A Reversed Phase Ultra-High-Performance Liquid Chromatography-Data Independent Mass Spectrometry Method for the Rapid Identification of Mycobacterial Lipids

Isin T. Sakallioglu,[1] Amith S. Maroli,[1,2] Aline De Lima Liete,[1,2] and Robert Powers[1,2,*]

[1]*Department of Chemistry, University of Nebraska-Lincoln, Lincoln NE 68588-0304*

[2]*Nebraska Center for Integrated Biomolecular Communication, University of Nebraska-Lincoln, Lincoln NE 68588-0304*

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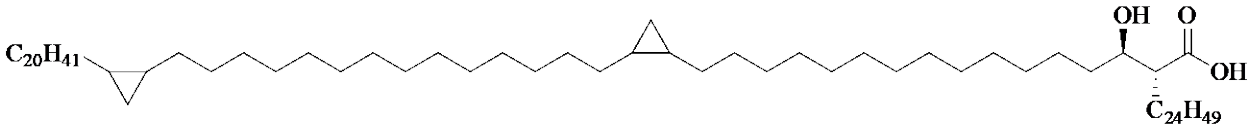
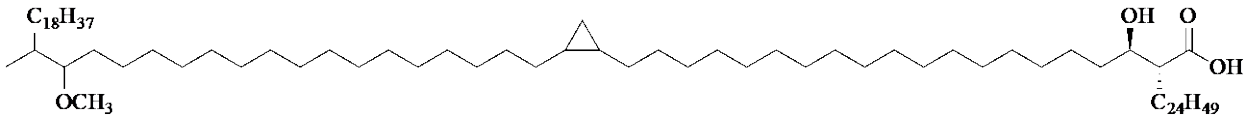
A)



Chemical Formula: $C_{80}H_{156}O_3$
Exact Mass: 1165.21
Molecular Weight: 1166.09
m/z: 1165.21 (100.0%), 1166.21 (88.4%), 1167.21 (37.7%), 1168.22 (11.1%), 1169.22 (2.6%), 1167.22 (1.6%)
Elemental Analysis: C, 82.40; H, 13.48; O, 4.12

B)



Chemical Formula: $C_{85}H_{168}O_4$
Exact Mass: 1253.29
Molecular Weight: 1254.24
m/z: 1253.29 (100.0%), 1254.30 (94.0%), 1255.30 (44.5%), 1256.30 (13.3%), 1257.31 (3.4%)
Elemental Analysis: C, 81.40; H, 13.50; O, 5.10

Figure S1. Chemical structures and predicted properties for **(A)** α-mycolic acid and **(B)** methoxy cis mycolic acid. ChemDraw v19.1 (PerkinElmer, Waltham, MA) was used to generate chemical structures and to predict chemical and mass spectrometry parameters, which included theoretical isotopic distribution.

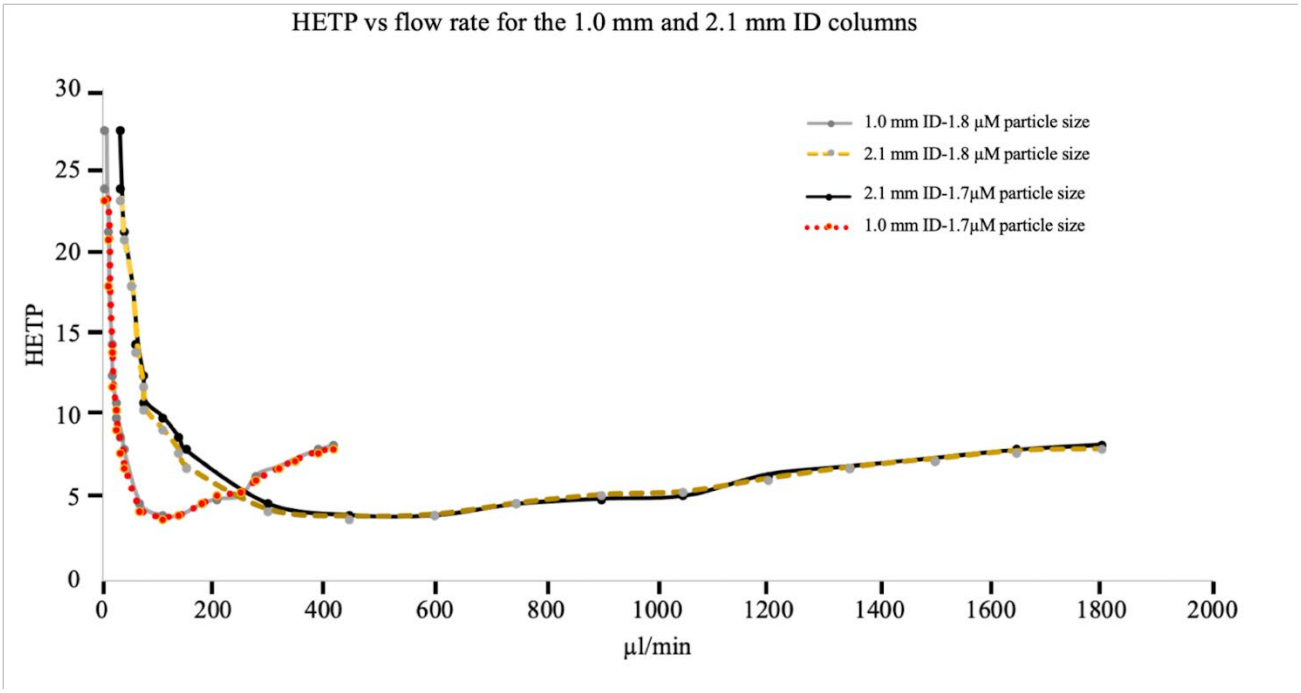


Figure S2. Height equivalent to a theoretical plate versus flow rate plots for different sized ultra-high-performance liquid chromatography columns. The plots correspond to 1 mm and 2.1 mm internal diameter ultra-high-performance liquid chromatography columns with 1.7 or 1.8 µm particle sizes. The particle sizes correspond to the charged surface hybrid and high strength silica columns, respectively. These plots were generated from available literature data [1-4].

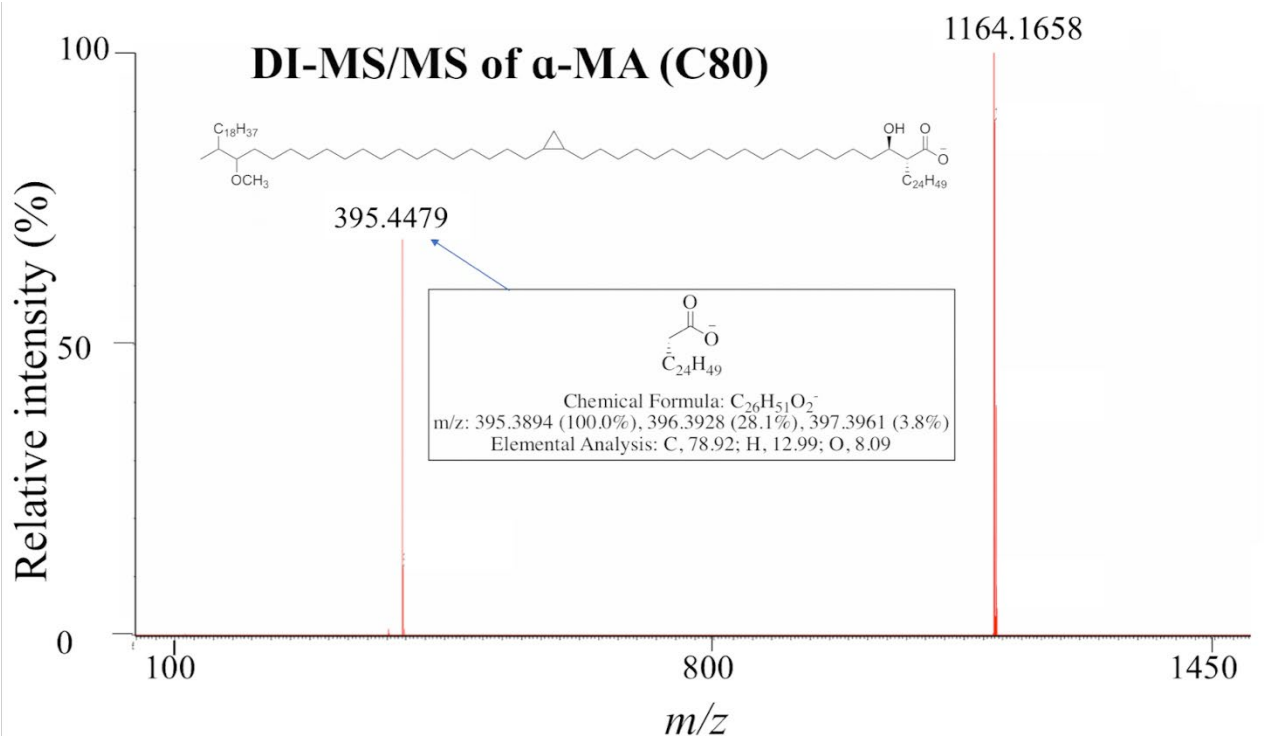


Figure S3. Direct-injection mass spectrometry-mass spectrometry spectrum of α-mycolic acid. The spectrum highlights the daughter ion at *m/z*:395, which provides information regarding the R_2 side chain length. The daughter ion is labeled with a chemical structure and mass spectrometry parameters predicted from ChemDraw v19.1 (PerkinElmer, Waltham, MA), which includes the theoretical isotopic distribution. The full structure of α-mycolic acid is shown as an insert. Abbreviations: DI-MS/MS: direct-injection mass spectrometry-mass spectrometry; α-MA: α-mycolic acid; C80: chain-length of 80 carbons.

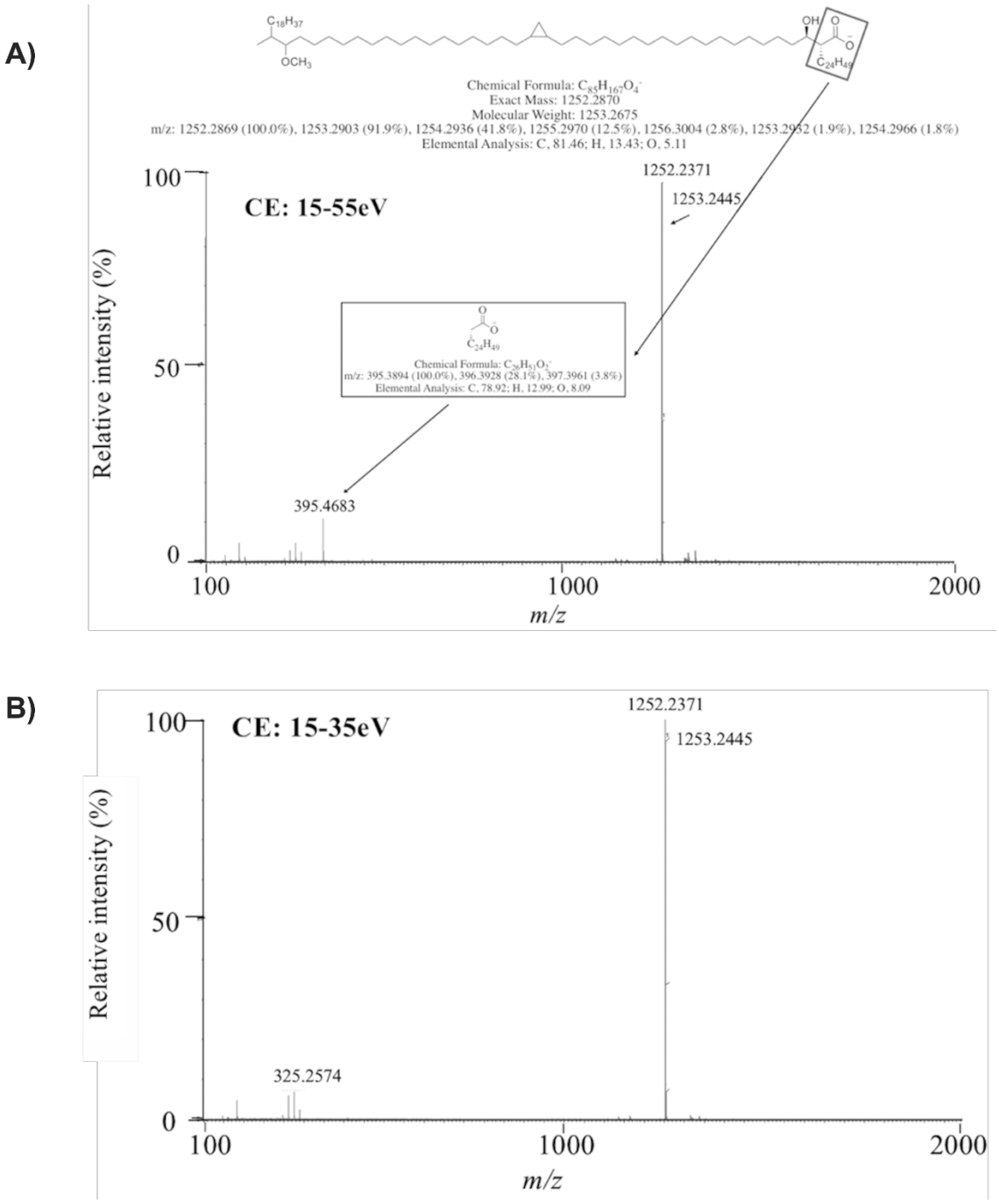


Figure S4. Mass spectrometry elevated collision energy spectrum of methoxy cis mycolic acid. The mass spectrometry elevated collision energy spectra were collected at a collision energy ramp of **(A)** 15 to 55eV, which highlighted the expected *m/z*:395 fragment that provides information regarding the R_2 side chain length and **(B)** 15 to 35eV, which lacks the daughter ion at *m/z*:395. The daughter ion is labeled with a chemical structure and mass spectrometry parameters predicted from ChemDraw v19.1 (PerkinElmer, Waltham, MA), which includes the theoretical isotopic distribution. The full structure of methoxy cis mycolic acid is shown as an insert. Abbreviations: CE: collision energy.

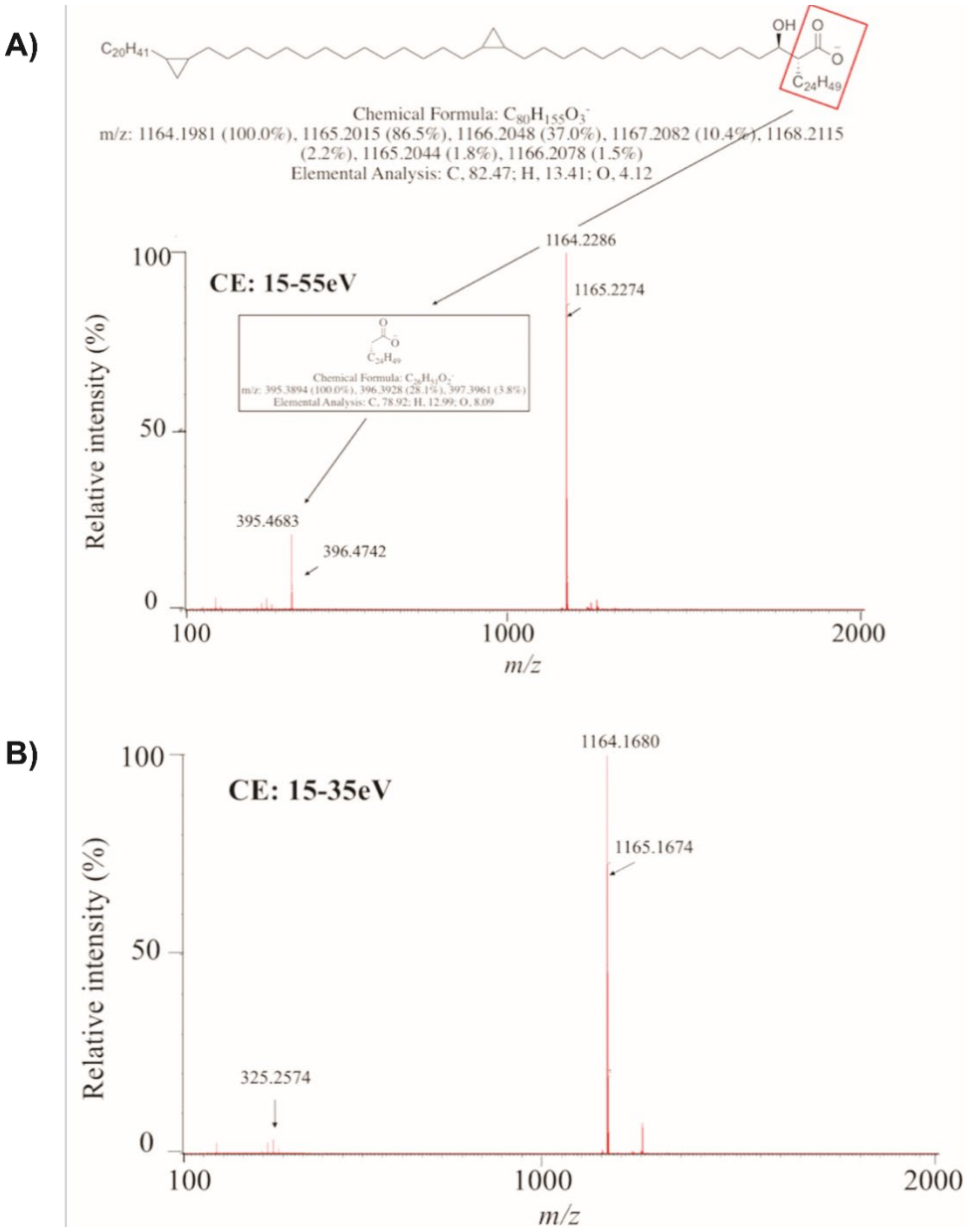


Figure S5. Mass spectrometry elevated collision energy spectrum of α-mycolic acid. The mass spectrometry elevated collision energy spectra were collected at a collision energy ramp of **(A)** 15 to 55eV, which highlighted the expected *m/z*:395 fragment that provides information regarding the R_2 side chain length and **(B)** 15 to 35eV, which lacks the daughter ion at *m/z*:395. The daughter ion is labeled with a chemical structure and mass spectrometry parameters predicted from ChemDraw v19.1 (PerkinElmer, Waltham, MA), which includes the theoretical isotopic distribution. The full structure and scaffold of α-mycolic acid is shown as an insert. Abbreviations: CE: collision energy.

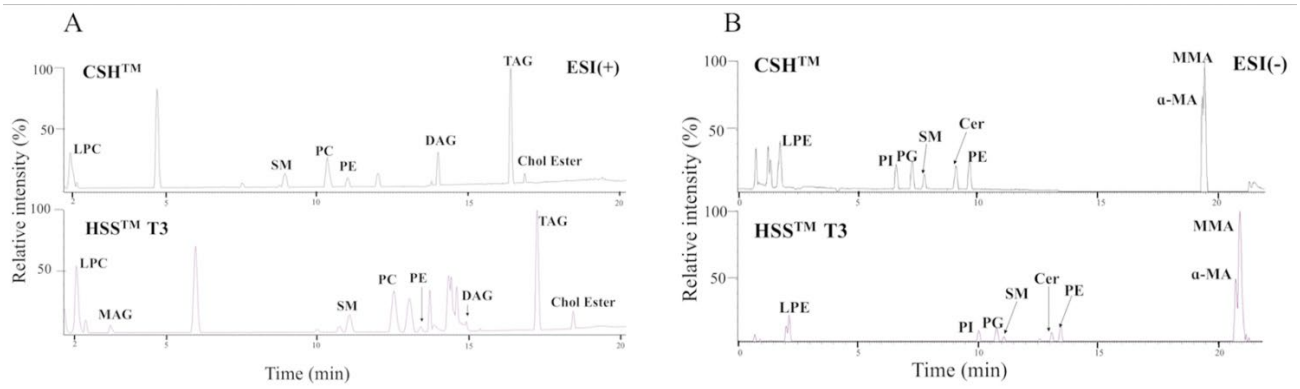


Figure S6. Ultra-high-performance liquid chromatography-quadrupole time of flight-mass spectrometry chromatogram of the mixture of the EquiSPLASH™ standard and mycolic acids. The chromatogram obtained in the **(A)** positive ionization mode. The analytes were separated in 22 minutes on a Acquity ultra-high-performance liquid chromatography system with a (*top*) charged surface hybrid column or (*bottom*) high strength silica column with acetonitrile/water (60/40, v/v), 10 mM of ammonium formate and 0.1% formic acid (Solvent A), and 2-propanol/acetonitrile (90/10, v/v) with 10 mM of ammonium formate and 0.1% formic acid (Solvent B). The chromatogram obtained in the **(B)** negative ionization mode. The analytes were separated in 14 minutes on an Acquity ultra-high-performance liquid chromatography system with a (*top*) charged surface hybrid column or (*bottom*) high strength silica column with acetonitrile/water (60/40, v/v), 10 mM of ammonium formate and 0.1% formic acid (Solvent A), and 2-propanol/acetonitrile (90/10, v/v) with 10 mM of ammonium formate and 0.1% formic acid (Solvent B).

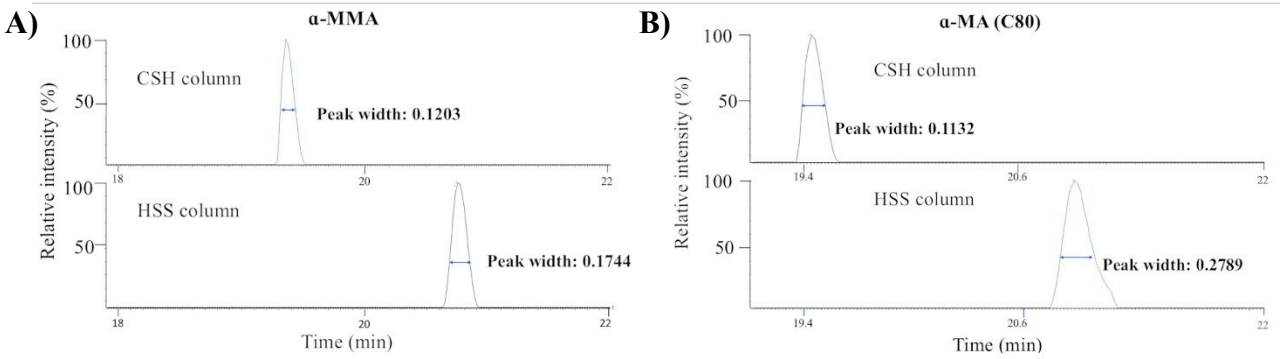


Figure S7. Extracted ion chromatogram of **A)** methoxy cis mycolic acid and **B)** α-mycolic acid. The extracted ion chromatograms highlight the peak widths on the (*top*) charged surface hybrid column or (*bottom*) high strength silica column with a 22-minute gradient elution using mobile phase A: acetonitrile/water (60/40, v/v), 10 mM of ammonium formate and 0.1% formic acid, and mobile phase B: 2-propanol/acetonitrile (90/10, v/v), with 10 mM of ammonium formate and 0.1% formic acid. Abbreviations: HSS, high strength silica; CSH, charged surface hybrid; α-MMA, methoxy cis mycolic acid; α-MA, α-mycolic acid; C80: chain-length of 80 carbons.

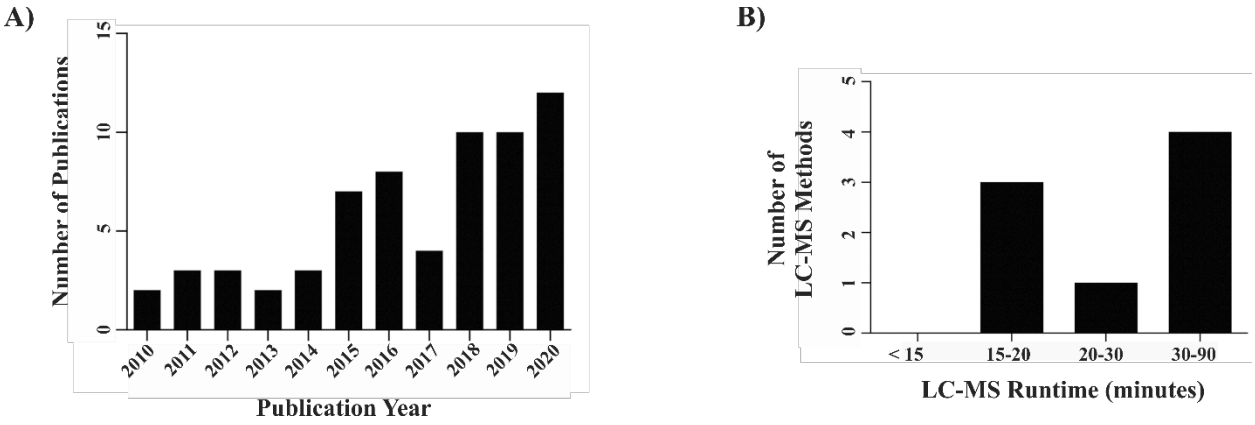


Figure S8. Bar plots of **(A)** the number of PubMed papers published per year containing the keywords: mycolic acid, liquid chromatography, and mass spectrometry, and **(B)** the runtimes of the published liquid chromatography-mass spectrometry methods for mycobacterial lipidomics studies. Abbreviations: LC-MS: liquid-chromatography-mass spectrometry

Table S1. Summary of Liquid Chromatography-Mass Spectrometry Data for Standard Lipids

Analyte[a]	Accurate Mass[b]	Expected *m/z*[c]	Observed *m/z*[d]			R.T[e]	Fragments (m/z) (15-55eV)[f]
			[M+H]+	[M-H]-	Other adduct with m/z		
15:0-18:1(d7) PC	752.6061	[M+H]+ 753.6134	753.6500	NA	[M+HCOO]-797.6603	7.03	184.0829
18:1(d7) Lyso PC	528.3921	[M+H]+ 529.3994	529.4276	NA	[M+HCOO]-573.4567	1.60	184.0829
15:0-18:1(d7) PE	710.5998	[M+H]+ 711.5634	711.5839	709.5873	NA	7.41	288.368; 241.2884
18:1(d7) Lyso PE	486.3451	[M+H]+ 487.3524	487.3642	485.4087	NA	1.64	288.368
15:0-18:1(d7)PG	741.5537	[M-H]- 740.5464	NA	740.5747	NA	6.02	288.368; 325.2563; 377.2825; 311.2412
15:0-18:1(d7) PI	829.5698	[M-H]- 828.5798	NA	828.5798	NA	5.63	288.368; 241.2884; 539.3309; 377.2825
15:0-18:1(d7) PS	754.5490	[M+H]+ 755.5562	755.5645	NA	NA	7.43	570.5732; 711.5966
15:0-18:1(d7)-15:0 TAG	811.7646	$[M+NH4]^+$ 829.7985	NA	NA	$[M+NH_4]$+ 829.8103	9.56	570.5473; 523.498; 355.0883; 281.0632
15:0-18:1(d7) DAG	587.5506	$[M+NH4]^+$ 605.5884	NA	NA	$[M+NH_4]$+ 605.5966	8.39	570.5732; 495.2889; 346.3519; 311.3161
18:1(d7) MAG	363.3366	$[M+H]^+$ 364.3429	364.3488	NA	[M+Na]+ 386.3327	2.16	328.2567
18:1(d7) Chol Ester	657.6441	[M+NH4]+ 675.6779	NA	NA	[M+Na]+ 680.6644	9.78	579.5624; 369.3717; 551.5365
d18:1-18:1(d9) SM	737.6397	[M+H]+ 738.6470	738.6642	NA	[M+Na]+ 760.6395 & [M+HCOO]-782.6973	6.22	577.5937; 701.5889
C15 Ceramide-d7	530.5404	[M+H]+ 531.5477	531.5612	NA	[M+HCOO]- 575.6102& [M+Na]+ 553.5405	7.15	271.3281; 289.3423; 513.5599
α-mycolic acid (C80)	1165.205	$[M-H]^-$ 1164.093	NA	1164.1680	[M+Na]+ 1188.1850	10.9	395.4683
α-mycolic acid, methoxy cis	1253.2904	$[M-H]^-$ 1252.241	NA	1252.2371	[M+Na]+ 1276.2723	10.8	395.4683

[a]Lipid analytes in the mixture of Equisplash and two mycolic acids.
[b]Accurate mass of the lipids in the mixture
[c]Expected *m/z* values of the lipid in the mixture.
[d]Observed *m/z* with the indicated adduct.
[e]Retention time on a charged surface hybrid column with a 14-minute elution gradient
[f]Fragment ions observed in 15 to 55 eV

Table S2. Peak Widths and Retention Times for Lipids from the Standard Mixture[a]

Lipid Name	Accurate Mass	HS22-LFR		CS22-LFR	
		Rt (min) (Mean±SD)	Peak Width (min) (Mean±SD)	Rt (min) (Mean±SD)	Peak Width (min) (Mean±SD)
15:0-18:1(d7) PC	752.6061	12.5235±0.008	0.5026±0.001	10.3275±0.008	0.51415±0.034
18:1(d7) Lyso PC	528.3921	2.024±0.009	0.4457±0.026	1.878±0.000	0.3884±0.0118
15:0-18:1(d7) PE	710.5998	13.45±0.010	0.3234±0.011	10.02±0.35	0.2866±0.001
18:1(d7) Lyso PE	486.3451	2.1375±0.003	0.2817±0.001	1.809±0.051	0.2651±0.009
15:0-18:1(d7)PG	741.5537	10.765±0.015	0.36265±0.014	7.535±0.275	0.31605±0.026
15:0-18:1(d7) PI	829.5698	10.035±0.005	0.3531±0.011	6.79±0.18	0.253±0.011
15:0-18:1(d7) PS	754.549	10.453±0.039	0.5764±0.007	N/O	N/O
15:0-18:1(d7)-15:0 TAG	811.7646	17.25±0.000	0.22205±0.001	16.3835±0.009	0.2153±0.005
15:0-18:1(d7) DAG	587.5506	14.591±0.000	0.246±0.002	13.9905±0.000	0.2097±0.000
18:1(d7) MAG	363.3366	3.1735±0.009	0.28085±0	2.6585±0.009	0.29385±0.000
18:1(d7) Chol Ester	657.6441	18.455±0	0.2065±0.002	16.84±0.000	0.1619±0.000
d18:1-18:1(d9) SM	737.6397	11.0485±0.009	0.4368±0.004	8.895±0.000	0.3817±0.009
C15 Ceramide-d7	530.5404	13.0385±0.009	0.3094±0.010	9.102±0.009	0.2641±0.003
α– mycolic acid (C80)	1165.205	20.755±0.165	0.26225±0.087	19.455±0.005	0.1807±0.002
α–mycolic acid, methoxy cis	1253.2904	20.63±0.120	0.1964±0.038	19.37±0.001	0.1922±0.002

[a]Lipids that were observed and reported in the negative ionization mode are in bold font; N/O: not observed

Table S3. Summary of Column Resolution

	Column Type and Runtime		
	CSH-14 minutes	**CS-22 minutes**	**HS-22 minutes**
MA Resolution	0.99 ± 0.06	0.8 ± 0.2	0.97 ± 0.01

Table S4. Summary of Spectral Features for the Four Liquid Chromatography-Mass Spectrometry Methods

	Method			
	CS-14 LFR	**HS-30 LFR**	**HS-22 HFR**	**HS-25 LFR**
Number of features	5436	8066	4682	3730
Average of the raw intensities	5.66E+04	1.79E+04	6.63E+03	8.44E+03
Median raw intensity	2.85E+03	2.69E+03	6.43E+02	8.13E+02
Standard deviation	2.66E+05	8.59E+04	5.90E+04	6.56E+04

Table S5. Summary of the Statistical Analysis of the Four Liquid Chromatography-Mass Spectrometry Methods

	Method			
	CS-14 LFR	**HS-30 LFR**	**HS-22 HFR**	**HS-25 LFR**
Number of Identified lipids	308	334	229	133
Average of the raw intensities	1.50E+05	3.5E+04	3.7E+04	5.6E+04
Median raw intensity	2.7E+03	4.9E+03	1.3E+03	3.4E+03
Standard deviation	7.5E+05	1.7E+05	2.4E+05	3.2E+05

Table S6. Retention Times Obtained for Lipids from the Standard Mixture for Each Liquid Chromatography-Mass Spectrometry Method[a]

Lipid Name	**Methods compared**			
	CS14-LFR	**HS25-LFR**	**HS22-HFR**	**HS30-LFR**
15:0-18:1(d7) PC	7.03	18.2	N/O	8.5
18:1(d7) Lyso PC	1.6	12.2	12.2	2.3
15:0-18:1(d7) PE	7.41	N/O	15.5	8.9
18:1(d7) Lyso PE	1.64	11.5	12.1	2.4
15:0-18:1(d7)PG	6.02	N/O	N/O	7.2
15:0-18:1(d7) PI	5.63	15.8	N/O	7.0
15:0-18:1(d7) PS	7.43	N/O	N/O	7.8
15:0-18:1(d7)-15:0 TAG	9.56	N/O	N/O	18.3
15:0-18:1(d7) DAG	8.39	N/O	N/O	11.5
18:1(d7) MAG	2.16	N/O	N/O	6.1
18:1(d7) Chol Ester	9.78	N/O	N/O	19.1
d18:1-18:1(d9) SM	6.22	N/O	N/O	7.5
C15 Ceramide-d7	7.15	N/O	N/O	8.0
α– mycolic acid (C80)	10.9	N/O	N/O	23.7
α–mycolic acid, methoxy cis	10.8	N/O	N/O	23.9

[a]Lipids that were observed and reported in the negative ionization mode are in bold font; N/O: not observed

Table S7. Lipid Retention Times Identified by Each of the Four Liquid Chromatography-Mass Spectrometry Methods[a]

LipidID	HS22-HFR RT (min)	CS14-LFR RT (min)	HS30-LFR RT (min)	HS25-LFR RT (min)
Ac1PIM1(46:1)	14.26	N/O	15.87	N/O
Ac1PIM1(46:2)	16.77	N/O	N/O	N/O
Ac1PIM1(47:1)	18.72	N/O	5.20	N/O
Ac1PIM1(47:2)	17.49	N/O	N/O	N/O
Ac1PIM1(48:1)	N/O	N/O	16.56	N/O
Ac1PIM1(48:2)	17.86	N/O	N/O	20.20
Ac1PIM1(48:3)	16.79	10.91	N/O	N/O
Ac1PIM1(48:3)	N/O	N/O	N/O	N/O
Ac1PIM1(48:4)	N/O	9.43	N/O	N/O
Ac1PIM1(49:2)	N/O	7.72	N/O	N/O
Ac1PIM1(49:2)	N/O	N/O	8.20	N/O
Ac1PIM1(49:4)	17.21	9.53	N/O	N/O
Ac1PIM1(50:2)	N/O	N/O	8.42	N/O
Ac1PIM1(50:3)	17.86	7.59	N/O	N/O
Ac1PIM1(50:5)	18.09	N/O	N/O	N/O
Ac1PIM1(51:2)	N/O	8.09	N/O	N/O
Ac1PIM1(51:3)	18.65	N/O	18.67	21.47
Ac1PIM1(51:4)	18.52	N/O	N/O	N/O
Ac1PIM1(51:5)	N/O	9.56	N/O	N/O
Ac1PIM1(52:2)	16.33	6.98	10.52	N/O
Ac1PIM1(52:3)	19.84	N/O	N/O	N/O
Ac1PIM1(52:5)	18.62	6.10	N/O	N/O
Ac1PIM1(53:2)	N/O	6.98	N/O	N/O
Ac1PIM1(53:3)	19.84	N/O	N/O	N/O
Ac1PIM1(53:4)	N/O	N/O	18.09	N/O
Ac1PIM1(53:5)	17.09	6.69	18.00	18.69

Ac1PIM1(54:3)	16.99	8.29	N/O	N/O
Ac1PIM1(55:1)	N/O	10.43	7.19	N/O
Ac1PIM1(55:2)	N/O	N/O	4.42	N/O
Ac1PIM1(55:4)	17.84	N/O	N/O	20.23
Ac1PIM1(55:5)	15.68	N/O	8.14	N/O
Ac1PIM1(56:1)	N/O	N/O	7.40	N/O
Ac1PIM1(56:3)	20.00	N/O	N/O	N/O
Ac1PIM1(56:4)	19.40	N/O	N/O	20.20
Ac1PIM1(57:1)	N/O	12.55	8.20	20.89
Ac1PIM1(57:2)	N/O	N/O	7.26	N/O
Ac1PIM1(57:3)	N/O	N/O	6.81	N/O
Ac1PIM1(57:4)	19.35	N/O	N/O	N/O
Ac1PIM1(C44)	N/O	N/O	16.00	N/O
Ac1PIM1(C45)	14.72	N/O	N/O	N/O
Ac1PIM1(C46)	14.77	N/O	6.13	N/O
Ac1PIM1(C47)	18.91	N/O	6.59	N/O
Ac1PIM1(C48)	N/O	N/O	17.14	22.32
Ac1PIM1(C49)	N/O	10.52	N/O	N/O
Ac1PIM1(C51)	N/O	10.63	N/O	N/O
Ac1PIM1(C52)	N/O	10.63	N/O	N/O
Ac1PIM1(C53)	17.49	10.21	8.66	N/O
Ac1PIM1(C55)	N/O	N/O	19.37	N/O
Ac1PIM1(C56)	N/O	N/O	8.77	N/O
Ac1PIM2(46:1)	18.11	N/O	N/O	N/O
Ac1PIM2(46:2)	N/O	6.69	N/O	N/O
Ac1PIM2(48:1)	N/O	N/O	N/O	19.94
Ac1PIM2(48:2)	N/O	7.67	N/O	N/O
Ac1PIM2(48:4)	18.16	N/O	N/O	N/O
Ac1PIM2(49:1)	N/O	N/O	8.90	21.62
Ac1PIM2(49:2)	19.60	N/O	N/O	N/O

Ac1PIM2(49:4)	N/O	7.62	18.95	N/O
Ac1PIM2(50:1)	13.29	N/O	8.85	N/O
Ac1PIM2(50:4)	N/O	10.19	N/O	N/O
Ac1PIM2(51:3)	N/O	8.02	N/O	N/O
Ac1PIM2(51:4)	N/O	N/O	19.13	N/O
Ac1PIM2(51:5)	N/O	7.67	N/O	N/O
Ac1PIM2(52:3)	N/O	8.09	N/O	N/O
Ac1PIM2(52:4)	N/O	12.15	N/O	N/O
Ac1PIM2(53:1)	N/O	N/O	15.60	N/O
Ac1PIM2(53:2)	N/O	8.33	20.16	N/O
Ac1PIM2(53:3)	N/O	N/O	21.97	N/O
Ac1PIM2(53:4)	N/O	8.03	N/O	N/O
Ac1PIM2(54:1)	N/O	N/O	20.31	N/O
Ac1PIM2(54:2)	N/O	8.38	19.00	N/O
Ac1PIM2(54:3)	N/O	10.02	N/O	N/O
Ac1PIM2(54:4)	10.49	12.42	N/O	N/O
Ac1PIM2(54:5)	N/O	7.62	N/O	N/O
Ac1PIM2(55:1)	N/O	N/O	5.69	N/O
Ac1PIM2(55:2)	N/O	8.43	19.13	N/O
Ac1PIM2(55:3)	N/O	8.35	N/O	N/O
Ac1PIM2(55:4)	16.28	12.58	N/O	N/O
Ac1PIM2(55:5)	N/O	8.07	N/O	N/O
Ac1PIM2(56:1)	16.24	N/O	16.50	N/O
Ac1PIM2(56:2)	14.65	N/O	N/O	N/O
Ac1PIM2(56:3)	N/O	8.40	N/O	N/O
Ac1PIM2(57:1)	N/O	7.62	3.35	N/O
Ac1PIM2(57:2)	N/O	N/O	7.97	N/O
Ac1PIM2(57:3)	N/O	8.45	2.83	N/O
Ac1PIM2(57:4)	N/O	12.95	N/O	N/O
Ac1PIM2(C44)	10.53	N/O	N/O	N/O

Ac1PIM2(C46)	11.64	N/O	N/O	N/O
Ac1PIM2(C48)	12.89	N/O	8.85	22.27
Ac1PIM2(C49)	N/O	12.18	N/O	N/O
Ac1PIM2(C50)	14.17	N/O	N/O	N/O
Ac1PIM2(C51)	16.23	N/O	7.44	N/O
Ac1PIM2(C52)	N/O	12.83	N/O	N/O
Ac1PIM2(C53)	N/O	5.69	8.42	N/O
Ac1PIM2(C55)	N/O	9.43	N/O	N/O
Ac1PIM2(C56)	N/O	N/O	16.88	N/O
Ac1PIM3(46:1)	N/O	7.87	N/O	19.99
Ac1PIM3(46:2)	N/O	N/O	8.47	N/O
Ac1PIM3(47:1)	16.98	7.94	22.00	N/O
Ac1PIM3(47:2)	N/O	8.18	N/O	N/O
Ac1PIM3(48:2)	N/O	12.56	N/O	N/O
Ac1PIM3(49:2)	N/O	8.37	N/O	N/O
Ac1PIM3(49:3)	6.86	N/O	N/O	N/O
Ac1PIM3(50:2)	N/O	12.95	N/O	N/O
Ac1PIM3(50:3)	N/O	8.43	20.41	N/O
Ac1PIM3(50:5)	N/O	N/O	16.38	N/O
Ac1PIM3(51:1)	N/O	10.99	19.18	N/O
Ac1PIM3(51:3)	14.94	10.59	N/O	N/O
Ac1PIM3(52:5)	N/O	8.43	N/O	N/O
Ac1PIM3(53:3)	N/O	N/O	20.21	N/O
Ac1PIM3(54:1)	N/O	3.52	N/O	N/O
Ac1PIM3(54:3)	8.97	N/O	N/O	N/O
Ac1PIM3(54:5)	N/O	N/O	20.94	N/O
Ac1PIM3(55:1)	N/O	N/O	20.81	N/O
Ac1PIM3(55:5)	16.89	N/O	N/O	N/O
Ac1PIM3(56:1)	N/O	10.59	N/O	N/O
Ac1PIM3(57:1)	N/O	10.69	N/O	N/O

Ac1PIM3(C44)	N/O	N/O	9.58	N/O
Ac1PIM3(C46)	16.24	N/O	18.75	N/O
Ac1PIM3(C48)	N/O	N/O	18.98	N/O
Ac1PIM3(C49)	N/O	N/O	19.20	N/O
Ac1PIM3(C50)	N/O	N/O	19.23	N/O
Ac1PIM3(C51)	N/O	N/O	19.31	N/O
Ac1PIM3(C55)	15.14	N/O	N/O	N/O
Ac1PIM4(46:2)	N/O	7.79	20.20	N/O
Ac1PIM4(48:3)	N/O	7.62	N/O	N/O
Ac1PIM4(48:4)	N/O	7.54	N/O	N/O
Ac1PIM4(50:2)	6.42	N/O	N/O	N/O
Ac1PIM4(50:3)	N/O	8.12	N/O	N/O
Ac1PIM4(50:5)	N/O	N/O	9.18	N/O
Ac1PIM4(51:2)	N/O	N/O	9.45	N/O
Ac1PIM4(51:3)	N/O	8.71	N/O	N/O
Ac1PIM4(51:4)	6.88	N/O	N/O	N/O
Ac1PIM4(52:2)	N/O	N/O	19.63	N/O
Ac1PIM4(53:1)	6.47	N/O	N/O	N/O
Ac1PIM4(53:3)	N/O	8.90	N/O	N/O
Ac1PIM4(53:4)	N/O	8.75	N/O	N/O
Ac1PIM4(54:1)	N/O	8.40	N/O	N/O
Ac1PIM4(54:5)	15.40	N/O	N/O	N/O
Ac1PIM4(55:4)	N/O	8.92	N/O	N/O
Ac1PIM4(55:5)	N/O	8.78	N/O	N/O
Ac1PIM4(56:3)	N/O	7.92	N/O	N/O
Ac1PIM4(57:4)	16.11	8.42	N/O	N/O
Ac1PIM4(C44)	N/O	N/O	19.92	N/O
Ac1PIM4(C46)	N/O	N/O	19.48	N/O
Ac1PIM4(C50)	N/O	11.62	N/O	N/O
Ac1PIM4(C51)	N/O	11.88	18.07	N/O

Ac1PIM4(C52)	N/O	11.90	N/O	N/O
Ac1PIM4(C55)	7.04	N/O	N/O	N/O
Ac1PIM5(50:4)	N/O	8.22	N/O	N/O
Ac1PIM5(51:5)	16.81	N/O	N/O	N/O
Ac1PIM5(52:3)	N/O	8.58	N/O	N/O
Ac1PIM5(52:4)	N/O	8.37	21.01	N/O
Ac1PIM5(53:1)	N/O	N/O	21.79	N/O
Ac1PIM5(53:5)	17.77	N/O	N/O	N/O
Ac1PIM5(54:3)	N/O	8.05	N/O	N/O
Ac1PIM5(54:4)	N/O	8.58	N/O	N/O
Ac1PIM5(56:4)	N/O	8.75	N/O	N/O
Ac1PIM5(C44)	16.89	N/O	N/O	N/O
Ac1PIM5(C49)	N/O	8.71	N/O	N/O
Ac1PIM5(C51)	N/O	8.86	N/O	N/O
Ac1PIM6(C44)	N/O	8.40	N/O	N/O
Ac1PIM6(C46)	N/O	8.53	N/O	N/O
Ac2PIM2(60:1)	16.58	N/O	N/O	N/O
Ac2PIM2(61:1)	N/O	10.34	7.31	N/O
Ac2PIM2(62:1)	N/O	12.22	N/O	N/O
Ac2PIM2(62:2)	N/O	N/O	N/O	21.62
Ac2PIM2(62:3)	14.10	N/O	N/O	N/O
Ac2PIM2(63:2)	14.73	5.43	19.81	N/O
Ac2PIM2(64:1)	N/O	N/O	5.40	N/O
Ac2PIM2(64:2)	N/O	N/O	7.37	N/O
Ac2PIM2(64:4)	14.66	10.67	N/O	N/O
Ac2PIM2(64:5)	N/O	11.19	N/O	N/O
Ac2PIM2(65:2)	N/O	10.57	N/O	N/O
Ac2PIM2(65:3)	N/O	N/O	2.79	N/O
Ac2PIM2(66:3)	17.50	10.92	20.40	N/O
Ac2PIM2(66:4)	15.43	N/O	N/O	N/O

Ac2PIM2(66:5)	N/O	N/O	N/O	16.23
Ac2PIM2(67:1)	N/O	N/O	8.42	N/O
Ac2PIM2(67:2)	N/O	12.98	N/O	N/O
Ac2PIM2(67:3)	N/O	11.00	20.49	N/O
Ac2PIM2(68:1)	N/O	11.74	N/O	N/O
Ac2PIM2(68:4)	16.14	N/O	N/O	N/O
Ac2PIM2(68:5)	N/O	N/O	N/O	16.98
Ac2PIM2(69:1)	N/O	11.75	9.94	N/O
Ac2PIM2(69:4)	N/O	6.43	7.07	N/O
Ac2PIM2(69:6)	N/O	N/O	9.53	N/O
Ac2PIM2(70:1)	N/O	12.02	N/O	N/O
Ac2PIM2(70:2)	N/O	N/O	8.77	N/O
Ac2PIM2(70:4)	16.84	N/O	N/O	N/O
Ac2PIM2(70:5)	16.45	N/O	6.41	N/O
Ac2PIM2(70:6)	11.02	4.62	N/O	N/O
Ac2PIM2(71:1)	N/O	12.03	8.63	N/O
Ac2PIM2(71:2)	N/O	N/O	8.14	N/O
Ac2PIM2(71:3)	N/O	N/O	2.86	N/O
Ac2PIM2(71:4)	N/O	7.46	7.37	16.93
Ac2PIM2(72:1)	N/O	12.03	8.12	N/O
Ac2PIM2(72:6)	N/O	N/O	6.34	N/O
Ac2PIM2(73:1)	N/O	7.89	N/O	N/O
Ac2PIM2(73:2)	N/O	7.75	N/O	N/O
Ac2PIM2(73:4)	N/O	12.12	8.09	17.95
Ac2PIM2(74:1)	N/O	N/O	8.18	N/O
Ac2PIM2(74:3)	N/O	N/O	8.07	N/O
Ac2PIM2(74:4)	N/O	12.23	N/O	N/O
Ac2PIM2(75:4)	N/O	N/O	8.85	N/O
Ac2PIM2(C60)	16.92	N/O	N/O	N/O
Ac2PIM2(C61)	N/O	N/O	7.70	17.04

Ac2PIM2(C63)	13.87	4.49	N/O	N/O
Ac2PIM2(C65)	N/O	8.05	20.66	N/O
Ac2PIM2(C66)	N/O	N/O	20.88	N/O
Ac2PIM2(C67)	N/O	N/O	9.12	N/O
Ac2PIM2(C68)	N/O	N/O	21.06	N/O
Ac2PIM2(C69)	N/O	N/O	7.29	N/O
Ac2PIM2(C70)	N/O	N/O	9.03	N/O
Ac2PIM2(C71)	N/O	N/O	8.09	N/O
Ac2PIM3(63:1)	11.02	N/O	N/O	N/O
Ac2PIM3(64:1)	16.12	N/O	N/O	N/O
Ac2PIM3(65:2)	N/O	5.71	N/O	N/O
Ac2PIM3(65:4)	16.91	N/O	N/O	N/O
Ac2PIM3(65:5)	16.79	N/O	N/O	N/O
Ac2PIM3(66:1)	16.84	N/O	N/O	N/O
Ac2PIM3(67:2)	N/O	N/O	3.77	N/O
Ac2PIM3(67:5)	17.23	N/O	N/O	N/O
Ac2PIM3(67:6)	17.11	N/O	N/O	N/O
Ac2PIM3(68:2)	17.11	N/O	N/O	N/O
Ac2PIM3(68:3)	16.86	N/O	N/O	17.89
Ac2PIM3(68:4)	16.77	N/O	N/O	N/O
Ac2PIM3(68:6)	N/O	N/O	19.46	N/O
Ac2PIM3(69:2)	N/O	4.07	4.60	N/O
Ac2PIM3(69:6)	18.11	N/O	N/O	N/O
Ac2PIM3(70:3)	N/O	N/O	5.43	N/O
Ac2PIM3(71:1)	19.81	N/O	N/O	N/O
Ac2PIM3(71:2)	N/O	11.42	6.36	N/O
Ac2PIM3(71:3)	16.96	N/O	N/O	N/O
Ac2PIM3(71:6)	19.30	N/O	N/O	N/O
Ac2PIM3(72:5)	N/O	5.55	N/O	N/O
Ac2PIM3(73:2)	N/O	11.62	N/O	N/O

Ac2PIM3(73:3)	N/O	5.48	5.35	N/O
Ac2PIM3(73:4)	N/O	10.43	N/O	N/O
Ac2PIM3(74:3)	N/O	10.43	N/O	N/O
Ac2PIM3(74:4)	N/O	N/O	5.36	N/O
Ac2PIM3(74:5)	N/O	6.76	N/O	N/O
Ac2PIM3(75:1)	N/O	N/O	6.39	22.24
Ac2PIM3(75:3)	N/O	N/O	6.72	N/O
Ac2PIM3(75:5)	N/O	N/O	23.88	N/O
Ac2PIM3(C60)	N/O	N/O	7.07	N/O
Ac2PIM3(C69)	N/O	N/O	4.58	N/O
Ac2PIM3(C72)	19.83	N/O	8.40	N/O
Ac2PIM3(C73)	N/O	N/O	7.74	N/O
Ac2PIM3(C74)	16.99	N/O	23.79	N/O
Ac2PIM4(67:3)	N/O	N/O	23.73	N/O
Ac2PIM4(67:4)	19.11	N/O	N/O	N/O
Ac2PIM4(68:3)	N/O	N/O	23.90	N/O
Ac2SGL(C53)	N/O	9.01	N/O	N/O
Ac2SGL(C56)	11.02	N/O	N/O	N/O
Ac2SGL(C58)	N/O	N/O	N/O	17.91
Ac2SGL(C60)	17.72	5.65	19.78	19.25
Ac2SGL(C62)	19.08	7.11	N/O	21.27
Ac2SGL(C65)	N/O	10.63	N/O	N/O
Ac2SGL(C68)	N/O	N/O	19.86	N/O
Ac2SGL(C70)	N/O	N/O	20.08	N/O
Ac2SGL(C71)	N/O	12.56	19.40	N/O
Ac2SGL(C72)	N/O	7.42	N/O	N/O
Ac2SGL(C73)	N/O	7.59	N/O	20.03
Ac2SGL(C74)	N/O	7.87	N/O	N/O
Ac2SGL(C75)	N/O	7.94	N/O	N/O
Alpha-MA(C79H158NO3)	N/O	12.98	N/O	N/O

Alpha-MA(C85H167O3)	N/O	7.87	N/O	N/O
Alpha-MA(C87H171O3)	N/O	7.19	5.96	N/O
Alpha-MA(C86H172NO3)	N/O	7.77	N/O	21.67
Alpha-MA(C93H183O3)	N/O	8.35	N/O	N/O
Alpha-MA(C94H188NO3)	N/O	8.02	N/O	N/O
Alpha-MA(C85H170NO3)	19.32	N/O	N/O	N/O
Alpha-MA(C83H161O3)	N/O	N/O	N/O	15.17
Alpha-MA(C84H165O3)	N/O	N/O	N/O	22.32
Alpha-MA(C94H183O3)	N/O	N/O	N/O	6.86
Alpha-MA(C75H145O3)	N/O	N/O	20.88	N/O
Alpha-MA(C74H144O3Na)	N/O	N/O	10.36	N/O
Alpha-MA(C76H147O3)	N/O	N/O	21.11	N/O
Alpha-MA(C77H149O3)	N/O	N/O	21.23	N/O
Alpha-MA(C79H153O3)	N/O	N/O	21.57	N/O
Alpha-MA(C88H172O3Na)	N/O	N/O	7.07	N/O
CL(58:2)	N/O	N/O	8.88	N/O
CL(59:2)	17.49	N/O	N/O	N/O
CL(59:3)	N/O	N/O	8.14	16.46
CL(60:2)	18.09	N/O	N/O	N/O
CL(61:1)	N/O	10.21	N/O	N/O
CL(61:3)	16.28	N/O	N/O	21.58
CL(62:2)	19.84	N/O	N/O	N/O
CL(62:3)	19.84	N/O	N/O	N/O
CL(62:4)	18.08	N/O	N/O	N/O
CL(63:2)	N/O	12.55	N/O	N/O
CL(63:3)	N/O	N/O	9.56	N/O
CL(63:4)	16.79	N/O	N/O	N/O
CL(64:1)	N/O	N/O	7.42	N/O
CL(64:2)	N/O	9.25	8.38	22.00
CL(64:3)	N/O	12.45	7.55	N/O

CL(65:2)	N/O	12.98	9.10	N/O
CL(65:3)	18.06	12.55	8.27	N/O
CL(66:1)	15.05	N/O	7.27	N/O
CL(66:2)	N/O	N/O	9.49	N/O
CL(66:4)	N/O	8.12	N/O	N/O
CL(67:3)	N/O	7.52	9.21	22.24
CL(68:3)	13.99	N/O	9.41	N/O
CL(69:2)	15.17	14.18	N/O	N/O
CL(69:3)	N/O	9.41	N/O	N/O
CL(69:4)	N/O	7.55	N/O	N/O
CL(70:1)	N/O	8.05	N/O	N/O
CL(70:3)	N/O	10.63	7.47	N/O
CL(71:1)	N/O	11.39	8.42	N/O
CL(71:4)	N/O	7.52	N/O	N/O
CL(72:1)	N/O	11.52	N/O	N/O
CL(72:3)	10.99	N/O	N/O	N/O
CL(72:4)	N/O	9.26	N/O	N/O
CL(73:1)	11.05	N/O	21.56	N/O
CL(73:3)	N/O	10.77	N/O	N/O
CL(73:4)	N/O	8.12	N/O	N/O
CL(75:3)	11.00	11.35	8.42	N/O
CL(76:3)	N/O	N/O	16.73	N/O
CL(78:3)	11.02	N/O	10.11	N/O
CL(80:2)	N/O	8.02	N/O	N/O
CL(82:1)	N/O	11.29	N/O	N/O
CL(90:2)	N/O	9.25	N/O	N/O
CL(C60)	N/O	10.44	N/O	N/O
CL(C61)	N/O	10.29	N/O	N/O
CL(C64)	N/O	7.37	N/O	N/O
CL(C67)	15.12	N/O	N/O	N/O

CL(C68)	N/O	N/O	21.29	N/O
CL(C69)	N/O	N/O	8.40	N/O
CL(C74)	N/O	8.35	16.73	N/O
CL(C76)	N/O	N/O	12.88	N/O
CL(C82)	N/O	11.37	N/O	N/O
CL(C84)	N/O	N/O	8.40	N/O
CL(C88)	N/O	9.26	N/O	N/O
DAT1(C52)	N/O	7.92	N/O	N/O
DAT1(C54)	14.63	N/O	N/O	N/O
DAT1(C56)	N/O	N/O	18.63	N/O
DAT2(C57)	N/O	9.45	N/O	N/O
DG(31:2)	N/O	N/O	N/O	19.42
DG(32:2)	14.94	N/O	N/O	N/O
DG(33:1)	16.42	4.92	5.68	17.34
DG(35:1)	20.00	N/O	N/O	N/O
DG(36:2)	19.95	N/O	N/O	19.33
DG(37:1)	15.03	N/O	N/O	N/O
DG(37:2)	17.72	N/O	N/O	19.28
DG(38:2)	14.96	N/O	8.00	N/O
DG(39:1)	15.36	N/O	N/O	N/O
DG(C34)	20.00	N/O	N/O	N/O
DG(C35)	16.06	N/O	N/O	N/O
DG(C40)	17.69	N/O	8.80	19.78
DG(C46)	N/O	4.92	N/O	N/O
DG(C47)	N/O	6.69	N/O	N/O
DG(C48)	N/O	7.31	N/O	N/O
DIMA(C105)	N/O	N/O	15.87	N/O
DIMA(C81)	N/O	N/O	8.23	N/O
DIMA(C82)	N/O	N/O	8.90	N/O
DIMA(C85)	N/O	N/O	N/O	20.69

DIMA(C86)	19.47	N/O	N/O	19.32
DIMA(C88)	17.47	N/O	N/O	N/O
DIMA(C90)	17.65	N/O	N/O	N/O
DIMA(C91)	N/O	N/O	4.90	N/O
DIMA(C92)	N/O	N/O	5.60	N/O
DIMA(C93)	N/O	7.42	6.24	N/O
DIMA(C94)	N/O	N/O	6.91	N/O
DIMA(C95)	N/O	7.79	N/O	N/O
DIMA(C96)	N/O	N/O	8.17	N/O
DIMB(C100)	N/O	8.29	N/O	N/O
DIMB(C101)	N/O	7.52	6.64	N/O
DIMB(C102)	N/O	8.40	8.80	20.20
DIMB(C103)	N/O	8.70	7.57	N/O
DIMB(C104)	19.86	8.83	8.20	22.24
DIMB(C105)	N/O	8.95	15.17	N/O
DIMB(C83)	N/O	N/O	8.35	20.68
DIMB(C85)	N/O	N/O	9.21	N/O
DIMB(C87)	18.11	N/O	N/O	N/O
DIMB(C88)	17.26	N/O	N/O	N/O
DIMB(C89)	19.30	N/O	N/O	N/O
DIMB(C90)	18.93	N/O	N/O	N/O
DIMB(C91)	18.93	N/O	N/O	N/O
DIMB(C92)	18.93	N/O	N/O	N/O
DIMB(C96)	N/O	N/O	15.67	N/O
DIMB(C98)	N/O	7.95	N/O	N/O
DIMB(C99)	N/O	8.05	8.70	N/O
DP-P(C)	14.91	N/O	N/O	N/O
DP-PP(C)	N/O	2.45	3.14	16.15
GMM(Alpha-MA)(C79)	N/O	N/O	15.75	N/O
GMM(Alpha-MA)(C81)	N/O	N/O	16.56	6.13

GMM(Alpha-MA)(C86)	N/O	N/O	17.76	N/O
GMM(Alpha-MA)(C87)	N/O	N/O	18.17	N/O
GMM(Alpha-MA)(C89)	N/O	N/O	18.49	N/O
GMM(keto-MA)(C91)	N/O	N/O	15.65	N/O
GMM(methoxy-MA)(C86)	N/O	N/O	N/O	6.48
GMM(methoxy-MA)(C92)	N/O	N/O	6.87	N/O
GPD(C106)	N/O	N/O	11.72	N/O
GPD(C111)	N/O	N/O	16.91	N/O
Hydroxyphthioceranic acid(C33)	N/O	N/O	N/O	19.75
Hydroxyphthioceranic acid(C36)	N/O	N/O	7.74	N/O
Keto-MA(C75)	N/O	9.41	N/O	N/O
Keto-MA(C77)	N/O	N/O	20.03	N/O
Keto-MA(C82)	N/O	N/O	N/O	15.15
Keto-MA(C83)	N/O	N/O	N/O	20.94
Keto-MA(C84)	18.57	7.72	N/O	N/O
Keto-MA(C85)	19.01	N/O	9.80	N/O
Keto-MA(C86)	19.35	N/O	N/O	21.04
Keto-MA(C87)	19.35	N/O	N/O	12.30
Keto-MA(C88)	18.58	7.89	N/O	N/O
Keto-MA(C90)	N/O	8.23	N/O	N/O
Keto-MA(C93)	N/O	N/O	N/O	6.54
LPE(16:1)	9.80	1.30	N/O	6.69
LPE(17:1)	14.63	N/O	N/O	N/O
LPE(18:1)	N/O	N/O	2.31	12.99
LPE(19:1)	11.53	1.96	2.65	12.66
LPE(C16)	14.40	1.55	1.98	11.46
LPE(C18)	11.87	2.19	2.10	6.63
LPE(C19)	11.31	2.38	9.68	13.19

LPE(C20)	11.94	2.10	2.81	13.97
LPG(16:1)	13.87	N/O	N/O	4.86
LPG(18:1)	N/O	N/O	N/O	7.31
LPG(19:1)	13.59	N/O	N/O	7.40
LPG(C16)	6.57	N/O	N/O	7.27
LPG(C17)	17.91	N/O	N/O	N/O
LPG(C18)	19.93	N/O	N/O	7.27
LPG(C19)	N/O	N/O	1.98	N/O
LPG(C20)	N/O	N/O	N/O	15.24
LPI(18:1)	11.48	1.27	1.63	10.49
LPI(18:2)	N/O	1.05	N/O	20.89
LPI(19:1)	N/O	N/O	N/O	5.84
LPI(19:2)	N/O	8.33	7.39	21.95
LPI(C18)	N/O	N/O	N/O	4.70
LPI(C19)	13.36	N/O	N/O	N/O
LPIM1(18:2)	N/O	3.49	N/O	N/O
LPIM1(19:2)	N/O	4.55	4.93	N/O
LPIM1(C19)	5.77	N/O	N/O	N/O
LPIM2(18:2)	N/O	N/O	9.68	N/O
LPIM2(19:1)	N/O	10.41	8.35	N/O
LPIM2(19:2)	N/O	10.32	N/O	N/O
LPIM2(C16)	14.94	N/O	N/O	6.54
LPIM2(C17)	15.01	10.16	16.91	N/O
LPIM2(C18)	15.77	N/O	N/O	N/O
LPIM2(C19)	5.33	10.28	17.43	N/O
LPIM3(18:1)	N/O	N/O	N/O	9.40
LPIM3(18:2)	N/O	N/O	14.08	N/O
LPIM3(19:1)	19.21	12.15	N/O	N/O
LPIM3(C16)	15.72	N/O	9.86	6.13
LPIM3(C17)	N/O	N/O	N/O	12.00

LPIM3(C18)	N/O	N/O	N/O	21.32
LPIM3(C19)	N/O	N/O	N/O	21.34
LPIM4(19:1)	N/O	N/O	N/O	9.51
LPIM5(19:2)	N/O	N/O	2.86	N/O
LPIM5(C18)	N/O	N/O	N/O	22.30
LPIM5(C19)	N/O	N/O	6.86	18.28
LPIM6(18:1)	19.84	9.13	N/O	N/O
LPIM6(18:2)	N/O	N/O	N/O	20.63
LPIM6(19:1)	N/O	9.18	N/O	N/O
LPIM6(C16)	N/O	8.47	N/O	N/O
LPIM6(C17)	N/O	8.60	N/O	N/O
LPIM6(C19)	N/O	8.90	6.36	N/O
Mbt -Fe(17:1)	15.50	7.04	7.29	N/O
Mbt -Fe(18:1)	N/O	N/O	10.22	N/O
Mbt -Fe(20:1)	N/O	7.85	N/O	N/O
Mbt -Fe(C17)	N/O	7.72	10.76	15.18
Mbt -Fe(C18)	N/O	8.78	8.22	N/O
Mbt -Fe(C19)	14.82	8.14	N/O	22.45
Mbt +Fe(17:1)	15.77	2.99	7.52	16.56
Mbt +Fe(18:1)	N/O	7.44	N/O	N/O
Mbt +Fe(19:1)	16.42	4.05	N/O	N/O
Mbt +Fe(20:1)	6.23	N/O	N/O	N/O
Mbt +Fe(C17)	N/O	4.16	8.63	N/O
Mbt +Fe(C18)	N/O	5.38	5.58	N/O
Mbt +Fe(C19)	N/O	N/O	8.30	N/O
Mbt +Fe(C20)	N/O	N/O	3.89	N/O
Methoxy-MA(C74)	N/O	N/O	8.09	N/O
Methoxy-MA(C83)	N/O	N/O	9.82	20.16
Methoxy-MA(C84)	N/O	N/O	N/O	21.06
Methoxy-MA(C85)	19.84	N/O	N/O	19.28

Methoxy-MA(C86)	17.81	7.87	N/O	19.88
Methoxy-MA(C87)	19.03	7.95	N/O	21.06
Methoxy-MA(C88)	19.84	N/O	N/O	N/O
Methoxy-MA(C89)	18.89	N/O	N/O	N/O
Methoxy-MA(C90)	19.84	N/O	N/O	22.32
Methoxy-MA(C91)	N/O	7.69	6.34	N/O
Methoxy-MA(C92)	N/O	7.85	N/O	N/O
Methoxy-MA(C93)	N/O	7.83	7.62	N/O
Methoxy-MA(C94)	N/O	8.18	8.37	N/O
MG(15:1)	11.48	N/O	N/O	N/O
MG(17:1)	15.35	N/O	N/O	9.33
MG(18:1)	14.82	N/O	N/O	N/O
MG(20:1)	5.11	N/O	N/O	19.81
MG(22:1)	N/O	N/O	N/O	12.55
MG(C15)	N/O	N/O	N/O	15.44
MG(C16)	14.22	N/O	N/O	N/O
MG(C17)	N/O	N/O	N/O	15.04
MG(C18)	14.82	N/O	N/O	N/O
MG(C19)	12.53	N/O	N/O	N/O
MG(C20)	15.77	N/O	N/O	N/O
MG(C22)	16.48	N/O	N/O	N/O
MG(C24)	N/O	N/O	N/O	11.53
MPM(C31)	N/O	2.16	9.49	N/O
MPM(C32)	N/O	N/O	7.81	N/O
Mycocerosic or Phthioceranic acid(C33)	17.70	N/O	N/O	19.75
Mycolipanolic acid(C24)	N/O	N/O	6.89	12.12
Mycolipanolic acid(C24)	N/O	N/O	N/O	N/O
Mycolipanolic acid(C26)	17.67	N/O	N/O	N/O
Mycolipenic acid(C25)	19.95	N/O	N/O	N/O

Mycolipenic acid(C27)	N/O	N/O	N/O	17.21
Mycolipenic acid(C28)	N/O	N/O	19.31	16.66
Mycosanoic or Mycocerosic acid(C24)	18.26	N/O	N/O	15.63
PE(30:1)	14.91	N/O	N/O	N/O
PE(31:1)	18.74	N/O	N/O	N/O
PE(32:2)	N/O	N/O	1.03	N/O
PE(33:1)	10.15	N/O	7.75	N/O
PE(33:2)	14.92	N/O	N/O	N/O
PE(34:1)	N/O	7.94	N/O	N/O
PE(34:2)	N/O	7.54	5.95	N/O
PE(35:2)	N/O	N/O	7.92	12.23
PE(36:2)	15.17	N/O	N/O	16.29
PE(37:2)	16.14	N/O	N/O	N/O
PE(C30)	N/O	7.27	N/O	19.20
PE(C31)	12.29	N/O	3.52	N/O
PE(C32)	N/O	N/O	N/O	20.21
PE(C37)	N/O	N/O	8.50	N/O
PE(C38)	N/O	N/O	10.76	N/O
PG(32:1)	N/O	5.58	5.05	N/O
PG(32:2)	N/O	1.05	1.23	11.39
PG(33:1)	16.50	6.38	N/O	N/O
PG(33:2)	16.89	1.25	N/O	N/O
PG(34:1)	N/O	7.19	7.04	N/O
PG(34:2)	N/O	N/O	6.23	14.04
PG(35:2)	19.21	7.35	2.86	N/O
PG(36:2)	N/O	N/O	N/O	15.18
PG(42:1)	10.97	N/O	N/O	N/O
PG(44:1)	N/O	N/O	18.57	N/O
PG(45:1)	14.63	N/O	N/O	N/O

PG(C30)	N/O	2.19	2.93	17.14
PG(C31)	10.99	N/O	N/O	N/O
PG(C32)	N/O	N/O	N/O	22.32
PG(C33)	N/O	N/O	10.67	N/O
PG(C34)	N/O	N/O	7.44	N/O
PG(C36)	N/O	N/O	7.50	N/O
PG(C44)	15.21	N/O	N/O	N/O
PGL-tb(C105)	N/O	N/O	21.64	N/O
Phthioceranic acid(C42)	N/O	1.05	N/O	N/O
Phthioceranic acid(C45)	6.79	N/O	N/O	N/O
PI(32:1)	N/O	7.46	9.51	N/O
PI(32:2)	N/O	N/O	6.89	N/O
PI(33:1)	N/O	5.41	2.69	N/O
PI(33:2)	N/O	7.62	7.35	N/O
PI(34:1)	N/O	N/O	9.53	16.20
PI(34:2)	15.92	N/O	7.44	20.99
PI(34:3)	N/O	N/O	N/O	17.29
PI(34:4)	N/O	8.35	18.06	N/O
PI(35:1)	N/O	N/O	11.42	16.96
PI(35:2)	N/O	N/O	8.02	19.31
PI(35:3)	N/O	7.52	7.44	18.30
PI(35:4)	N/O	8.51	8.05	N/O
PI(36:2)	N/O	N/O	8.58	N/O
PI(36:3)	N/O	8.78	7.55	N/O
PI(37:1)	N/O	8.30	5.58	N/O
PI(37:2)	N/O	8.22	9.18	21.91
PI(37:3)	N/O	7.92	8.40	19.37
PI(C31)	N/O	8.43	9.63	N/O
PI(C32)	11.05	7.75	N/O	8.25
PI(C33)	15.45	N/O	17.23	N/O

PI(C34)	15.87	N/O	N/O	N/O
PIM1(32:1)	N/O	7.00	9.51	21.49
PIM1(33:1)	N/O	7.12	9.54	N/O
PIM1(34:1)	N/O	7.52	N/O	N/O
PIM1(34:3)	N/O	N/O	N/O	18.04
PIM1(34:4)	N/O	N/O	N/O	16.86
PIM1(35:1)	N/O	8.60	N/O	N/O
PIM1(35:3)	N/O	N/O	8.14	N/O
PIM1(36:1)	10.99	N/O	N/O	N/O
PIM1(36:2)	10.99	8.83	N/O	N/O
PIM1(C30)	6.22	N/O	9.54	20.77
PIM1(C31)	N/O	N/O	9.73	N/O
PIM1(C32)	N/O	N/O	N/O	12.00
PIM1(C34)	N/O	N/O	N/O	21.77
PIM2(32:1)	N/O	N/O	N/O	19.83
PIM2(33:1)	5.06	N/O	N/O	N/O
PIM2(33:2)	N/O	7.19	N/O	N/O
PIM2(34:2)	N/O	8.30	N/O	N/O
PIM2(34:4)	N/O	N/O	N/O	22.32
PIM2(35:2)	N/O	9.08	N/O	N/O
PIM2(35:3)	N/O	8.30	N/O	N/O
PIM2(35:4)	6.10	N/O	N/O	N/O
PIM2(36:1)	N/O	N/O	16.05	N/O
PIM2(36:2)	N/O	8.23	N/O	N/O
PIM2(37:1)	N/O	N/O	16.23	N/O
PIM2(37:2)	N/O	8.71	N/O	N/O
PIM2(37:3)	N/O	8.60	N/O	N/O
PIM2(C30)	N/O	N/O	19.40	N/O
PIM2(C32)	10.99	7.62	N/O	N/O
PIM2(C33)	18.01	N/O	N/O	N/O

PIM2(C34)	N/O	7.85	15.98	N/O
PIM2(C35)	N/O	N/O	N/O	6.34
PIM2(C36)	N/O	8.22	16.66	N/O
PIM2(C37)	15.91	N/O	N/O	N/O
PIM3(32:2)	N/O	N/O	9.80	N/O
PIM3(33:2)	N/O	N/O	10.06	N/O
PIM3(34:1)	N/O	3.16	N/O	N/O
PIM3(34:2)	N/O	N/O	14.97	N/O
PIM3(34:3)	N/O	N/O	14.11	19.57
PIM3(34:4)	N/O	N/O	6.06	N/O
PIM3(35:1)	6.59	6.31	N/O	N/O
PIM3(35:3)	16.54	N/O	N/O	17.82
PIM3(36:1)	6.32	6.92	N/O	N/O
PIM3(36:2)	N/O	N/O	7.35	N/O
PIM3(36:3)	17.09	N/O	11.55	18.69
PIM3(37:1)	17.52	7.35	18.42	19.38
PIM3(37:2)	16.79	N/O	16.18	N/O
PIM3(37:3)	N/O	N/O	15.53	N/O
PIM3(C30)	N/O	2.43	N/O	N/O
PIM3(C31)	N/O	N/O	16.16	N/O
PIM3(C32)	17.12	N/O	N/O	N/O
PIM3(C34)	18.50	N/O	N/O	N/O
PIM3(C36)	18.30	N/O	7.42	20.68
PIM4(32:2)	N/O	9.30	N/O	N/O
PIM4(33:1)	6.49	N/O	N/O	N/O
PIM4(33:2)	N/O	8.29	N/O	N/O
PIM4(34:1)	17.63	7.50	N/O	N/O
PIM4(34:3)	N/O	8.14	N/O	N/O
PIM4(35:1)	N/O	2.96	8.40	N/O
PIM4(35:2)	16.98	N/O	N/O	N/O

PIM4(35:4)	N/O	N/O	5.63	N/O
PIM4(36:1)	N/O	7.89	N/O	N/O
PIM4(37:1)	N/O	7.92	N/O	N/O
PIM4(37:3)	18.52	N/O	17.34	N/O
PIM4(C31)	N/O	2.31	N/O	N/O
PIM4(C32)	17.50	7.42	N/O	N/O
PIM4(C33)	17.86	7.57	N/O	N/O
PIM4(C34)	N/O	7.64	N/O	N/O
PIM4(C35)	N/O	8.30	N/O	N/O
PIM4(C36)	N/O	N/O	21.65	N/O
PIM4(C37)	N/O	8.30	10.67	N/O
PIM5(32:1)	17.91	1.78	17.64	N/O
PIM5(33:1)	18.89	N/O	N/O	N/O
PIM5(34:2)	N/O	7.40	N/O	N/O
PIM5(35:2)	N/O	N/O	9.53	N/O
PIM5(35:4)	N/O	N/O	7.52	20.69
PIM5(36:1)	15.73	2.74	N/O	N/O
PIM5(36:3)	N/O	N/O	8.60	N/O
PIM5(37:1)	N/O	N/O	11.05	N/O
PIM5(37:2)	N/O	7.81	10.32	N/O
PIM5(37:3)	N/O	N/O	8.25	N/O
PIM5(C30)	17.86	1.65	N/O	N/O
PIM5(C31)	18.91	N/O	N/O	N/O
PIM5(C32)	N/O	2.21	N/O	N/O
PIM5(C33)	N/O	N/O	18.07	N/O
PIM5(C34)	15.96	N/O	N/O	N/O
PIM6(32:2)	N/O	N/O	7.60	N/O
PIM6(33:2)	N/O	7.89	8.23	N/O
PIM6(34:1)	N/O	N/O	19.46	N/O
PIM6(34:3)	N/O	7.92	8.29	N/O

PIM6(35:1)	N/O	N/O	19.55	N/O
PIM6(35:4)	N/O	7.97	8.35	N/O
PIM6(36:1)	N/O	7.35	N/O	N/O
PIM6(C31)	N/O	N/O	8.22	20.69
PIM6(C32)	N/O	6.03	N/O	N/O
PIM6(C33)	N/O	2.15	N/O	N/O
PIM6(C36)	N/O	8.35	N/O	N/O
SL-III(C104)	N/O	N/O	12.95	N/O
SL-III(C106)	N/O	N/O	16.41	N/O
SL-III(C107)	N/O	N/O	16.48	N/O
SL-III(C92)	N/O	11.40	N/O	N/O
SL-III(C95)	N/O	N/O	8.40	N/O
TG(47:3)	15.70	N/O	N/O	N/O
TG(52:1)	N/O	10.06	17.99	N/O
TG(52:3)	N/O	N/O	N/O	22.33
TG(57:1)	N/O	N/O	N/O	N/O
TG(58:1)	N/O	10.52	N/O	N/O
TG(67:1)	N/O	7.64	N/O	N/O
TG(67:2)	N/O	N/O	4.42	N/O
TG(67:3)	N/O	11.95	N/O	N/O
TG(68:1)	N/O	7.59	6.84	N/O
TG(69:1)	N/O	N/O	6.59	N/O
TG(70:1)	N/O	8.14	N/O	N/O
TG(70:2)	N/O	7.17	6.44	N/O
TG(72:1)	N/O	N/O	7.27	N/O
TG(78:1)	N/O	7.77	N/O	N/O
TG(79:1)	N/O	7.92	N/O	N/O
TG(80:1)	N/O	8.12	N/O	N/O
TG(81:1)	N/O	8.25	9.76	N/O
TG(C53)	N/O	N/O	17.69	N/O

TG(C58)	N/O	10.39	N/O	N/O
TG(C66)	N/O	7.41	N/O	N/O
TG(C67)	N/O	N/O	N/O	21.31
TG(C68)	N/O	N/O	6.81	N/O
TG(C70)	N/O	7.35	N/O	N/O
TG(C74)	N/O	6.98	N/O	N/O
TG(C75)	N/O	7.39	N/O	N/O
TG(C76)	N/O	7.74	8.02	N/O
TG(C77)	N/O	7.87	N/O	N/O
TG(C78)	N/O	8.10	N/O	N/O
TG(C81)	N/O	N/O	8.20	N/O
TG(C82)	N/O	N/O	8.42	N/O
TG(C85)	18.06	N/O	N/O	N/O
TG(C86)	18.32	N/O	N/O	N/O
TMM(Alpha-MA(monoenoic or monocyclopropanoic))(C76)	N/O	8.03	N/O	N/O
TMM(Alpha-MA(monoenoic or monocyclopropanoic))(C85)	N/O	N/O	16.50	N/O
TMM(Alpha-MA)(C86)	N/O	N/O	19.58	N/O
TMM(Alpha-MA)(C87)	N/O	N/O	16.51	N/O
TMM(keto-MA)(C75)	N/O	N/O	16.58	N/O
TMM(keto-MA)(C81)	N/O	N/O	15.75	N/O
TMM(keto-MA)(C86)	N/O	N/O	19.42	N/O
TMM(keto-MA)(C87)	N/O	N/O	17.23	N/O
TMM(keto-MA)(C89)	N/O	N/O	16.66	N/O
TMM(keto-MA)(C90)	N/O	N/O	16.88	N/O
TMM(keto-MA)(C92)	N/O	N/O	15.17	N/O
TMM(keto-MA)(C93)	N/O	N/O	17.23	N/O

TMM(keto-MA)(C94)	N/O	N/O	17.36	N/O
TMM(methoxy-MA)(C79)	N/O	N/O	15.73	N/O
TMM(methoxy-MA)(C83)	N/O	N/O	16.53	N/O
TMM(methoxy-MA)(C84)	N/O	N/O	16.20	N/O
TMM(methoxy-MA)(C87)	N/O	N/O	16.66	N/O
TMM(methoxy-MA)(C88)	N/O	N/O	16.86	N/O
TMM(methoxy-MA)(C90)	N/O	N/O	17.14	N/O
TMM(methoxy-MA)(C91)	N/O	N/O	17.19	N/O
TMM(methoxy-MA)(C92)	N/O	N/O	17.32	N/O

[a]LipidID: lipid identifiers from LipidMaps-MtbDB (https://www.lipidmaps.org/tools/ms/Mtb_batch_bulk.html); RT: retention time; N/O: the lipid was not detected by the liquid-chromatography mass spectrometry method listed in **Tables 1** and **2**.

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