH	215.1655	215.1653	0.9	16:1	253.2176	253.2173	1.2	538.3151	538.315	0.2	562.3179	562.315	5.2	24.00	9Δ	ω-7
674.4408	674.4402	0.9	12.27	PE	14:1 OH	241.1811	241.1809	0.8	16:1	253.2175	253.2173	0.8	564.3303	564.3307	-0.7	588.3312	588.3307	0.8	24.00	9Δ(16:1), 7Δ(14:1 OH)	ω-7, ω-7
662.4404	662.4402	0.3	12.90	PE	12:0 OH	215.1653	215.1653	0.0	17:1	267.2330	267.2330	0.0	550.3122	550.315	-5.1	564.3274	564.3307	-5.8	14.02	9Δ	ω-7
676.4567	676.4559	1.2	13.73	PE	12:0 OH	215.1654	215.1653	0.5	18:1	281.2488	281.2486	0.7	566.3472	566.3463	1.6	590.3513	590.3463	8.5	24.00	9Δ	ω-7
702.4720	702.4715	0.7	14.76	PE	14:1 OH	241.1809	241.1809	0.0	18:1	281.2487	281.2486	0.4	592.36	592.362	-3.4	616.362	616.3625	-0.8	24.00	9Δ(18:1), 7Δ(14:1 OH)	ω-7, ω-7
690.4728	690.4715	1.9	15.80	PE	14:0 OH	243.1969	243.1966	1.2	17:1	267.2333	267.2330	1.1	578.3434	578.3463	-5.0	592.3608	592.362	-2.0	14.02	9Δ	ω-7
717.4717	717.4712	0.7	15.87	PG	16:1	253.2175	253.2173	0.8	16:1	253.2175	253.2173	0.8	607.3635	607.3617	3.0	631.361	631.3617	-1.1	24.00	9Δ, 9Δ	ω-7, ω-7
730.5035	730.5028	1.0	17.73	PE	16:1	253.2174	253.2173	0.4	18:1 OH	297.2437	297.2435	0.7	644.3871	644.3933	-9.6	620.3916	620.3933	-2.7	24.00	9Δ(16:1), 11Δ(18:1 OH)	ω-7, ω-7
					16:1 OH	269.2124	269.2122	0.7	18:1	281.2488	281.2486	0.7								9Δ(16:1 OH), 11Δ(18:1)	ω-7, ω-7
719.4875	719.4869	0.8	19.13	PG	16:0	255.2329	255.2330	-0.4	16:1	253.2175	253.2173	0.8	609.3801	609.3773	4.6	633.3797	633.3773	3.8	24.00	9Δ	ω-7
674.4774	674.4766	1.2	20.74	PE	15:0	241.2174	241.2173	0.4	16:1	253.2175	253.2173	0.8	564.3681	564.3671	1.8	588.3682	588.3671	1.9	24.00	9Δ	ω-7
674.4769		0.4	21.63		14:0	227.2016	227.2017	-0.4	17:1	267.2329	267.2330	-0.4	562.3511	562.3514	-0.5	576.3646	576.3671	-4.3	14.01	9Δ	ω-7
733.5065	733.5025	5.5	21.85	PG	16:0	255.2338	255.2330	3.1	17:1	267.2340	267.2330	3.7	621.3762	621.3773	-1.8	635.3917	635.393	-2.0	14.02	9Δ	ω-7
688.491	688.4923	-1.9	23.27	PE	16:1	253.2185	253.2173	4.7	16:0	255.2332	255.2330	0.8	578.3802	578.3827	-4.3	602.3826	602.3827	-0.2	24.00	9Δ	ω-7
688.493		1.0	24.10		15:0	241.2174	241.2173	0.4	17:1	267.2331	267.2330	0.4	576.3658	576.3671	-2.3	590.3787	590.3827	-6.8	14.01	9Δ	ω-7
747.5201	747.5182	2.5	23.54	PG	16:0	255.2334	255.2330	1.6	18:1	281.2491	281.2486	1.8	637.4125	637.4086	6.1	661.4036	661.4086	-7.6	23.99	9Δ	ω-7
714.5081	714.5079	0.3	25.55	PE	17:1	267.2329	267.2330	-0.4	17:1	267.2329	267.2330	-0.4	602.3801	602.3827	-4.3	616.3959	616.3984	-4.1	14.02	9Δ, 9Δ	ω-7, ω-7
702.5082	702.5079	0.4	26.74	PE	16:0	255.2330	255.2330	0.0	17:1	267.2330	267.2330	0.0	590.3793	590.3827	-5.8	604.3981	604.3984	-0.5	14.02	9Δ	ω-7
728.5245	728.5236	1.2	27.60	PE	16:1	253.2175	253.2173	0.8	19:1	295.2644	295.2639	1.7	618.4084	618.414	-9.1	642.4077	642.414	-9.8	24.00	9Δ(16:1), 11Δ(19:1)	ω-7, ω-7
					17:1	267.2331	267.2330	0.4	18:1	281.2488	281.2486	0.7	616.3965	616.3984	-3.1	630.4106	630.414	-5.4	14.01	9Δ(17:1), 11Δ(18:1)	ω-7, ω-7
716.5234	716.5236	-0.3	29.95	PE	15:0	241.2173	241.2173	0.0	19:1	295.2642	295.2639	1.0	604.3959	604.3984	-4.1	618.4109	618.414	-5.0	14.02	11Δ	ω-7
					17:1	267.2329	267.2330	-0.4	17:0	269.2485	269.2486	-0.4								9Δ	ω-7
730.5394	730.5392	0.3	33.68	PE	16:0	255.2329	255.2330	-0.4	19:1	295.2642	295.2639	1.0	618.41	618.414	-6.5	632.428	632.4297	-2.7	14.02	11Δ	ω-7
					17:1	267.2329	267.2330	-0.4	18:0	283.2643	283.2643	0.0								9Δ	ω-7

Table S5. List of all identified unsaturated lipids in *P. mirabilis* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

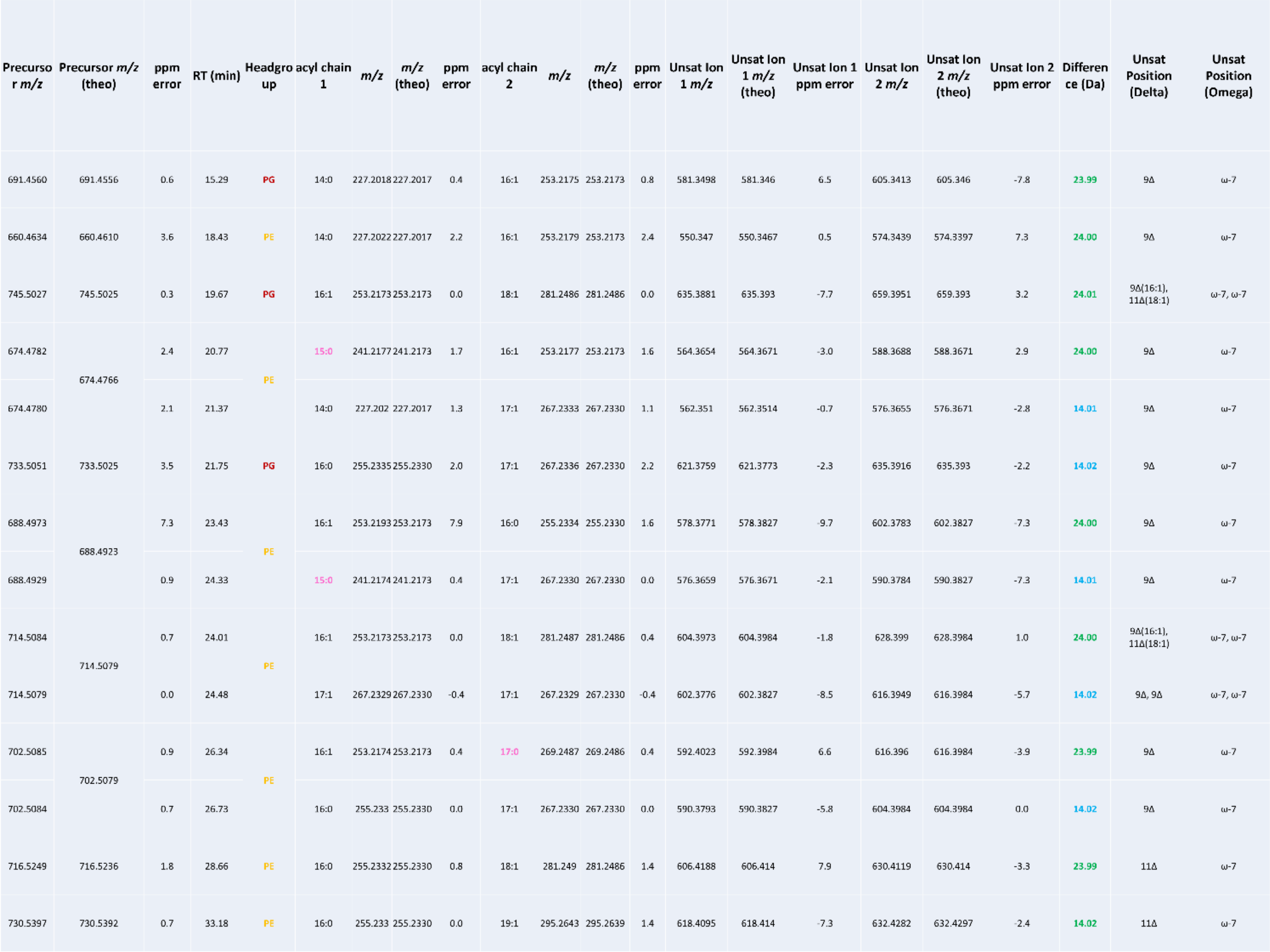
P. aeruginosa



Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
717.4713	717.4712	0.1	15.89	PG	16:1	253.2173	253.2173	0.0	16:1	253.2173	253.2173	0.0	607.3667	607.3617	8.2	631.3561	631.3617	-8.9	23.99	9Δ, 9Δ	ω-7, ω-7
719.4873	719.4869	0.6	18.61	PG	14:0	227.2017	227.2017	0.0	18:1	281.2487	281.2486	0.4	609.3801	609.3773	4.6	633.3816	633.3773	6.8	24.00	11Δ	ω-7
719.4877		1.1	19.14		16:1	253.2176	253.2173	1.2	16:0	255.2329	255.2330	-0.4	609.3807	609.3773	5.6	633.3797	633.3773	3.8	24.00	9Δ	ω-7
745.5027	745.5025	0.3	19.67	PG	16:1	253.2173	253.2173	0.0	18:1	281.2486	281.2486	0.0	635.39	635.393	-4.7	659.3934	659.393	0.6	24.00	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
733.5023	733.5025	-0.3	22.05	PG	16:0	255.2329	255.2330	-0.4	17:1	267.2328	267.2330	-0.7	621.3734	621.3773	-6.3	635.3887	635.393	-6.8	14.02	9Δ	ω-7
747.5201	747.5182	2.5	23.28	PG	16:0	255.233	255.2330	0.0	18:1	281.2487	281.2486	0.4	637.4117	637.4086	4.9	661.4043	661.4086	-6.5	23.99	11Δ	ω-7
747.5184		0.3	23.75		16:1	253.2175	253.2173	0.8	18:0	283.2644	283.2643	0.4	637.4125	637.4086	6.1	661.4031	661.4086	-8.3	23.99	9Δ	ω-7
773.5363	773.5338	3.2	24.04	PG	18:1	281.2487	281.2486	0.4	18:1	281.2487	281.2486	0.4	663.4236	663.4243	-1.1	687.4175	687.4243	-9.9	23.99	11Δ, 11Δ	ω-7, ω-7
714.5089	714.5079	1.4	24.77	PE	16:1	253.2175	253.2173	0.8	18:1	281.2489	281.2486	1.1	604.3975	604.3984	-1.5	628.3958	628.3984	-4.1	24.00	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
702.5084	702.5079	0.7	25.63	PE	15:0	241.2174	241.2173	0.4	18:1	281.2487	281.2486	0.4	592.3995	592.3984	1.9	616.3941	616.3984	-7.0	23.99	11Δ	ω-7
702.5087		1.1	27.07		16:0	255.2331	255.2330	0.4	17:1	267.2332	267.2330	0.7	590.3789	590.3827	-6.4	604.3978	604.3984	-1.0	14.02	9Δ	ω-7
761.5361	761.5338	3.0	27.00	PG	16:0	255.2335	255.2330	2.0	19:1	295.2649	295.2639	3.4	649.4072	649.4086	-2.2	663.423	663.4243	-2.0	14.02	11Δ	ω-7
716.5258	716.5236	3.1	29.14	PE	16:0	255.2335	255.2330	2.0	18:1	281.2493	281.2486	2.5	606.4199	606.414	9.7	630.4124	630.414	-2.5	23.99	11Δ	ω-7
742.5399	742.5392	0.9	29.71	PE	18:1	281.2487	281.2486	0.4	18:1	281.2487	281.2486	0.4	632.4242	632.4297	-8.7	656.4308	656.4297	1.7	24.01	11Δ, 11Δ	ω-7
742.5393		0.1	31.88		17:1	267.2329	267.2330	0.4	19:1	295.2642	295.2639	1.0	630.4113	630.414	-4.3	644.4264	644.4297	-5.1	14.02	9Δ(17:1), 11Δ(19:1)	ω-7
730.54	730.5392	1.1	31.13	PE	17:0	269.2488	269.2486	0.7	18:1	281.2488	281.2486	0.7	620.4337	620.4297	6.4	644.4255	644.4297	-6.5	23.99	11Δ	ω-7
730.5396		0.5	33.09		16:0	255.233	255.2330	0.0	19:1	295.2643	295.2639	1.4	618.4099	618.414	-6.6	632.4283	632.4297	-2.2	14.02	11Δ	ω-7
818.5877	818.5917	-4.9	31.59	PC	16:0	255.2329	255.2330	-0.4	19:1	295.2642	295.2639	1.0	706.4655	706.4665	-1.4	720.4819	720.4821	-0.3	14.02	11Δ	ω-7

Table S6. List of all identified unsaturated lipids in *P. aeruginosa* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

S. Typhimurium



Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
691.4560	691.4556	0.6	15.29	PG	14:0	227.2018	227.2017	0.4	16:1	253.2175	253.2173	0.8	581.3498	581.346	6.5	605.3413	605.346	-7.8	23.99	9Δ	ω-7
660.4634	660.4610	3.6	18.43	PE	14:0	227.2022	227.2017	2.2	16:1	253.2179	253.2173	2.4	550.347	550.3467	0.5	574.3439	574.3397	7.3	24.00	9Δ	ω-7
745.5027	745.5025	0.3	19.67	PG	16:1	253.2173	253.2173	0.0	18:1	281.2486	281.2486	0.0	635.3881	635.393	-7.7	659.3951	659.393	3.2	24.01	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
674.4782	674.4766	2.4	20.77	PE	15:0	241.2177	241.2173	1.7	16:1	253.2177	253.2173	1.6	564.3654	564.3671	-3.0	588.3688	588.3671	2.9	24.00	9Δ	ω-7
674.4780		2.1	21.37		14:0	227.202	227.2017	1.3	17:1	267.2333	267.2330	1.1	562.351	562.3514	-0.7	576.3655	576.3671	-2.8	14.01	9Δ	ω-7
733.5051	733.5025	3.5	21.75	PG	16:0	255.2335	255.2330	2.0	17:1	267.2336	267.2330	2.2	621.3759	621.3773	-2.3	635.3916	635.393	-2.2	14.02	9Δ	ω-7
688.4973	688.4923	7.3	23.43	PE	16:1	253.2193	253.2173	7.9	16:0	255.2334	255.2330	1.6	578.3771	578.3827	-9.7	602.3783	602.3827	-7.3	24.00	9Δ	ω-7
688.4929		0.9	24.33		15:0	241.2174	241.2173	0.4	17:1	267.2330	267.2330	0.0	576.3659	576.3671	-2.1	590.3784	590.3827	-7.3	14.01	9Δ	ω-7
714.5084	714.5079	0.7	24.01	PE	16:1	253.2173	253.2173	0.0	18:1	281.2487	281.2486	0.4	604.3973	604.3984	-1.8	628.399	628.3984	1.0	24.00	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
714.5079		0.0	24.48		17:1	267.2329	267.2330	-0.4	17:1	267.2329	267.2330	-0.4	602.3776	602.3827	-8.5	616.3949	616.3984	-5.7	14.02	9Δ, 9Δ	ω-7, ω-7
702.5085	702.5079	0.9	26.34	PE	16:1	253.2174	253.2173	0.4	17:0	269.2487	269.2486	0.4	592.4023	592.3984	6.6	616.396	616.3984	-3.9	23.99	9Δ	ω-7
702.5084		0.7	26.73		16:0	255.233	255.2330	0.0	17:1	267.2330	267.2330	0.0	590.3793	590.3827	-5.8	604.3984	604.3984	0.0	14.02	9Δ	ω-7
716.5249	716.5236	1.8	28.66	PE	16:0	255.2332	255.2330	0.8	18:1	281.249	281.2486	1.4	606.4188	606.414	7.9	630.4119	630.414	-3.3	23.99	11Δ	ω-7
730.5397	730.5392	0.7	33.18	PE	16:0	255.233	255.2330	0.0	19:1	295.2643	295.2639	1.4	618.4095	618.414	-7.3	632.4282	632.4297	-2.4	14.02	11Δ	ω-7

Table S7. List of all identified unsaturated lipids in *S.* Typhimurium lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

V. cholerae

Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
702.4725	702.4715	1.4	15.33	PE	16:1	253.2174	253.2173	0.4	16:1 OH	269.2124	269.2122	0.7	592.3627	592.362	1.2	616.3635	616.362	2.4	24.00	9Δ, 9Δ	ω-7, ω-7
658.4467	658.4453	2.1	15.70	PE	14:1	225.1863	225.1860	1.3	16:1	253.2177	253.2173	1.6	548.3331	548.3358	-4.9	572.334	572.3358	-3.1	24.00	9Δ(16:1), 7Δ(14:1)	ω-7, ω-7
717.4714	717.4712	0.3	15.99	PG	16:1	253.2174	253.2173	0.4	16:1	253.2174	253.2173	0.4	607.3594	607.3617	-3.8	631.3571	631.3617	-7.3	24.00	9Δ, 9Δ	ω-7, ω-7
660.4634	660.4610	3.6	18.40	PE	14:0	227.2022	227.2017	2.2	16:1	253.2179	253.2173	2.4	550.3478	550.3467	2.0	574.3442	574.3397	7.8	24.00	9Δ	ω-7
660.4621		1.7	19.17		14:1	225.1863	225.1860	1.3	16:0	255.2332	255.2330	0.8	550.3476	550.3467	1.6	574.3418	574.3397	3.7	23.99	7Δ	ω-7
686.4772	686.4766	0.9	19.69	PE	16:1	253.2174	253.2173	0.4	16:1	253.2174	253.2173	0.4	576.364	576.3671	-5.4	600.3627	600.3671	-7.3	24.00	9Δ, 9Δ	ω-7, ω-7
745.5051	745.5025	3.5	19.84	PG	16:1	253.2175	253.2173	0.8	18:1	281.2488	281.2486	0.7	635.3879	635.393	-8.0	659.3923	659.393	-1.1	24.00	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
733.5051	733.5025	3.5	21.75	PG	16:1	253.2175	253.2173	0.8	17:0	269.2487	269.2486	0.4	609.3726	609.3773	-7.7	633.3804	633.3773	4.9	24.01	8Δ	w-8
688.4974	688.4923	7.4	23.33	PE	16:1	253.2194	253.2173	8.3	16:0	255.2335	255.2330	2.0	578.3769	578.3827	-10.0	602.3805	602.3827	-3.7	24.00	9Δ	ω-7
714.5088	714.5079	1.3	24.50	PE	16:1	253.2175	253.2173	0.8	18:1	281.2488	281.2486	0.7	604.3972	604.3984	-2.0	628.4002	628.3984	2.9	24.00	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
747.5193	747.5182	1.5	23.98	PG	16:1	253.2177	253.2173	1.6	18:0	283.2646	283.2643	1.1	637.4127	637.4086	6.4	661.4046	661.4086	-6.0	23.99	9Δ	ω-7
716.5275	716.5236	5.4	28.77	PE	16:0	255.234	255.2330	3.9	18:1	281.2498	281.2486	4.3	606.4196	606.414	9.2	630.4099	630.414	-6.5	23.99	11Δ	ω-7
716.524		0.6	30.19		16:1	253.2174	253.2173	0.4	18:0	283.2644	283.2643	0.4	606.4142	606.414	0.3	630.4128	630.414	-1.9	24.00	9Δ	ω-7

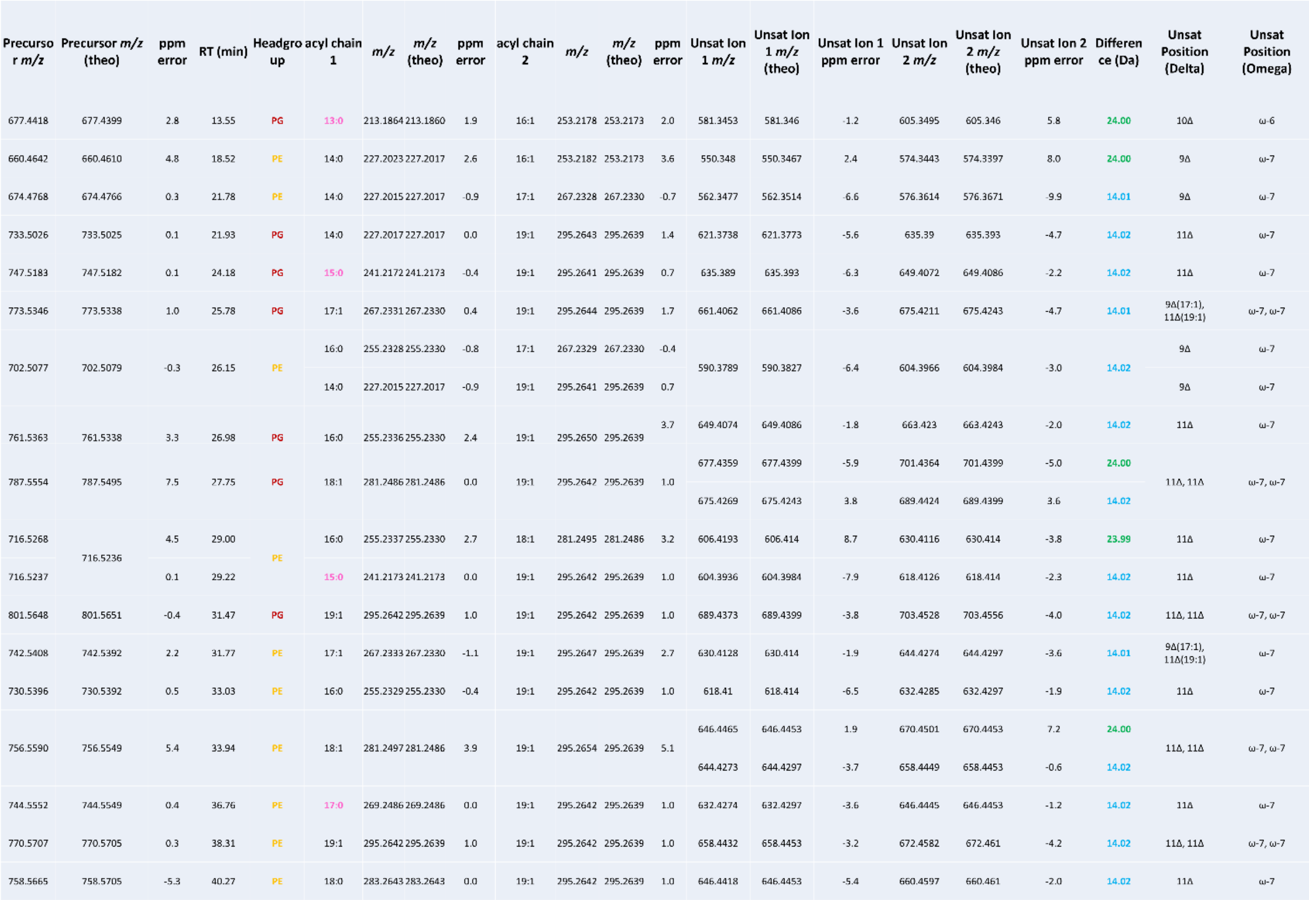
Table S8. List of all identified unsaturated lipids in *V. cholera* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

S. marcescens

Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
717.4711	717.4712	-0.1	15.82	PG	16:1	253.2173	253.2173	0.0	16:1	253.2173	253.2173	0.0	607.3582	607.3617	-5.8	631.3618	631.3617	0.2	24.00	9Δ, 9Δ	ω-7, ω-7
705.4710	705.4712	-0.3	17.53	PG	14:0	227.2016	227.2017	-0.4	17:1	267.2329	267.2330	-0.4	593.342	593.346	-6.7	607.3587	607.3617	-4.9	14.02	9Δ	ω-7
686.4782	686.4766	2.3	19.16	PE	16:1	253.2176	253.2173	1.2	16:1	253.2176	253.2173	1.2	576.3704	576.3671	5.7	600.3626	600.3671	-7.5	23.99	9Δ, 9Δ	ω-7, ω-7
674.4767	674.4766	0.1	20.70	PE	15:0	241.2173	241.2173	0.0	16:1	253.2173	253.2173	0.0	564.3691	564.3671	3.5	588.3692	588.3671	3.6	24.00	9Δ	ω-7
674.4777		1.6	21.37		14:0	227.2019	227.2017	0.9	17:1	267.2332	267.2330	0.7	562.3506	562.3514	-1.4	576.3652	576.3671	-3.3	14.01	9Δ	ω-7
733.5068	733.5025	5.9	21.76	PG	16:0	255.2339	255.2330	3.5	17:1	267.2341	267.2330	4.1	621.3763	621.3773	-1.6	635.3918	635.393	-1.9	14.02	9Δ	ω-7
714.5082	714.5079	0.4	23.33	PE	17:1	267.233	267.2330	0.0	17:1	267.233	267.2330	0.0	602.3804	602.3827	-3.8	616.3964	616.3984	-3.2	14.02	9Δ, 9Δ	ω-7, ω-7
688.4931	688.4923	1.2	24.18	PE	15:0	241.2175	241.2173	0.8	17:1	267.2331	267.2330	0.4	576.3672	576.3671	0.2	590.3781	590.3827	-7.8	14.01	9Δ	ω-7
702.5086	702.5079	1.0	26.22	PE	16:1	253.2175	253.2173	0.8	17:0	269.2487	269.2486	0.4	592.3994	592.3984	1.7	616.3947	616.3984	-6.0	24.00	9Δ	ω-7
702.5084		0.7	26.72		16:0	255.233	255.2330	0.0	17:1	267.2330	267.2330	0.0	590.3792	590.3827	-5.9	604.3984	604.3984	0.0	14.02	9Δ	ω-7
716.5248	716.5236	1.7	28.68	PE	16:0	255.2332	255.2330	0.8	18:1	281.2490	281.2486	1.4	606.4199	606.414	9.7	630.4133	630.414	-1.1	23.99	11Δ	ω-7
716.5242		0.8	29.31		16:1	253.2175	253.2173	0.8	18:0	283.2644	283.2643	0.4	606.4144	606.414	0.7	630.4102	630.414	-6.0	24.00	9Δ	ω-7
730.5394	730.5392	0.3	33.25	PE	16:0	255.2329	255.2330	-0.4	19:1	295.2642	295.2639	1.0	618.4095	618.414	-7.3	632.4277	632.4297	-3.2	14.02	11Δ	ω-7
730.5392		0.0	33.48		17:1	267.2329	267.2330	-0.4	18:0	283.2642	283.2643	-0.4	618.4093	618.414	-7.6	632.4289	632.4297	-1.3	14.02	9Δ	ω-7

Table S9. List of all identified unsaturated lipids in *S. marcescens* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

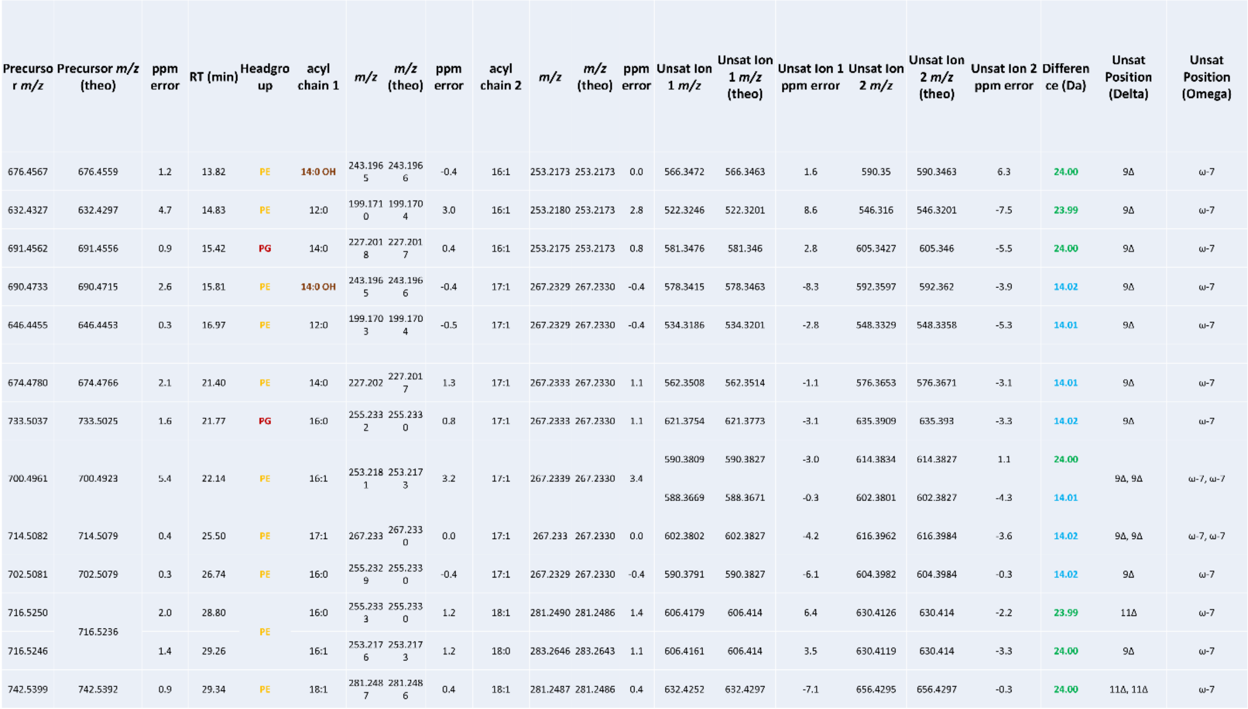
C. jejuni



Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
677.4418	677.4399	2.8	13.55	PG	13:0	213.1864	213.1860	1.9	16:1	253.2178	253.2173	2.0	581.3453	581.346	-1.2	605.3495	605.346	5.8	24.00	10Δ	ω-6
660.4642	660.4610	4.8	18.52	PE	14:0	227.2023	227.2017	2.6	16:1	253.2182	253.2173	3.6	550.348	550.3467	2.4	574.3443	574.3397	8.0	24.00	9Δ	ω-7
674.4768	674.4766	0.3	21.78	PE	14:0	227.2015	227.2017	-0.9	17:1	267.2328	267.2330	-0.7	562.3477	562.3514	-6.6	576.3614	576.3671	-9.9	14.01	9Δ	ω-7
733.5026	733.5025	0.1	21.93	PG	14:0	227.2017	227.2017	0.0	19:1	295.2643	295.2639	1.4	621.3738	621.3773	-5.6	635.39	635.393	-4.7	14.02	11Δ	ω-7
747.5183	747.5182	0.1	24.18	PG	15:0	241.2172	241.2173	-0.4	19:1	295.2641	295.2639	0.7	635.389	635.393	-6.3	649.4072	649.4086	-2.2	14.02	11Δ	ω-7
773.5346	773.5338	1.0	25.78	PG	17:1	267.2331	267.2330	0.4	19:1	295.2644	295.2639	1.7	661.4062	661.4086	-3.6	675.4211	675.4243	-4.7	14.01	9Δ(17:1), 11Δ(19:1)	ω-7, ω-7
702.5077	702.5079	-0.3	26.15	PE	16:0	255.2328	255.2330	-0.8	17:1	267.2329	267.2330	-0.4	590.3789	590.3827	-6.4	604.3966	604.3984	-3.0	14.02	9Δ	ω-7
					14:0	227.2015	227.2017	-0.9	19:1	295.2641	295.2639	0.7								9Δ	ω-7
761.5363	761.5338	3.3	26.98	PG	16:0	255.2336	255.2330	2.4	19:1	295.2650	295.2639	3.7	649.4074	649.4086	-1.8	663.423	663.4243	-2.0	14.02	11Δ	ω-7
787.5554	787.5495	7.5	27.75	PG	18:1	281.2486	281.2486	0.0	19:1	295.2642	295.2639	1.0	677.4359	677.4399	-5.9	701.4364	701.4399	-5.0	24.00	11Δ, 11Δ	ω-7, ω-7
													675.4269	675.4243	3.8	689.4424	689.4399	3.6	14.02		
716.5268	716.5236	4.5	29.00	PE	16:0	255.2337	255.2330	2.7	18:1	281.2495	281.2486	3.2	606.4193	606.414	8.7	630.4116	630.414	-3.8	23.99	11Δ	ω-7
716.5237		0.1	29.22		15:0	241.2173	241.2173	0.0	19:1	295.2642	295.2639	1.0	604.3936	604.3984	-7.9	618.4126	618.414	-2.3	14.02	11Δ	ω-7
801.5648	801.5651	-0.4	31.47	PG	19:1	295.2642	295.2639	1.0	19:1	295.2642	295.2639	1.0	689.4373	689.4399	-3.8	703.4528	703.4556	-4.0	14.02	11Δ, 11Δ	ω-7, ω-7
742.5408	742.5392	2.2	31.77	PE	17:1	267.2333	267.2330	-1.1	19:1	295.2647	295.2639	2.7	630.4128	630.414	-1.9	644.4274	644.4297	-3.6	14.01	9Δ(17:1), 11Δ(19:1)	ω-7
730.5396	730.5392	0.5	33.03	PE	16:0	255.2329	255.2330	-0.4	19:1	295.2642	295.2639	1.0	618.41	618.414	-6.5	632.4285	632.4297	-1.9	14.02	11Δ	ω-7
756.5590	756.5549	5.4	33.94	PE	18:1	281.2497	281.2486	3.9	19:1	295.2654	295.2639	5.1	646.4465	646.4453	1.9	670.4501	670.4453	7.2	24.00	11Δ, 11Δ	ω-7, ω-7
													644.4273	644.4297	-3.7	658.4449	658.4453	-0.6	14.02		
744.5552	744.5549	0.4	36.76	PE	17:0	269.2486	269.2486	0.0	19:1	295.2642	295.2639	1.0	632.4274	632.4297	-3.6	646.4445	646.4453	-1.2	14.02	11Δ	ω-7
770.5707	770.5705	0.3	38.31	PE	19:1	295.2642	295.2639	1.0	19:1	295.2642	295.2639	1.0	658.4432	658.4453	-3.2	672.4582	672.461	-4.2	14.02	11Δ, 11Δ	ω-7, ω-7
758.5665	758.5705	-5.3	40.27	PE	18:0	283.2643	283.2643	0.0	19:1	295.2642	295.2639	1.0	646.4418	646.4453	-5.4	660.4597	660.461	-2.0	14.02	11Δ	ω-7

Table S10. List of all identified unsaturated lipids in *C. jejuni* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

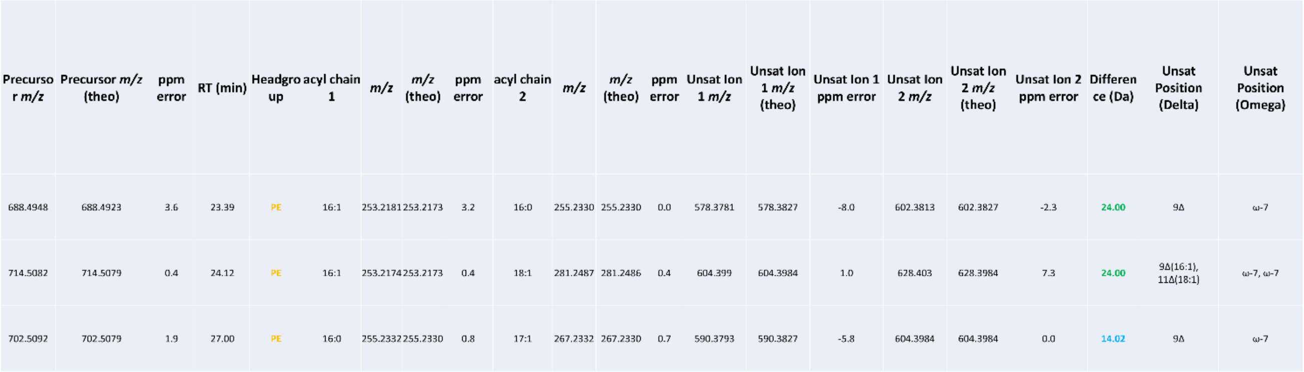
Y. pseudotuberculosis



Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
676.4567	676.4559	1.2	13.82	PE	14:0 OH	243.1965	243.1966	-0.4	16:1	253.2173	253.2173	0.0	566.3472	566.3463	1.6	590.35	590.3463	6.3	24.00	9Δ	ω-7
632.4327	632.4297	4.7	14.83	PE	12:0	199.1710	199.1704	3.0	16:1	253.2180	253.2173	2.8	522.3246	522.3201	8.6	546.316	546.3201	-7.5	23.99	9Δ	ω-7
691.4562	691.4556	0.9	15.42	PG	14:0	227.2018	227.2017	0.4	16:1	253.2175	253.2173	0.8	581.3476	581.346	2.8	605.3427	605.346	-5.5	24.00	9Δ	ω-7
690.4733	690.4715	2.6	15.81	PE	14:0 OH	243.1965	243.1966	-0.4	17:1	267.2329	267.2330	-0.4	578.3415	578.3463	-8.3	592.3597	592.362	-3.9	14.02	9Δ	ω-7
646.4455	646.4453	0.3	16.97	PE	12:0	199.1703	199.1704	-0.5	17:1	267.2329	267.2330	-0.4	534.3186	534.3201	-2.8	548.3329	548.3358	-5.3	14.01	9Δ	ω-7
674.4780	674.4766	2.1	21.40	PE	14:0	227.202	227.2017	1.3	17:1	267.2333	267.2330	1.1	562.3508	562.3514	-1.1	576.3653	576.3671	-3.1	14.01	9Δ	ω-7
733.5037	733.5025	1.6	21.77	PG	16:0	255.2332	255.2330	0.8	17:1	267.2333	267.2330	1.1	621.3754	621.3773	-3.1	635.3909	635.393	-3.3	14.02	9Δ	ω-7
700.4961	700.4923	5.4	22.14	PE	16:1	253.2181	253.2173	3.2	17:1	267.2339	267.2330	3.4	590.3809 588.3669	590.3827 588.3671	-3.0 -0.3	614.3834 602.3801	614.3827 602.3827	1.1 -4.3	24.00 14.01	9Δ, 9Δ	ω-7, ω-7
714.5082	714.5079	0.4	25.50	PE	17:1	267.233	267.2330	0.0	17:1	267.233	267.2330	0.0	602.3802	602.3827	-4.2	616.3962	616.3984	-3.6	14.02	9Δ, 9Δ	ω-7, ω-7
702.5081	702.5079	0.3	26.74	PE	16:0	255.2329	255.2330	-0.4	17:1	267.2329	267.2330	-0.4	590.3791	590.3827	-6.1	604.3982	604.3984	-0.3	14.02	9Δ	ω-7
716.5250	716.5236	2.0	28.80	PE	16:0	255.2333	255.2330	1.2	18:1	281.2490	281.2486	1.4	606.4179	606.414	6.4	630.4126	630.414	-2.2	23.99	11Δ	ω-7
716.5246		1.4	29.26		16:1	253.2176	253.2173	1.2	18:0	283.2646	283.2643	1.1	606.4161	606.414	3.5	630.4119	630.414	-3.3	24.00	9Δ	ω-7
742.5399	742.5392	0.9	29.34	PE	18:1	281.2487	281.2486	0.4	18:1	281.2487	281.2486	0.4	632.4252	632.4297	-7.1	656.4295	656.4297	-0.3	24.00	11Δ, 11Δ	ω-7

Table S11. List of all identified unsaturated lipids in *Y. pseudotuberculosis* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

B. subtilis



Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)
688.4948	688.4923	3.6	23.39	PE	16:1	253.2181	253.2173	3.2	16:0	255.2330	255.2330	0.0	578.3781	578.3827	-8.0	602.3813	602.3827	-2.3	24.00	9Δ	ω-7
714.5082	714.5079	0.4	24.12	PE	16:1	253.2174	253.2173	0.4	18:1	281.2487	281.2486	0.4	604.399	604.3984	1.0	628.403	628.3984	7.3	24.00	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
702.5092	702.5079	1.9	27.00	PE	16:0	255.2332	255.2330	0.8	17:1	267.2332	267.2330	0.7	590.3793	590.3827	-5.8	604.3984	604.3984	0.0	14.02	9Δ	ω-7

Table S12. List of all identified unsaturated lipids in *B. subtilis* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

L. plantarum

Precursor *m/z*	Precursor *m/z* (theo)	ppm error	RT (min)	Headgroup	acyl chain 1	*m/z*	*m/z* (theo)	ppm error	acyl chain 2	*m/z*	*m/z* (theo)	ppm error	Unsat Ion 1 *m/z*	Unsat Ion 1 *m/z* (theo)	Unsat Ion 1 ppm error	Unsat Ion 2 *m/z*	Unsat Ion 2 *m/z* (theo)	Unsat Ion 2 ppm error	Difference (Da)	Unsat Position (Delta)	Unsat Position (Omega)	Precursor *m/z*
717.4712	717.4712	0.0	1823	15.85	PG	16:1	253.2173	253.2173	0.0	16:1	253.2173	253.2173	0.0	607.3586	607.3617	-5.1	631.3595	631.3617	-3.5	24.00	9Δ	ω-7
719.4888	719.4869	2.6	2015	18.80	PG	14:0	227.2021	227.2017	1.8	18:1	281.2492	281.2486	2.1	609.3845	609.3773	11.8	633.3824	633.3773	8.1	24.00	11Δ	ω-7
719.4879		1.4	2024	19.03		16:1	253.2177	253.2173	1.6	16:0	255.233	255.2330	0.0	609.3815	609.3773	6.9	633.3845	633.3773	11.4	24.00	9Δ	ω-7
745.5040	745.5025	2.0	2067	20.23	PG	16:1	253.2179	253.2173	2.4	18:1	281.2491	281.2486	1.8	635.3878	635.393	-8.2	659.3986	659.393	8.5	24.01	9Δ(16:1), 11Δ(18:1)	ω-7, ω-7
733.5024	733.5025	-0.1	2128	21.70	PG	14:0	227.2016	227.2017	-0.4	19:1	295.2642	295.2639	1.0	621.3737	621.3773	-5.8	635.3885	635.393	-7.1	14.01	11Δ	ω-7
														593.3429	593.346	-5.2	607.3611	607.3617	-1.0	14.02	9Δ	ω-9
747.5201	747.5182	2.5	2227	24.59	PG	16:1	253.2174	253.2173	0.4	18:0	283.2643	283.2643	0.0	637.4096	637.4086	1.6	661.4095	661.4086	1.4	24.00	9Δ	ω-7
						16:0	255.2329	255.2330	-0.4	18:1	281.2487	281.2486	0.4								11Δ	ω-7
761.5354	761.5338	2.1	2333	27.45	PG	16:0	255.2334	255.2330	1.6	19:1	295.2647	295.2639	2.7	649.4067	649.4086	-2.9	663.4225	663.4243	-2.7	14.02	11Δ	ω-7
														621.3784	621.3773	1.8	635.3928	635.393	-0.3	14.01	9Δ	ω-9
775.5500	775.5495	0.6	2396	29.02	PG	18:1	281.2489	281.2486	1.1	18:0	283.2643	283.2643	0.0	665.4409	665.4399	1.5	689.4399	689.4399	0.0	24.00	11Δ	ω-7

Table S13. List of all identified unsaturated lipids in *L. plantarum* lipid extract with all precursor and fragment ion ppm error values for acyl chain product ions and unsaturation element fragment ions (within 10 ppm error). Features are color coded by headgroup (PGs in red, PEs in yellow, PCs in purple), unsaturation type (cyclopropane rings in blue, double bonds in green), and unique acyl chain modifications (odd-carbon branched acyl chains in pink, hydroxyl acyl chains in brown).

Polyunsaturated fatty acids within GPLs

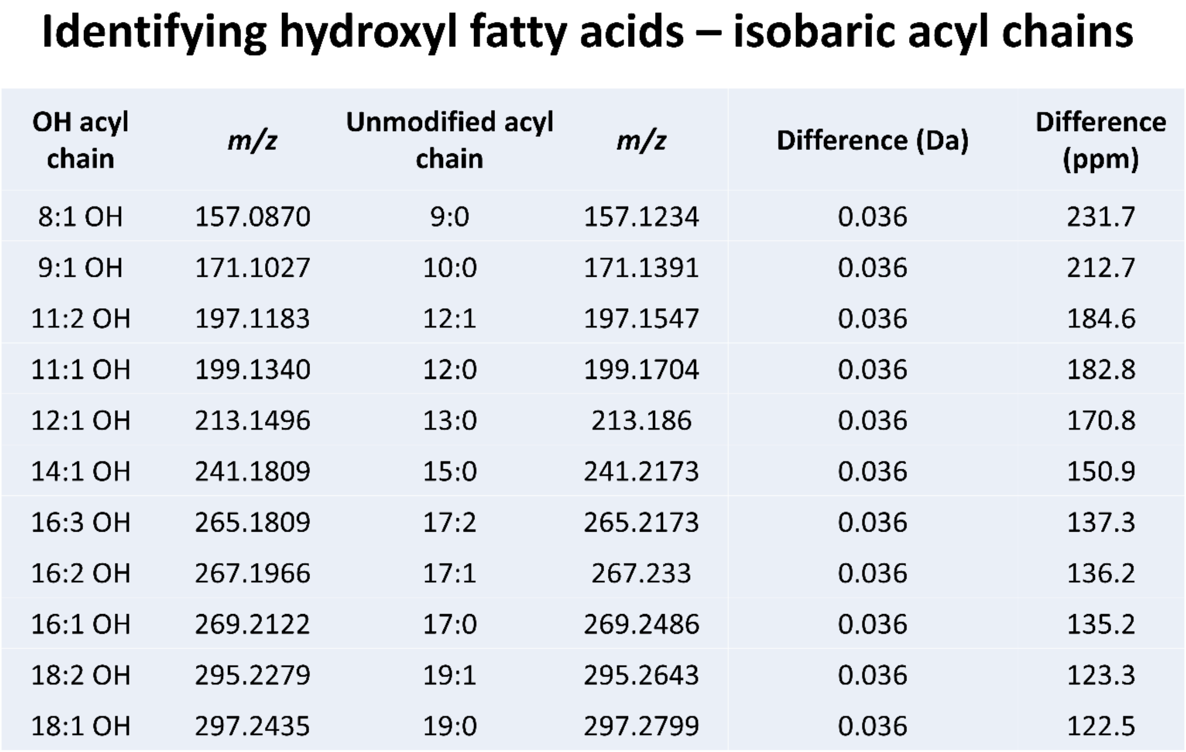
Acyl Chain	$m/z_{\text{theoretical}}$	m/z_{observed}	error (ppm)	Sample
11:2 OH	197.1183	197.1183	0.00	*Escherichia coli*
		197.1183	0.00	*Salmonella enterica Typhimurium*
16:4	247.1704	247.1705	0.40	*Klebsiella pneumoniae*
		247.1705	0.40	*Bacillus subtilis*
16:2	251.2017	251.2016	-0.40	*Klebsiella pneumoniae*
		251.2019	0.80	*Proteus mirabilis*
		251.2017	0.00	*Vibrio cholerae*
		251.2017	0.00	*Lactobacillus plantarum*
		251.2013	-1.59	*Escherichia coli*
		251.2016	-0.40	*Pseudomonas aeruginosa*
16:3 OH	265.1809	265.1810	0.38	*Vibrio cholerae*
		265.1810	0.38	*Escherichia coli*
17:2	265.2173	265.2173	0.00	*Klebsiella pneumoniae*
16:2 OH	267.1967	267.1966	0.37	*Escherichia coli*
		267.1966	0.37	*Enterobacter cloacae*
18:4	275.2017	275.2017	0.00	*Klebsiella pneumoniae*
		275.2018	0.36	*Bacillus subtilis*
18:3	277.2173	277.2171	-0.72	*Campylobacter jejuni*
18:2	279.2330	279.2329	-0.36	*Klebsiella pneumoniae*
		279.2328	-0.72	*Proteus mirabilis*
		279.233	0.00	*Vibrio cholerae*
		279.2328	-0.72	*Campylobacter jejuni*
		279.2329	-0.36	*Escherichia coli*
		279.2331	0.36	*Lactobacillus plantarum*
		279.2327	-1.07	*Enterobacter cloacae*
		279.2330	0.00	*Pseudomonas aeruginosa*
19:2	293.2486	293.2486	0.00	*Klebsiella pneumoniae*
18:2 OH	295.2279	295.2281	0.68	*Vibrio cholerae*
		295.2277	-0.68	*Escherichia coli*
		295.2277	-0.68	*Yersinia pseudotuberculosis*
20:4	303.2330	303.2330	0.00	*Klebsiella pneumoniae*

Table S14. List of identified polyunsaturated fatty acids (PUFAs) within GPLs with observed and theoretical acyl chain product ion *m/z* values along with the bacterial lipid extract they were identified in.

Hydroxyl fatty acids within GPLs

Acyl Chain	$m/z_{\text{theoretical}}$	m/z_{observed}	error (ppm)	Sample
8:1 OH	157.0870	157.0870	0.00	*Escherichia coli*
9:1 OH	171.1027	171.1027	0.00	*Escherichia coli*
		171.1027	0.00	*Enterobacter cloacae*
		171.1027	0.00	*Klebsiella pneumoniae*
		171.1027	0.00	*Proteus mirabilis*
		171.1028	-0.58	*Salmonella enterica Typhimurium*
		171.1027	0.00	*Vibrio cholerae*
		171.1026	0.58	*Serratia marcescens*
		171.1026	0.58	*Yersinia pseudotuberculosis*
10:0 OH	187.1340	187.1339	0.53	*Escherichia coli*
		187.1340	0.00	*Proteus mirabilis*
		187.1340	0.00	*Salmonella enterica Typhimurium*
		187.1340	0.00	*Yersinia pseudotuberculosis*
11:2 OH	197.1183	197.1183	0.00	*Escherichia coli*
		197.1183	0.00	*Salmonella enterica Typhimurium*
11:1 OH	199.1340	199.1339	0.50	*Escherichia coli*
12:1 OH	213.1496	213.1496	0.00	*Proteus mirabilis*
12:0 OH	215.1653	215.1653	0.00	*Escherichia coli*
		215.1655	-0.93	*Proteus mirabilis*
		215.1654	-0.46	*Salmonella enterica Typhimurium*
14:1 OH	241.1809	241.1811	-0.83	*Proteus mirabilis*
		241.1811	-0.83	*Vibrio cholerae*
14:0 OH	243.1966	243.1966	0.00	*Escherichia coli*
		243.1966	0.00	*Proteus mirabilis*
		243.1967	-0.41	*Salmonella enterica Typhimurium*
		243.1969	-1.23	*Vibrio cholerae*
		243.1965	0.41	*Yersinia pseudotuberculosis*
16:3 OH	265.1809	265.1810	-0.38	*Vibrio cholerae*
		265.1810	-0.38	*Escherichia coli*
16:2 OH	267.1966	267.1967	-0.37	*Escherichia coli*
		267.1966	0.00	*Enterobacter cloacae*
		267.1965	0.37	*Salmonella enterica Typhimurium*
		267.1967	-0.37	*Vibrio cholerae*
		267.1967	-0.37	*Serratia marcescens*
		267.1966	0.00	*Yersinia pseudotuberculosis*
16:1 OH	269.2122	269.2124	-0.74	*Escherichia coli*
		269.2121	0.37	*Klebsiella pneumoniae*
		269.2123	-0.37	*Proteus mirabilis*
		269.2123	-0.37	*Pseudomonas aeruginosa*
		269.2121	0.37	*Salmonella enterica Typhimurium*
		269.2124	-0.74	*Vibrio cholerae*
		269.2122	0.00	*Serratia marcescens*
		269.2120	0.74	*Yersinia pseudotuberculosis*
16:0 OH	271.2279	271.2281	-0.74	*Proteus mirabilis*
		271.2277	0.74	*Campylobacter jejuni*
		271.2278	0.37	*Yersinia pseudotuberculosis*
18:2 OH	295.2279	295.2281	-0.68	*Vibrio cholerae*
		295.2277	0.68	*Escherichia coli*
		295.2277	0.68	*Yersinia pseudotuberculosis*
18:1 OH	297.2435	297.2437	-0.67	*Proteus mirabilis*
		297.2436	-0.34	*Pseudomonas aeruginosa*
18:0 OH	299.2592	299.2590	0.67	*Vibrio cholerae*

Table S15. List of identified hydroxyl acyl chains within GPLs with observed and theoretical acyl chain product ion *m/z* values along with the bacterial lipid extract they were identified in.



Identifying hydroxyl fatty acids – isobaric acyl chains

OH acyl chain	*m/z*	Unmodified acyl chain	*m/z*	Difference (Da)	Difference (ppm)
8:1 OH	157.0870	9:0	157.1234	0.036	231.7
9:1 OH	171.1027	10:0	171.1391	0.036	212.7
11:2 OH	197.1183	12:1	197.1547	0.036	184.6
11:1 OH	199.1340	12:0	199.1704	0.036	182.8
12:1 OH	213.1496	13:0	213.186	0.036	170.8
14:1 OH	241.1809	15:0	241.2173	0.036	150.9
16:3 OH	265.1809	17:2	265.2173	0.036	137.3
16:2 OH	267.1966	17:1	267.233	0.036	136.2
16:1 OH	269.2122	17:0	269.2486	0.036	135.2
18:2 OH	295.2279	19:1	295.2643	0.036	123.3
18:1 OH	297.2435	19:0	297.2799	0.036	122.5

Table S16. List of identified OH acyl chains with their respective acyl chain product ion *m/z* values along with unmodified (non-hydroxyl) acyl chains which are isobaric with each hydroxyl acyl chain. The small difference in mass between hydroxyl acyl chains and unmodified acyl chains showcases the need for high-resolution high-mass accuracy instrumentation for identification of hydroxyl acyl chains.

Lysyl-PGs in Gram-negative and Gram-positive bacteria

Bacterium	Precursor *m/z* (exp)	ID
Campylobacter jejuni	779.5192	Lysyl PG 13:0_14:0
	793.535	Lysyl PG 13:0_15:0
	807.5516	Lysyl PG 13:0_16:0
	821.5665	Lysyl PG 13:0_17:0
	835.5818	Lysyl PG 15:0_16:0
Bacillus subtilis	821.5665	Lysyl PG 15:0/15:0
	821.5659	Lysyl PG 15:0/15:0
Lactobacillus plantarum	875.6149	Lysyl PG 16:0_18:1
	889.6292	Lysyl PG 16:0_19:1
	877.6284	Lysyl PG 16:0_18:0

Table S17. List of identified lysyl-PGs with their respective precursor *m/z* values in Gram-negative *C. jejuni* and Gram-positive *B. subtilis* and *L. plantarum*.