Example imaging calculation for a 3 x 3 pixel area with 3 compounds (A, B,C):

A

Spectra #	Position X	Position Y
1	0	0
2	0	1
3	0	2
4	1	0
5	1	1
6	1	2
7	2	0
8	2	1
9	2	2

B

Absolute Intensity (Counts)[1]		
Compound A	Compound B	Compound C
50	50	0
0	100	25
100	50	50
50	70	80
0	50	75
25	75	0
500	500	0
0	1000	250
1000	500	500

C

Relative Units (mol %)		
Compound A	Compound B	Compound C
50	50	0
0	80	20
50	25	25
25	35	40
0	40	60
25	75	0
50	50	0
0	80	20
50	25	25

D

Spectra #	X	Y	Greyscale Color (Red = Green = Blue)[3]		
1	0	0	242	242	255
2	0	1	255	229	242
3	0	2	229	242	229
4	1	0	242	237	214
5	1	1	255	242	217
6	1	2	249	236	255
7	2	0	127	127	255
8	2	1	255	0	127
9	2	2	0	127	0

E

Greyscale Color (Red = Green = Blue)[2,3]		
96	96	255
255	0	170
96	175	149
175	143	85
255	127	0
175	16	255
96	96	255
255	0	170
96	175	149

Notes:

1-Maximum value for Compound A, B, C will be 1000, 1000, 500 counts respectively

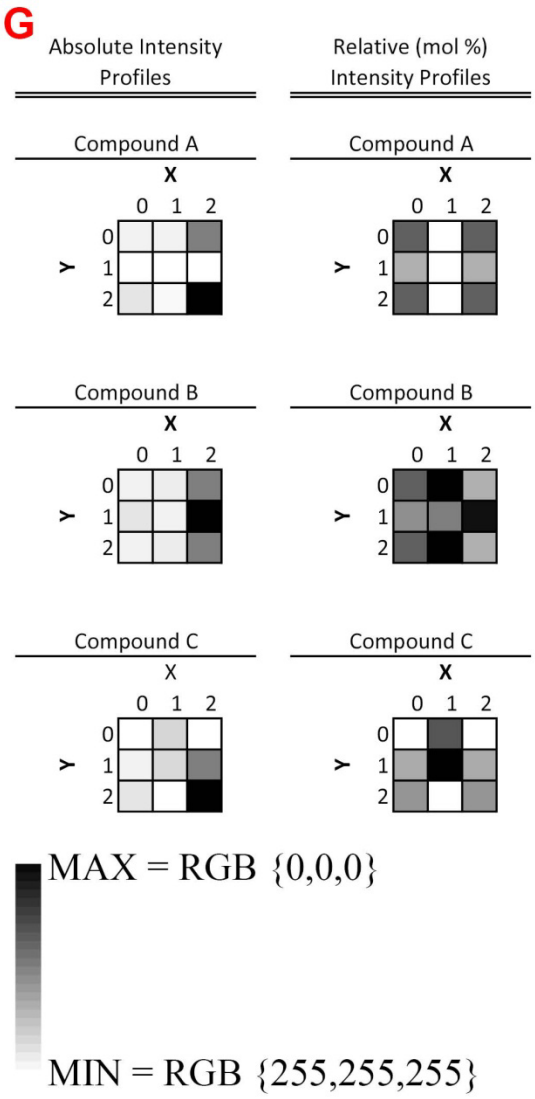
2-Maximum (relative) value for all compounds set to 80 mol %.

3-Example Microsoft Excel formula for greyscale conversion:
Color = 255 - ROUND((255 * value / maxValue),0)

F

Y position \ X position	0	1	2
0	{0,0}	{1,0}	{2,0}
1	{0,1}	{1,1}	{2,1}
2	{0,2}	{1,2}	{2,2}

G



Supplemental Figure 1.

Example conversion of raw MS data to a set of MS images on an absolute and relative scale.

(A) Imaging setup: MALDI-MS spectra are acquired at each x, y position within a 3 x 3 square for a total of 9 spectra (#1-9). Each spectrum will have an absolute x, y position associated with it as the laser rasterizes across each individual position. For example, in spectrum #1 the x, y position is {0, 0} and for spectrum #6 the x, y position is {1, 2}.

(B) Data Acquisition: Within each spectrum the absolute intensity (in counts) of 3 compounds (Compound A, Compound B, and Compound C) is acquired (see column Absolute Intensity (Counts)). For example, in spectra #5: Compound A's intensity was 0 counts, Compound B's intensity was 50 counts, and Compound C's intensity was 75 counts.

(C) Calculation of relative compound values: For each individual spectrum the relative units of each compound can be calculated as follows:

1) Determine the absolute intensity units of selected compounds within a spectrum: In spectrum #3 Compound A has 100 counts, Compound B has 50 counts, and Compound C has 50 counts
2) Calculate the sum of the total counts for the selected spectrum: In spectrum #3 the total counts are 200 counts (Compound A counts + Compound B counts + Compound C counts = 100 counts + 50 counts + 50 counts).
3) Divide a compound's absolute units by the total units within that spectrum. In spectrum #3 Compound A = 100 counts with the total counts for that spectrum 200 counts. Therefore Compound A is 50 mol % (100 counts / 200 counts * 100% = 50 mol %). The counts can be converted to mol % since these are relative amounts calculated within a spectrum and are not absolute quantities. For Compounds B and C a similar calculation can be made to get 25 and 25 mol %, respectively. Therefore the maximum and minimum mol % a compound can be is 100 and 0%, respectively for a particular spectra.

(D) Convert absolute counts into pixel RGB values: To create a MS image representing the absolute distribution of a compound within the 3 x 3 area we need to convert the absolute intensity (in counts) into a Red-Green-Blue (RGB) value that can visually represent the absolute intensity.

1) Determine the maximum absolute intensity for a compound. For example, Compound A, B, and C's maximum intensities are 1000, 1000, and 500 counts respectively.
2) Greyscale colors are generated by setting the Red = Green = Blue value with an 8-bit color system (0-255) (e.g. white = {255, 255, 255} and black {0, 0, 0}). The formula to convert an absolute intensity into a linear greyscale RGB value is: greyscale value = 255 – 255 * absolute intensity / maximum absolute intensity. The final greyscale value should be rounded to an integer before image generation. For example for spectrum #1, Compound A: the greyscale value will equal 242 where the absolute intensity is 50 counts and the maximum intensity is 1000 counts

(= 255 – 255 * 50 counts / 1000 counts). This will correspond to a very light grey RGB representation {242, 242, 242}.

3) A similar image could be created (as done in the manuscript) by normalizing the counts for each compound relative to the total counts acquired for entire spectrum (i.e. including all other compounds identified and non-identified).

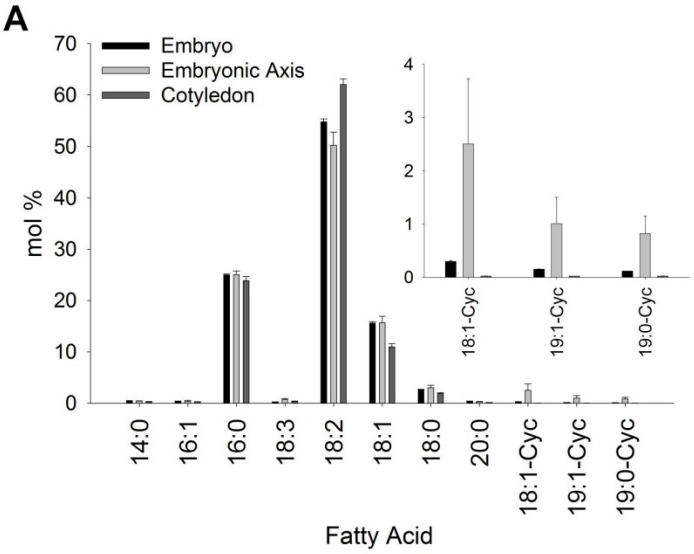
(E) Convert relative mol % values into pixel RGB values: To create an MS image representing the relative distribution of a compound within the 3 x 3 area we need to convert the relative intensity (in mol %) into a RGB value that can visually represent the relative units (in mol %).

1) Find the maximum value within all spectra across all compounds. While one could use a separate maximum mol % value for each compound this would not normalize the images to each other. Therefore in this case we choose a value that is either the maximum for all compounds over the entire area sampled. For example in this case the maximum mol % value is 80 (found in spectrum #8 of Compound B).
2) Convert each relative value as shown in Part D step 2 above into a greyscale value (= 255 – 255 * relative units / maximum relative units). In example, for spectrum #1 for Compound A, the greyscale value is 96 where the relative units for this compound 50 mol % and the maximum mol % is 80 (= 255 – 255 * 50 units / 80 units).

(F) Imaging position setup: Now that we have greyscale values for each x, y position we can create a 3 x 3 image using these values. Shown here is how each pixel of the box will correspond to the absolute x, y position.

(G) Absolute intensity and relative intensity profiles can be generated using the greyscale values for each individual x, y position. These images were generated using Microsoft Excel while images in the manuscript were generated using the LipidImager application using identical principles.

A



B

	Embryo		Embryonic Axis		Cotyledon		Embryonic Axis vs. Cotyledon
	Mean	StDev	Mean	StDev	Mean	StDev	
Fatty Acid (Common Name)	(mol %)		(mol %)		(mol %)		p-value
14:0 (Myristic)	0.48	0.03	0.43	0.04	0.32	0.03	0.01
16:1 (Palmitoleic)	0.42	0.01	0.34	0.20	0.31	0.02	0.80
16:0 (Palmitic)	25.01	0.22	25.05	0.74	23.91	0.77	0.11
18:3 (Linolenic)	0.21	0.05	0.72	0.18	0.35	0.05	0.03
18:2 (Linoleic)	54.77	0.58	50.21	2.55	62.03	1.11	0.02
18:1 (Oleic)	15.56	0.31	15.64	1.27	10.98	0.65	0.001
18:0 (Stearic)	2.69	0.03	2.99	0.51	1.89	0.16	0.002
20:0 (Arachidic)	0.32	0.11	0.28	0.06	0.14	0.02	0.02
18:1-Cyc (Malvalic)	0.30	0.02	2.51	1.22	0.02	0.01	0.03
19:1-Cyc (Sterculic)	0.15	0.01	1.01	0.50	0.02	0.00	0.02
19:0-Cyc (Dihydrosterculic)	0.12	0.00	0.82	0.33	0.02	0.00	0.01

Supplemental Figure 2. Fatty acid composition of total cottonseed lipid extracts.

(A) Fatty acid composition of total lipids extracted separately from mature (complete) cotton embryos in addition to hand-dissected embryonic axis and cotyledon tissues. The base-catalyzed, fatty acids methyl esters were analyzed by gas chromatography-mass spectrometry. The inset demonstrates the exclusive localization of cyclic fatty acids in the embryonic axis. Fatty acid abbreviations: myristic (14:0), palmitoleic (16:1), palmitic (16:0), linolenic (18:3), linoleic (18:2), oleic (18:1), stearic (18:0), arachidic (20:0), malvalic (18:1-Cyc), sterculic (19:1-Cyc), dihydrosterculic (19:0-Cyc).

(B) Table of results from part (A) presented as mean and standard deviation (StDev) mol % of total seed fatty acids (n = 3 to 4 sample replicates with each replicate representing pooled lipid extracts of 5 to 10 embryos or hand-dissected tissues). A student's t-test (two-tailed, unpaired) confirms the embryonic axis and cotyledon tissue comprise of significantly different fatty acid compositions.

Supplemental Table 1. Triacylglycerol molecular species analyzed by MALDI-MSI

					Cross Section (Na^+ Adducts)			Longitudinal Section (Na^+ Adducts)				Cross Section (K^+ Adducts)			Longitudinal Section (K^+ Adducts)		
Abbreviated Name	**Formula**	**Adduct(s)**	**Common Name[1,2]**	**$[M + Na]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**$[M + K]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**
TAG-48:2	C51H94O6	Na^+, K^+	TAG-MPL-(14:0/16:0/18:2)	825.695	825.696	0.003	1.0	825.693	0.004	1.6	841.669	841.669	0.006	0.6	841.670	0.010	1.9
TAG-48:1	C51H96O6	Na^+, K^+	TAG-MPO-(14:0/16:0/18:1)	827.710	827.709	0.006	1.2	827.709	0.008	1.7	843.684	843.679	0.011	6.0	843.681	0.014	4.3
TAG-48:0	C51H98O6	Na^+, K^+	TAG-PPP-(16:0/16:0/16:0)	829.726	829.730	0.004	5.2	829.726	0.005	0.2	845.700	845.697	0.013	3.9	845.702	0.013	1.8
TAG-50:4	C53H94O6	Na^+, K^+	TAG-MLL-(14:0/18:2/18:2)	849.695	849.696	0.002	1.1	849.693	0.004	1.8	865.669	865.666	0.007	2.8	865.677	0.012	9.4
TAG-50:3	C53H96O6	Na^+, K^+	TAG-MLO-(14:0/18:2/18:1)	851.710	851.712	0.002	2.1	851.710	0.003	0.4	867.684	867.681	0.009	3.9	867.692	0.011	9.0
TAG-50:2	C53H98O6	Na^+, K^+	TAG-PPL-(16:0/16:0/18:2)	853.726	853.728	0.002	2.0	853.726	0.001	0.7	869.700	869.695	0.006	6.0	869.695	0.005	5.8
TAG-50:1	C53H100O6	Na^+, K^+	TAG-PPO-(16:0/16:0/18:1)	855.742	855.739	0.003	3.5	855.738	0.003	4.7	871.716	871.715	0.012	0.4	871.714	0.011	1.4
TAG-52:5	C55H96O6	Na^+, K^+	TAG-PLLn-(16:0/18:2/18:3)	875.710	875.712	0.002	1.7	875.710	0.003	0.0	891.684	891.676	0.007	9.5	891.699	0.009	16.3
TAG-52:4	C55H98O6	Na^+, K^+	TAG-PLL-(16:0/18:2/18:2)	877.726	877.728	0.002	2.3	877.725	0.001	0.8	893.700	893.693	0.007	8.1	893.691	0.007	9.9
TAG-52:3	C55H100O6	Na^+, K^+	TAG-PLO-(16:0/18:2/18:1)	879.742	879.741	0.002	0.4	879.740	0.002	2.3	895.716	895.715	0.013	0.7	895.711	0.011	4.8
TAG-52:2	C55H102O6	Na^+, K^+	TAG-POO-(16:0/18:1/18:1) > TAG-SLP-(18:0/18:2/16:0)	881.757	881.755	0.003	2.4	881.754	0.003	4.1	897.731	897.735	0.012	4.0	897.729	0.010	2.5
TAG-54:7	C57H96O6	Na^+, K^+	TAG-LLLn-(18:2/18:2/18:3)	899.710	899.711	0.004	0.5	899.709	0.006	1.4	915.684	915.677	0.009	7.6	915.702	0.004	19.3
TAG-54:6	C57H98O6	Na^+, K^+	TAG-LLL-(18:2/18:2/18:2)	901.726	901.727	0.002	1.4	901.724	0.001	1.9	917.700	917.691	0.008	9.4	917.689	0.007	11.7
TAG-54:5	C57H100O6	Na^+, K^+	TAG-LLO-(18:2/18:2/18:1)	903.742	903.742	0.002	0.3	903.739	0.001	2.9	919.716	919.713	0.012	2.6	919.707	0.009	9.1
TAG-54:4	C57H102O6	Na^+, K^+	TAG-LOO-(18:2/18:1/18:1) > TAG-SLL-(18:0/18:2/18:2)	905.757	905.756	0.002	1.2	905.754	0.002	3.7	921.731	921.735	0.013	3.5	921.728	0.011	3.6
TAG-54:3	C57H104O6	Na^+, K^+	TAG-OOO-(18:1/18:1/18:1) > TAG-SLO-(18:0/18:2/18:1)	907.773	907.770	0.004	3.7	907.768	0.004	5.3	923.747	923.752	0.011	5.0	923.746	0.010	1.6
TAG-54:2	C57H106O6	Na^+, K^+	TAG-SOO-(18:0/18:1/18:1) > TAG-ALP-(20:0/18:2/16:0) > TAG-SSL-(18:0/18:0/18:2)	909.789	909.783	0.005	6.1	909.783	0.006	6.1	925.763	925.759	0.010	4.1	925.760	0.010	2.8
TAG-54:1	C57H108O6	Na^+, K^+	TAG-SSO-(18:0/18:0/18:1)	911.804	911.799	0.007	5.5	911.803	0.010	1.4	927.778	927.773	0.011	5.4	927.778	0.011	0.8
TAG-56:4	C59H106O6	Na^+, K^+	TAG-ALL-(20:0/18:2/18:2)/GLO-(20:1/18:2/18:1)	933.789	933.785	0.004	4.4	933.785	0.007	4.0	949.763	949.761	0.015	1.4	949.765	0.011	2.2
TAG-56:3	C59H108O6	Na^+, K^+	TAG-ALO-(20:0/18:2/18:1)	935.804	935.797	0.006	7.7	935.801	0.009	3.4	951.778	951.774	0.013	4.6	951.780	0.012	1.9
TAG-56:2	C59H110O6	Na^+, K^+	TAG-AOO-(20:0/18:1/18:1)	937.820	937.818	0.006	2.2	937.817	0.010	3.0	953.794	953.792	0.009	2.4	953.793	0.011	0.8
TAG-58:4	C61H110O6	Na^+, K^+	TAG-BLL-(22:0/18:2/18:2)	961.820	961.821	0.006	1.2	961.819	0.010	1.5	977.794	977.792	0.011	2.0	977.791	0.012	2.7
TAG-53:3-Cyc	C56H100O6	Na^+, K^+	TAG-LScP	891.742	891.739	0.005	3.0	891.739	0.005	2.6	907.716	907.709	0.006	6.9	907.707	0.006	10.1
TAG-53:2-Cyc	C56H102O6	Na^+, K^+	TAG-LDscP (OScP)	893.757	893.748	0.006	10.3	893.747	0.006	11.4	909.731	909.726	0.008	5.4	909.725	0.004	7.3
TAG-53:1-Cyc	C56H104O6	Na^+, K^+	TAG-ODScP	895.773	895.764	0.007	9.8	895.762	0.006	12.1	911.747	911.738	0.007	9.4	911.735	0.004	13.6
TAG-55:5-Cyc	C58H100O6	Na^+, K^+	TAG-LLSc	915.742	915.738	0.008	4.3	915.737	0.007	5.2	931.716	931.709	0.007	7.0	931.705	0.006	11.1
TAG-55:4-Cyc	C58H102O6	Na^+, K^+	TAG-LLDsc > OLSc	917.757	917.749	0.007	9.7	917.741	0.004	18.2	933.731	933.725	0.007	6.5	933.725	0.004	7.0
TAG-55:3-Cyc	C58H104O6	Na^+, K^+	TAG-LODsc > OOSc	919.773	919.761	0.003	13.4	919.758	0.006	16.1	935.747	935.739	0.008	8.2	935.738	0.004	10.0
TAG-56:5-Cyc	C59H102O6	Na^+, K^+	TAG-LScSc >> LnDScSc	929.757	929.747	0.004	11.7	929.746	0.009	12.2	945.731	945.723	0.010	8.8	945.730	0.011	1.9
TAG-56:4-Cyc	C59H104O6	Na^+, K^+	LDscSc > LnDscDsc	931.773	931.771	0.008	2.6	931.772	0.010	1.3	947.747	947.754	0.011	7.5	947.749	0.012	1.8
TAG-56:3-Cyc	C59H106O6	Na^+, K^+	LDscDsc	933.789	933.785	0.004	4.4	933.785	0.007	4.0	949.763	949.761	0.015	1.4	949.765	0.011	2.2

[1] Determined from ESI-MS/MS and literature

[2] Fatty Acid Abbreviations: M-14:0 Myristic; P-16:0 palmitic; Po-16:1 palmitoleic, Ln-18:3 linolenic; L-18:2 linoleic; O-18:1 oleic acid; S-18:0 stearic; A-20:0 arachidic; B-22:0 behenic; Sc-19:1 sterculic; Dsc-19:0 dihydrosterculic acid

[3] PPM = parts per million; (|measured mean *m/z* - theoretical monoisotopic *m/z* | / theoreticalmonisotopic *m/z* * 10^6)

Supplemental Table 2. Phosphatidylcholine molecular species analyzed by MALDI-MSI

				Cross Section (H^+ Adducts)			Longitudinal Section (H^+ Adducts)			Cross Section (K^+ Adducts)			Longitudinal Section (K^+ Adducts)			Cross Section (Na^+ Adducts)			Longitudinal Section (Na^+ Adducts)		
Abbreviated Name	**Formula**	**Adduct(s)**	**Common Name[1,2]**	**$[M+H]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**$[M+K]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**$[M+Na]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**
LysoPC-16:1	C24H48O7PN	H^+, Na^+, K^+	PC(16:1/0:0)	494.325	494.324	0.002	1.5	494.323	0.009	3.0	532.281	532.280	0.004	1.0	532.279	0.008	3.4	516.307	516.305	0.005	2.4	516.304	0.008	4.6
LysoPC-16:0	C24H50O7PN	H^+, Na^+, K^+	PC(16:0/0:0)	496.340	496.340	0.001	1.4	496.338	0.001	3.6	534.296	534.296	0.001	1.2	534.296	0.005	0.6	518.322	518.322	0.001	0.7	518.321	0.005	3.4
LysoPC-18:3	C26H48O7PN	H^+, Na^+, K^+	PC(18:3/0:0)	518.325	518.322	0.001	5.4	518.321	0.005	6.7	556.281	556.272	0.006	15.1	556.280	0.008	0.9	540.307	540.304	0.007	5.4	540.308	0.007	1.9
LysoPC-18:2	C26H50O7PN	H^+, Na^+, K^+	PC(18:2/0:0)	520.340	520.340	0.001	1.3	520.338	0.001	3.5	558.296	558.296	0.001	1.2	558.294	0.004	3.2	542.322	542.321	0.001	1.5	542.320	0.004	3.8
LysoPC-18:1	C26H52O7PN	H^+, Na^+, K^+	PC(18:1/0:0)	522.356	522.356	0.001	0.3	522.355	0.001	2.6	560.312	560.312	0.002	0.2	560.310	0.007	3.9	544.338	544.338	0.001	0.2	544.336	0.006	4.0
LysoPC-18:0	C26H54O7PN	H^+, Na^+, K^+	PC(18:0/0:0)	524.372	524.372	0.002	0.8	524.370	0.005	2.9	562.328	562.330	0.006	3.6	562.329	0.009	3.2	546.354	546.353	0.003	0.3	546.353	0.009	0.1
PC-32:2	C40H76O8PN	H^+, Na^+, K^+	PC(14:0/18:2)	730.539	730.539	0.002	0.2	730.537	0.003	2.2	768.495	768.495	0.002	0.2	768.495	0.007	0.1	752.521	752.519	0.002	1.5	752.517	0.003	4.9
PC-32:1	C40H78O8PN	H^+, Na^+, K^+	PC(14:0/18:1)	732.554	732.555	0.002	1.0	732.552	0.005	2.5	770.510	770.512	0.003	2.3	770.519	0.007	11.9	754.536	754.536	0.003	0.7	754.533	0.005	4.2
PC-32:0	C40H80O8PN	H^+, Na^+, K^+	Not Identified	734.570	734.571	0.002	1.0	734.569	0.005	1.7	772.526	772.528	0.002	2.2	772.525	0.007	0.9	756.552	756.555	0.002	3.5	756.552	0.003	0.6
PC-34:3	C42H78O8PN	H^+, Na^+, K^+	PC(16:0/18:3)	756.554	756.555	0.002	0.3	756.552	0.003	2.5	794.510	794.510	0.002	0.3	794.509	0.007	0.9	778.536	778.536	0.002	0.8	778.535	0.006	2.0
PC-34:2	C42H80O8PN	H^+, Na^+, K^+	PC(16:0/18:2)	758.570	758.571	0.001	1.4	758.568	0.001	2.2	796.526	796.527	0.001	1.4	796.524	0.001	2.0	780.552	780.553	0.001	2.0	780.551	0.001	1.7
PC-34:1	C42H82O8PN	H^+, Na^+, K^+	PC(16:0/18:1)	760.586	760.585	0.002	1.4	760.584	0.001	2.2	798.542	798.542	0.002	0.2	798.542	0.002	0.0	782.568	782.571	0.002	3.8	782.568	0.001	0.8
PC-35:1-Cyc	C43H82O8PN	H^+, Na^+, K^+	PC-Cyc-PSc	772.586	772.586	0.001	0.9	772.585	0.004	1.3	810.542	810.544	0.003	2.5	810.540	0.007	2.3	794.568	794.569	0.005	1.9	794.566	0.007	2.3
PC-35:0-Cyc	C43H84O8PN	H^+, Na^+, K^+	PC-Cyc-PDSc	774.601	774.600	0.004	1.2	774.600	0.006	2.1	812.557	812.559	0.005	2.0	812.557	0.008	0.5	796.583	796.582	0.002	1.8	796.584	0.005	0.4
PC-36:6	C44H76O8PN	H^+, Na^+, K^+	PC(18:3/18:3)	778.539	778.536	0.002	3.9	778.536	0.006	3.8	816.495	816.493	0.009	2.3	816.493	0.009	1.7	800.521	800.524	0.008	4.5	800.528	0.007	9.4
PC-36:5	C44H78O8PN	H^+, Na^+, K^+	PC(18:3/18:2)	780.554	780.553	0.001	1.1	780.551	0.001	4.8	818.510	818.510	0.002	0.4	818.511	0.009	0.7	802.536	802.537	0.004	0.3	802.536	0.008	0.2
PC-36:4	C44H80O8PN	H^+, Na^+, K^+	PC(18:2/18:2),PC(18:1/18:3)	782.570	782.571	0.002	0.7	782.568	0.001	2.2	820.526	820.527	0.001	0.9	820.524	0.001	2.1	804.552	804.553	0.001	1.1	804.550	0.001	2.0
PC-36:3	C44H82O8PN	H^+, Na^+, K^+	PC(18:1/18:2),PC(18:0/18:3)	784.586	784.586	0.002	0.1	784.584	0.001	1.9	822.542	822.541	0.001	0.1	822.541	0.001	0.9	806.568	806.567	0.003	0.9	806.566	0.001	2.0
PC-36:2	C44H84O8PN	H^+, Na^+, K^+	PC(18:0/18:2),PC(18:1/18:1)	786.601	786.600	0.002	1.2	786.600	0.001	2.2	824.557	824.557	0.002	0.0	824.557	0.002	0.2	808.583	808.582	0.003	2.0	808.581	0.002	2.3
PC-36:1	C44H86O8PN	H^+, Na^+, K^+	PC(18:1/18:0)	788.617	788.612	0.002	5.7	788.612	0.004	6.1	826.573	826.569	0.004	4.1	826.570	0.006	3.7	810.599	810.596	0.004	3.4	810.595	0.005	4.2
PC-37:3-Cyc	C45H82O8PN	H^+, Na^+, K^+	PC-Cyc-LSc	796.586	796.582	0.002	4.8	796.584	0.005	2.1	834.542	834.542	0.003	0.5	834.540	0.007	1.5	818.568	818.568	0.004	0.2	818.569	0.008	2.2
PC-37:2-Cyc	C45H84O8PN	H^+, Na^+, K^+	PC-Cyc-LDsc,OSc	798.601	798.597	0.003	5.2	798.599	0.004	2.3	836.557	836.557	0.003	0.3	836.556	0.005	1.6	820.583	820.580	0.011	4.0	820.583	0.006	0.5
PC-37:1-Cyc	C45H86O8PN	H^+, Na^+, K^+	PC-Cyc-ODsc	800.617	800.614	0.004	4.2	800.615	0.005	2.4	838.573	838.574	0.005	1.3	838.572	0.007	1.5	822.599	822.597	0.007	2.3	822.597	0.008	1.9
PC-38:4/PC-38:2-Cyc	C46H84O8PN	H^+, Na^+, K^+	PC(20:1/18:3), PC(20:2/18:2), PC-Cyc-ScSc	810.601	810.596	0.004	6.3	810.596	0.005	6.7	848.557	848.555	0.008	2.4	848.552	0.007	6.4	832.583	832.572	0.003	13.7	832.583	0.008	0.8
PC-38:3/PC-38:1-Cyc	C46H86O8PN	H^+, Na^+, K^+	PC(20:1/18:2), PC(20:0/18:3), PC-Cyc-ScDsc	812.617	812.617	0.005	0.3	812.617	0.007	0.1	850.573	850.573	0.004	0.1	850.576	0.007	3.3	834.599	834.600	0.007	0.8	834.600	0.010	1.9
PC-38:2/PC-38:0-Cyc	C46H88O8PN	H^+, Na^+, K^+	Not Identified ,PC-Cyc-DscDsc	814.633	814.632	0.002	0.3	814.631	0.005	2.1	852.588	852.589	0.003	0.2	852.586	0.009	3.3	836.615	836.616	0.004	1.5	836.616	0.007	1.2

[1] Determined from ESI-MS/MS and literature

[2]Fatty Acid Abbreviations: M-14:0 Myristic; P-16:0 palmitic; Po-16:1 palmitoleic, Ln-18:3 linolenic; L-18:2 linoleic; O-18:1 oleic acid; S-18:0 stearic; A-20:0 arachidic; B-22:0 behenic; Sc-19:1 sterculic; Dsc-19:0 dihydrosterculic acid

[3]PPM = parts per million; (|measured mean*m/z* - theoretical monoisotopic*m/z* | / theoreticalmonisotopic*m/z* * 10^6)

Supplemental Table 3. Phosphatidylethanolamine molecular species analyzed by MALDI-MSI

				Cross Section (H^+ Adducts)			Longitudinal Section (H^+ Adducts)			Cross Section (K^+ Adducts)			Longitudinal Section (K^+ Adducts)			Cross Section (Na^+ Adducts)			Longitudinal Section (Na^+ Adducts)		
Abbreviated Name	**Formula**	**Adduct(s)**	**Common Name[1,2]**	**$[M+H]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**$[M+K]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**$[M+Na]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**
LysoPE-16:0	C21H44O7PN	H^+, K^+, Na^+	PE(16:0/0:0)	454.293	454.297	0.006	7.3	454.292	0.009	3.4	492.249	492.247	0.007	3.8	492.249	0.011	1.2	476.275	476.275	0.005	1.2	476.274	0.011	2.2
LysoPE-18:3	C23H42O7PN	H^+, K^+, Na^+	PE(18:3/0:0)	476.278	476.275	0.005	5.4	476.277	0.012	2.2	514.234	514.226	0.009	14.9	514.229	0.012	9.5	498.260	498.256	0.009	6.7	498.262	0.011	4.6
LysoPE-18:2	C23H44O7PN	H^+, K^+, Na^+	PE(18:2/0:0)	478.293	478.293	0.002	1.0	478.292	0.008	2.3	516.249	516.248	0.007	1.5	516.248	0.012	1.7	500.275	500.275	0.004	1.5	500.275	0.013	1.5
LysoPE-18:1	C23H46O7PN	H^+, K^+, Na^+	PE(18:1/0:0)	480.309	480.309	0.007	0.8	480.309	0.011	1.0	518.265	518.270	0.012	10.4	518.263	0.012	3.9	502.291	502.294	0.011	6.4	502.292	0.011	2.8
PE-34:2	C39H74O8PN	H^+, K^+, Na^+	PE(18:2/16:0)	716.523	716.523	0.001	0.3	716.521	0.002	2.3	754.479	754.480	0.001	1.3	754.477	0.002	1.9	738.505	738.505	0.001	0.3	738.504	0.002	2.0
PE-34:1	C39H76O8PN	H^+, K^+, Na^+	PE(18:1/16:0)	718.539	718.536	0.006	4.4	718.536	0.007	4.1	756.495	756.493	0.008	1.9	756.493	0.008	1.8	740.521	740.524	0.002	4.1	740.522	0.003	1.3
PE-36:5	C41H72O8PN	H^+, K^+, Na^+	PE(18:3/18:2)	738.507	738.505	0.002	3.0	738.504	0.002	5.2	776.463	776.462	0.002	1.5	776.460	0.004	4.7	760.489	760.489	0.002	0.4	760.486	0.005	3.8
PE-36:4	C41H74O8PN	H^+, K^+, Na^+	PE(18:2/18:2)	740.523	740.524	0.002	0.8	740.522	0.003	1.9	778.479	778.480	0.001	1.7	778.477	0.003	1.9	762.505	762.505	0.002	0.2	762.503	0.003	2.1
PE-36:3	C41H76O8PN	H^+, K^+, Na^+	PE(18:2/18:1)	742.539	742.539	0.004	0.4	742.537	0.006	1.9	780.495	780.500	0.004	6.7	780.493	0.005	1.5	764.521	764.519	0.003	1.5	764.519	0.006	2.4
PE-36:2	C41H78O8PN	H^+, K^+, Na^+	PE(18:1/18:1, 18:2/18:0)	744.554	744.555	0.004	0.9	744.552	0.009	3.6	782.510	782.518	0.007	10.2	782.511	0.011	1.2	766.536	766.536	0.006	0.1	766.534	0.010	2.8
PE-36:1	C41H80O8PN	H^+, K^+, Na^+	PE(18:1/18:0)	746.570	746.572	0.007	2.6	746.573	0.013	3.7	784.526	784.532	0.005	7.6	784.524	0.011	2.2	768.552	768.554	0.005	2.7	768.550	0.011	2.7

[1] Determined from ESI-MS/MS and literature

[2]Fatty Acid Abbreviations: M-14:0 Myristic; P-16:0 palmitic; Po-16:1 palmitoleic, Ln-18:3 linolenic; L-18:2 linoleic; O-18:1 oleic acid; S-18:0 stearic; A-20:0 arachidic; B-22:0 behenic; Sc-19:1 sterculic; Dsc-19:0 dihydrosterculic acid

[3]PPM = parts per million; (|measured mean*m/z* - theoretical monoisotopic*m/z* | / theoreticalmonisotopic*m/z* * 10^6)

Supplemental Table 4. Phosphatidic acid molecular species analyzed by MALDI-MSI

				Cross Section (Na^+ Adducts)			Longitudinal Section (Na^+ Adducts)			Cross Section (K^+ Adducts)			Longitudinal Section (K^+ Adducts)		
Abbreviated Name	**Formula**	**Adduct(s)**	**Common Name[1,2]**	**$[M + Na]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**$[M + K]^+$ Theoretical monoisotopic *m/z***	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**	**Measured mean *m/z***	**Measured standard deviation *m/z***	**Mean error of measured vs. theoretical *m/z* (in ppm)[3]**
PA-34:3	C37H67O8P	K^+, Na^+	PA(16:0/18:3)	693.447	693.447	0.005	0.5	693.448	0.010	0.6	709.421	709.421	0.003	0.4	709.422	0.011	0.7
PA-34:2	C37H69O8P	K^+, Na^+	PA(16:0/18:2)	695.463	695.463	0.002	0.6	695.461	0.002	2.1	711.437	711.437	0.002	0.9	711.435	0.002	2.0
PA-34:1	C37H71O8P	K^+, Na^+	PA(16:0/18:1)	697.478	697.479	0.004	0.9	697.477	0.008	1.5	713.452	713.455	0.003	4.1	713.451	0.008	2.2
PA-36:5	C39H67O8P	K^+, Na^+	PA(18:3/18:2)	717.447	717.446	0.003	2.1	717.445	0.006	3.6	733.421	733.420	0.002	1.3	733.418	0.006	3.7
PA-36:4	C39H69O8P	K^+, Na^+	PA(18:2/18:2)	719.463	719.463	0.002	0.1	719.461	0.003	2.3	735.437	735.437	0.001	1.0	735.435	0.003	2.1
PA-36:3	C39H71O8P	K^+, Na^+	PA(18:2/18:1)	721.478	721.479	0.001	0.6	721.477	0.002	2.2	737.452	737.453	0.001	1.0	737.451	0.001	1.9
PA-36:2	C39H73O8P	K^+, Na^+	PA(18:1/18:1,18:2/18:0)	723.494	723.495	0.002	0.8	723.493	0.003	1.8	739.468	739.470	0.002	2.9	739.468	0.003	0.5

[1] Determined from ESI-MS/MS and literature

[2]Fatty Acid Abbreviations: M-14:0 Myristic; P-16:0 palmitic; Po-16:1 palmitoleic, Ln-18:3 linolenic; L-18:2 linoleic; O-18:1 oleic acid; S-18:0 stearic; A-20:0 arachidic; B-22:0 behenic; Sc-19:1 sterculic; Dsc-19:0 dihydrosterculic acid

[3]PPM = parts per million; (|measured mean *m/z* - theoretical monoisotopic *m/z* | / theoreticalmonisotopic *m/z* * 10^6)