Supplementary Information

Enhanced *in situ* detection and imaging of lipids in biological tissues by using 2,3-dicyanohydroquinone as a novel matrix for positive-ion MALDI-MS Imaging

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Supplementary Information--Experimental Section

Chemicals and Materials. 2,3-dicyanohydroquinone (DCH), 2,5-dihydroxybenzoic acid (DHB), 2,5-dihydroxyacetophenone (DHA), para-nitroaniline (PNA), 2,4-dinitrophenylhydrazine (DNPH), 2-mercaptobenzothiazole (2-MBT), α-cyano-4-hydroxycinnamic acid (CHCA), LC/MS-grade acetonitrile (ACN), methanol, ethanol, trifluoroacetic acid (TFA), formic acid (FA), and hematoxylin and eosin (H&E) staining solutions were purchased from Sigma-Aldrich (St. Louis, MO). One lipid standard compound of PC(16:0/18:2) was purchased from Avanti Polar Lipids, Inc. (Birmingham, AL). Ultrapure water used throughout the experiment was obtained from a Milli-Q system (Millipore, Milford, MA). Germinating Chinese-yew seeds were collected from Jiujiang city, Jiangxi Province, China, in November 2016. Camelina seeds were purchased from ExportGrain Corp. Ltd (Hei Longjiang, China). An 8-week-old adult male Sprague-Dawley rat was purchased from Shanghai Super-B&K laboratory animal Corp. Ltd (Shanghai, China) for rat liver harvest, and a 6-week-old male Kunming mouse was purchased from National Institutes for Food and Drug Control (Beijing, China) for mouse brain obtaining. For tissue frozen, all the harvested animal organs were slowly immersed into liquid nitrogen to avoid shattering, and then stored at -80 °C until use. All of the animal organs used in this study were approved by the Ethics Committee of College of Life and Environmental Sciences, Minzu University of China.

UV-Vis Absorption Spectroscopy. Ultraviolet-visible (UV-Vis) absorption spectra of DCH, DHB, PNA, DNPH, 2-MBT, and CHCA solutions at the concentration of 2×10^{-5} mol/L were acquired on a UV-vis spectrometer (TU-1901, Jasco, Japan). For preparation of these solutions, 0.0320 g of DCH was dissolved in 1 mL solvent of ACN/H_2O/TFA (90:10:0.3, v/v/v), 0.0308 g of DHB was dissolved in 1 mL solvent of methanol/H_2O/TFA (80:20:0.1, v/v/v), 0.0276 g of PNA was dissolved in 1 mL solvent of methanol/H_2O/TFA (85:15:0.1, v/v/v), 0.0396 g of DNPH was dissolved in 1 mL solvent of ACN/H_2O/TFA (50:50:0.1, v/v/v), 0.0334 g of 2-MBT was dissolved in 1 mL solvent of methanol/H_2O/TFA (80:20:0.1, v/v/v), and 0.0378 g of CHCA was dissolved in 1 mL solvent of methanol/H_2O/TFA (85:15:0.1, v/v/v). These matrices solutions were then diluted to the final concentration of 2×10^{-5} mol/L with the corresponding solvents. The wavelength scanning range from 250 to 500 nm was used for UV-vis absorption spectrum acquirement.

Optimization of Matrix Solution Composition. To establish the optimal DCH matrix solution, L9 (3^3) orthogonal array testing was carried out. According to previously studies,[1,2] the concentration of DCH, the % ACN, and the % TFA were used as the three variables for the optimization of matrix DCH solution. For each variable, three levels were chosen for the matrix optimization. The concentrations of DCH were prepared at 8, 10, and 12 mg/mL; the % ACN was prepared at 70%, 80%, and 90% in H_2O; the % TFA was prepared at 0.1%, 0.2 %, and 0.3%. Serial parallel-sectioned tissue slices (12-μm thickness) of homogeneous rat liver were used for the DCH matrix optimization.

Chemical Stability Evaluation. For the preparation of the matrix solutions, DCH was prepared at the optimal concentration of 10 mg/mL in ACN/H_2O/TFA (90:10:0.3, v/v/v), DHB was prepared at 10 mg/mL in 80:20 (v/v) methanol/H_2O containing 0.1% TFA, and DHA at a concentration of 10 mg/mL was dissolved in 50:50 (v/v) ethanol/H_2O containing 0.05% TFA. An air-brush sprayer (model 200, Badger Air-brush) was used for the matrix coating. Each matrix solution was sprayed for a total of 45 cycles (5 s of spraying and 60 s of drying time) on the surfaces of a clean glass slide (2.5×2.5 cm) and rat liver tissue section. After air-drying in a vented fume hood, three matrix-coated glass slides were loaded into and kept inside the high-vacuum MALDI ion source ($\sim10^{-}$

^{7} mbar) with a modified standby mode (the high voltage on target plate is switched off, and the UV laser in MALDI source is in a non-excited state) for chemical stability evaluation. Optical images of matrix-coated glass slides were captured using an Epson Perfection V550 Photo Flatbed Scanner (Epson, Suwa, Japan) at different time points during vacuum-storage (*i.e.*, 0, 4, 8, 16, 24, 32, 40, and 48 h). Subsequently, optical images of these matrix-coated glass slides were also taken after the atmospheric pressure storage at room temperature for 5, 10, 20, and 30 days. Meanwhile, all the weights of these matrix-coated glass slides at each storage time point were also measured with an electronic balance (MS105DU, Mettler-Toledo, USA). Microscopic images of dried DCH, DHB, PNA, DNPH, 2-MBT, and CHCA matrix particles formed by spraying were captured with a Nikon ECLIPSE Ti2-E inverted microscope (Nikon, Tokyo, Japan) under three different magnifications (10×, 20×, and 60×).

Quantitative Analysis of PC(16:0/18:2) Standard using DCH as the MALDI Matrix. A series of standard solutions of PC(16:0/18:2) with twenty-eight different concentrations in the range from 0.0 to 6.0 μg/μL were prepared in H_2O containing 0.1% TFA for quantitative evaluation for the use of DCH as the MALDI matrix. The detail concentrations of these solutions are 0.0, 0.0002, 0.0004, 0.0006, 0.0008, 0.001, 0.002, 0.004, 0.006, 0.008, 0.01, 0.02, 0.04, 0.06, 0.08, 0.1, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 4.0, and 6.0 μg/μL. DCH was dissolved at the optimal concentration of 10 mg/mL in 90% aqueous ACN containing 0.3% TFA. Before MS analysis, 1 μL of the series PC(16:0/18:2) standard solutions were spotted onto a MTP Anchorchip 384-well target plate (Bruker Daltonics, Billerica, MA) for air-drying at room temperature (25 ^{o}C), and then 1 μL of DCH matrix solution was added onto each air-dried PC(16:0/18:2) standard solution spot. After air-drying in a vented fume hood, quantitative detection were performed using an Autoflex Speed MALDI TOF/TOF mass spectrometer equipped with a 2000 Hz solid-state Smart beam Nd:YAG/355 nm UV laser (Bruker Daltonics, Billerica, MA). The Microsoft Excel 2016 was used for the construction of linear regression plots by plotting the peak intensities of the target standard compound of PC(16:0/18:2) versus the concentrations of the standard solutions.

Tissue Sectioning. All the selected fresh frozen tissues, including rat liver, mouse brain, camelina seed, and germinating Chinese-yew seed, were cryo-sectioned into 12 μm thickness slices with a Leica CM1860 cryostat (Leica Microsystems Inc., Wetzlar, Germany) at the chamber temperature of -20 °C, and then these serial cryo-sectioned tissue slices were immediately thaw-mounted on the indium tin oxide (ITO)-coated microscope glass slides purchased from Bruker Daltonics (Bremen, Germany).

Matrix Coating. DCH was prepared at the optimal concentration of 10 mg/mL in ACN/H_2O/TFA (90:10:0.3, v/v/v). DHB at a concentration of 25 mg/mL was prepared in 80:20 methanol/H_2O containing 0.1% TFA. 2-MBT at a concentration of 12 mg/mL was prepared in 80:20 methanol/H_2O containing 2% FA. CHCA at a concentration of 20 mg/mL was prepared in 85:15 methanol/H_2O containing 0.1% TFA. DNPH at a concentration of 4 mg/mL was prepared in 50:50 ACN/H_2O containing 0.1% TFA. PNA at a concentration of 20 mg/mL was prepared in 85:15 methanol/H_2O containing 0.1% TFA. Two standard peptide solutions, including Bradykinin 1-7 (*m/z* 757.40, 900 ng/ml) and Angiotensin II (*m/z* 1046.54, 750 ng/ml), were added to each above mentioned matrix solution for the lipid *in situ* analysis on tissue sections. Bradykinin 1-7 and Angiotensin II signal ions were used in combination with the matrix ions of $[M+H]^+$ as the internal standard to calibrate and improve the accuracy of the detectable lipid ion signals. For matrix deposition, all the matrix solutions were coated onto the surface of the rat liver, mouse brain, camelina seed, and germinating Chinese-yew seed tissue sections using a Badger Air-brush sprayer (model 200, Franklin Park, IL). Forty-five cycles (2s spray, 30s incubation and 60s drying time) were carried out for matrix coating. After matrix drying, optical images of the matrix-coated tissue sections were captured by using an Epson Perfection V550 Photo Scanner (Epson, Suwa, Japan).

MALDI-MS. The MALDI-MS measurements were performed in positive-ion reflection mode on an Autoflex Speed MALDI-TOF/TOF mass spectrometer (Bruker Daltonics, Billerica, MA). For MALDI-MS profiling, all mass spectra were acquired over the mass range from 100 to 1700 Da, and recorded by accumulating 200 scans at 500 laser shots per scan. Each spectrum was acquired by applying the optimized laser power for each matrix, in the range of 45% to 55% of the full scale of the Nd:YAG UV laser power with a global attenuator offset of 20%, which is ca. 1.6 mJ per pulse according to the manufacturer's product specification. Thus, 45% to 55% of the full scale of the Nd:YAG UV laser power with a global attenuator offset of 20% is equivalent to 720 to 880 μJ per laser shot. MS images of endogenous lipids in mouse brain and germinating Chinese-yew seed were obtained over a window of *m/z* range from 500 to 1100 at a spatial resolution of 100 μm with 500 laser shots per position. For MALDI-MS data acquisition, a mixed standard solution, including Bradykinin 1-7 ($[M+H]^+$, *m/z* 757.40), Angiotensin II ($[M+H]^+$, *m/z* 1046.54), Angiotensin I ($[M+H]^+$, *m/z* 1296.68), Substance P ($[M+H]^+$, *m/z* 1347.74), and Bombesin ($[M+H]^+$, *m/z* 1619.82), was used for external mass calibration. The matrix ions of DCH ($[M+H]^+$, *m/z* 161.03), DHB ($[M+H]^+$, *m/z* 155.03), 2-MBT ($[M+H]^+$, *m/z* 167.99), CHCA ($[M+H]^+$, *m/z* 190.05), DNPH ($[M+H]^+$, *m/z* 199.05), and PNA ($[M+H]^+$, *m/z* 139.05), were chosen in combination with two standard compound ions of Bradykinin 1-7 ($[M+H]^+$, *m/z* 757.40) and Angiotensin II ($[M+H]^+$, *m/z* 1046.54) for internal mass calibration. The cubic enhanced mode was chosen for both external and internal mass calibration processing.

Data Analysis. According to previous studies,[1, 3, 4] *FlexAnalysis* 3.4 software (Bruker Daltonics) was used for the MALDI-MS profiling data viewing and processing, such as peak alignment, batch internal mass calibration, monoisotopic "peak picking", and so on. The lipid ions were manually characterized by matching experimental precursors with theoretical values for parent ion spectra and experimental fragment ions with theoretical ones in MS/MS. Three databases, including METLIN (https://metlin.scripps.edu/), LIPID MAPS (www.lipidmaps.org), and LipidBlast (https://fiehnlab.ucdavis.edu/), were used for the lipid entity matching, within an allowable mass error of ±10 ppm. Three ion adduct forms of $[M+H]^+$, $[M+ Na]^+$, and $[M+K]^+$ were considered during the database searching in the positive-ion mode. *FlexImaging* 4.1 software (Bruker Daltonics) was used to reconstruct the ion maps of the detected lipids, with an allowable mass filter width of 10 ppm.

Histological Staining. After MALDI-MSI experiments, the same tissue sections were sequentially washed with 70%, 90%, and 100% methanol solutions to remove the matrix, and then hematoxylin and eosin (H&E) staining was performed to obtain standard histological optical images, according to a previously study.[5]

Lipids Extraction. Based on the previous reported procedure,[1,3,4] lipids were extracted from serial parallel-sectioned tissue slices (total ca. 250 mg, and 25 μm thickness for each tissue slice) of the same samples (rat liver, mouse brain, camelina seed, germinating Chinese-yew seed) which were used for MALDI profiling or imaging. Briefly, each tissue sample was added into five clean 2-mL Eppendorf tubes and homogenization was carried out by adding 200 μL H_2O in each Eppendorf tube with four 5 mm stainless steel balls on a Precellys 24 tissue homogenizer (Bertin Technologies, France) for 60 s × 3. Next, 800 μL of a mixed chloroform/methanol (1:3, v/v) solvent was added in each Eppendorf tube and the solution was homogenized for another 30 s. The vibrating frequency was set as 30 Hz during homogenization process. The tubes were then centrifuged at 10,000 × g in an Eppendorf 5430 R centrifuge (Hamberg, Germany) for 20 min at the temperature of 4 °C. The organic phase layer (chloroform layer) was carefully collected into a new 2-mL Eppendorf tube and then dried in the Savant SPD111 SpeedVac concentrator (Thermo Scientific, Waltham, USA) at 4 °C. The dried lipid sample was dissolved in 500 μL of 50% ACN with 10-min ultrasonic treatment. Finally, the lipid solution was filtered using 0.22 μm filter membrane for the following LC-MS/MS analysis.

LC-MS/MS Data Acquisition and Analysis. The structural confirmation of most of the detected mass-matched lipid compounds was accomplished by LC/MS/MS analysis. A Waters ACQUITY UPLC system coupled online to an Orbitrap Fusion Lumos Tribrid mass spectrometer (Thermo Fisher Scientific, Bremen, Germany), equipped with an ESI source was used. The mobile phase consisted of 0.01% formic acid in water (solvent A) and 0.01% formic acid in ACN/isopropanol (1:1) (solvent B) for binary gradient elution. An elution gradient of 5% to 45% B in 5 min; 45% to 100% B in 15 min and 100% B for 2 min was used to separate the lipids on a Waters BEH C8 column (2.1 × 50 mm, 1.7 μm) with the flow rate of 0.35 mL/min and a column temperature of 45 °C before the next injection. The FTMS detection mode was set at a mass resolution of 15,000 FWHM (*m/z* 400) for LC-MS survey scan data within a mass range of *m/z* 30 to 2000. MS/MS experiments on the top 5 most abundant ions in the survey scan were performed using collision-induced dissociation (CID) at a normalized collision energy of 30%. The automatic gain control and the time limit for each ion injection were 2×10^5 ion counts, and 100 ms in the ion trap. During the MS/MS data acquisitions, dynamic exclusion was applied with an ion exclusion time of 15 s. the assignment of the lipids was obtained by comparison of the acquired MS/MS spectra with those in the standard MS/MS libraries of the METLIN, HMDB, or LIPID MAPS database, with the aid of some manual spectral interpretation.

Supplementary Information--Results and Discussion

A 355 nm Nd:YAG ultraviolet (UV) laser was installed on the MALDI-TOF/TOF mass spectrometer used in this study, and UV absorption is a prerequisite for any new MALDI matrix screening.[2] The UV absorption spectra of DCH, DHB, PNA, DNPH, 2-MBT, and CHCA were first measured by an UV-vis spectrometer (Fig. S1). As shown, DCH shows the strongest UV absorption at 355 nm, indicating that DCH has the potential for use as a new MALDI matrix for lipid *in situ* detection and MSI studies.

Supplementary Information Figures

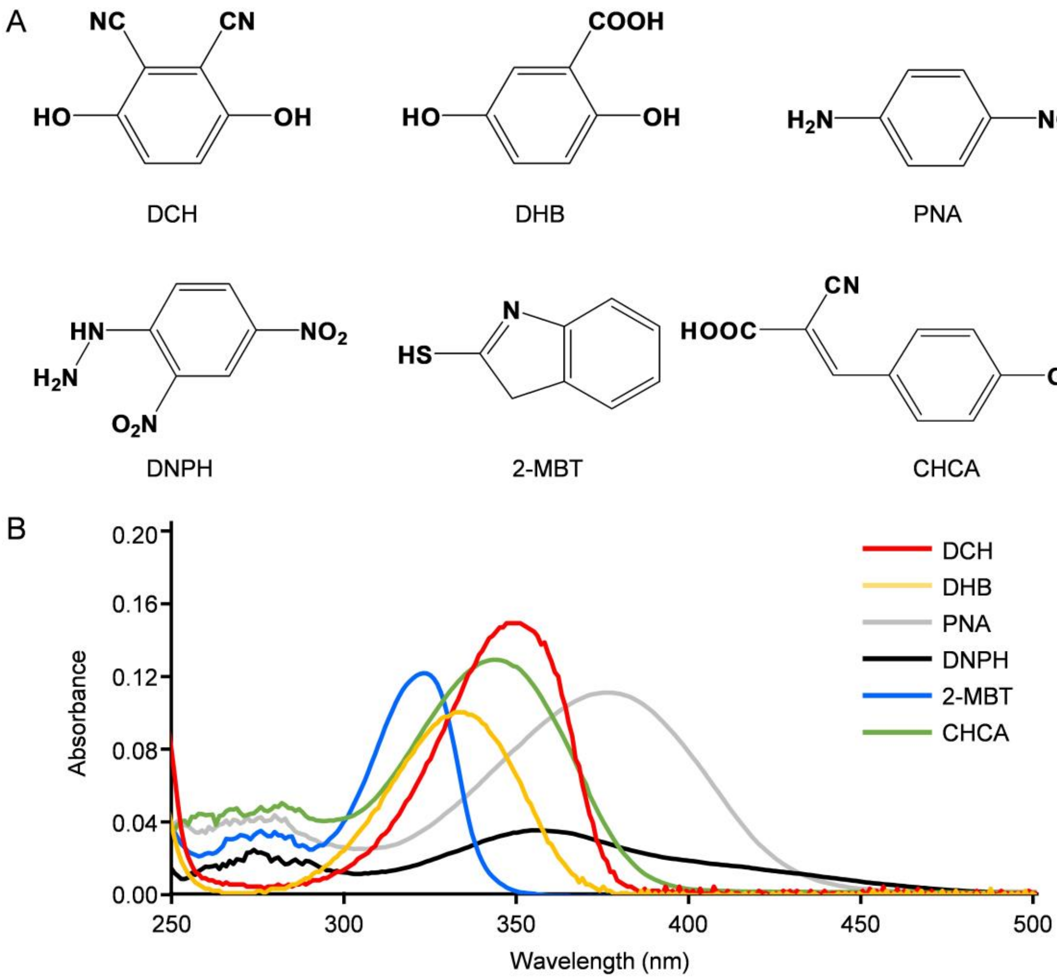


Fig. S1 Chemical structures (A) and the corresponding UV-vis absorption spectra (B) of the DCH, DHB, 2-MBT, CHCA, DNPH, and PNA matrices.

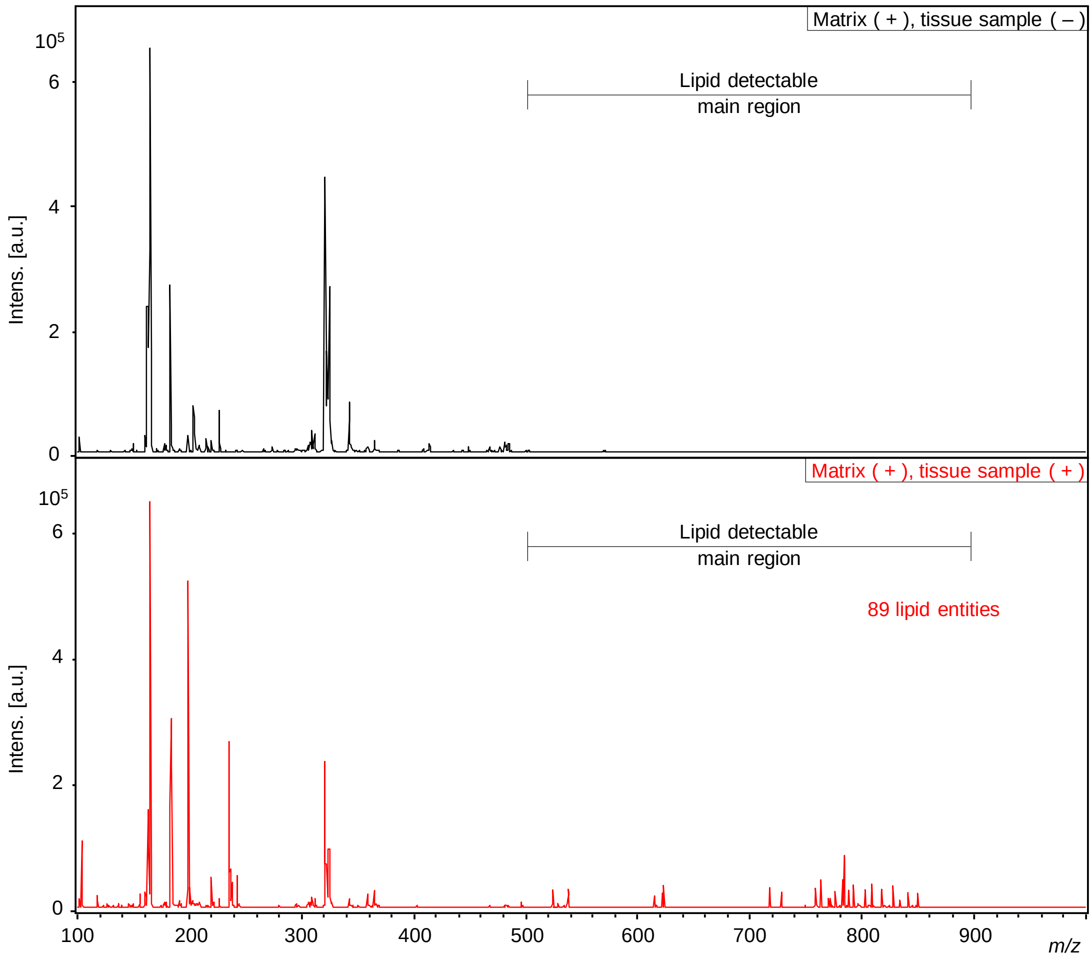


Fig. S2 Comparison of mass spectra acquired using DCH as the matrix from the laser irradiation of glass slides coated with (red) and without (black) tissue sections of the same rat liver by MALDI-TOF MS in the positive detection ion mode. The matrix solution containing 8 mg/mL DCH, prepared in 70% ACN solution containing 0.1% TFA, without optimization.

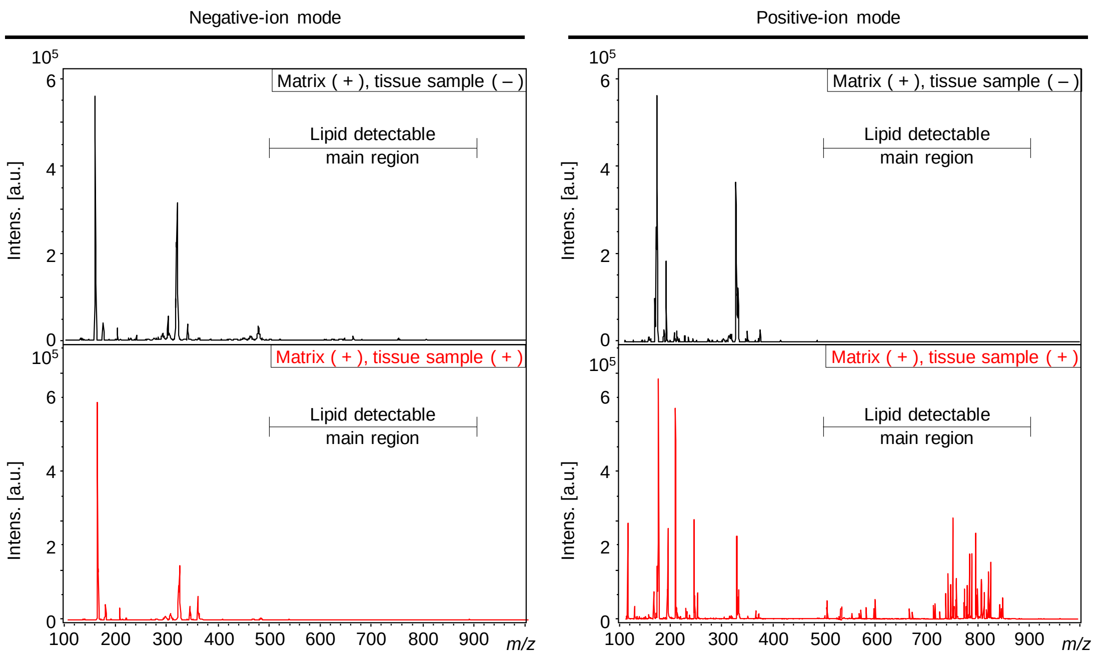
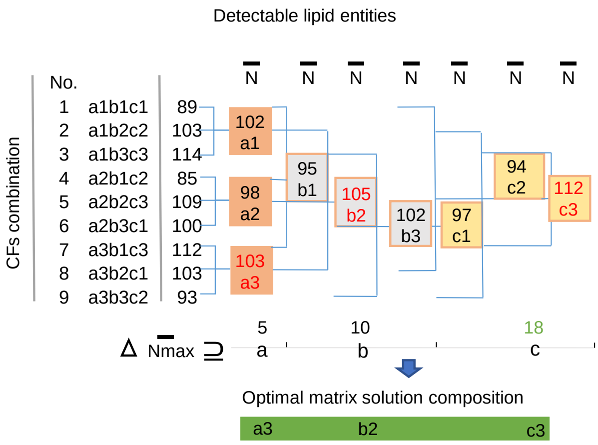


Fig. S3 Comparison of mass spectra acquired from UV laser irradiation of glass slides coated with (red mass spectra) and without (black mass spectra) rat liver tissue sections of the same by MALDI-TOF MS in both positive (right) and negative (left) ionization modes using DCH as the matrix. The optimized matrix solution, containing 10 mg/mL DCH, prepared in 90% ACN solution containing 0.3% TFA, was prepared for these detections.

A

Components	Concentration factors (CFs)		
ACN (%)	70.0 (a1)	80.0 (a2)	90.0 (a3)
DCH (mg/ml)	8.0 (b1)	10.0 (b2)	12.0 (b3)
TFA (%)	0.1 (c1)	0.2 (c2)	0.3 (c3)

B



C

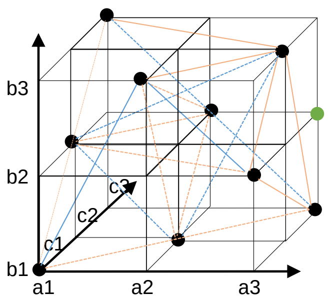


Fig. S4 Orthogonal array testing for the optimization of DCH matrix solution compositions. Three variables (% of ACN in water, DCH concentration, and % of TFA) and three levels of each variable were tested. The numbers of detected lipids were the average numbers from nine independent detection results (n=3*3).

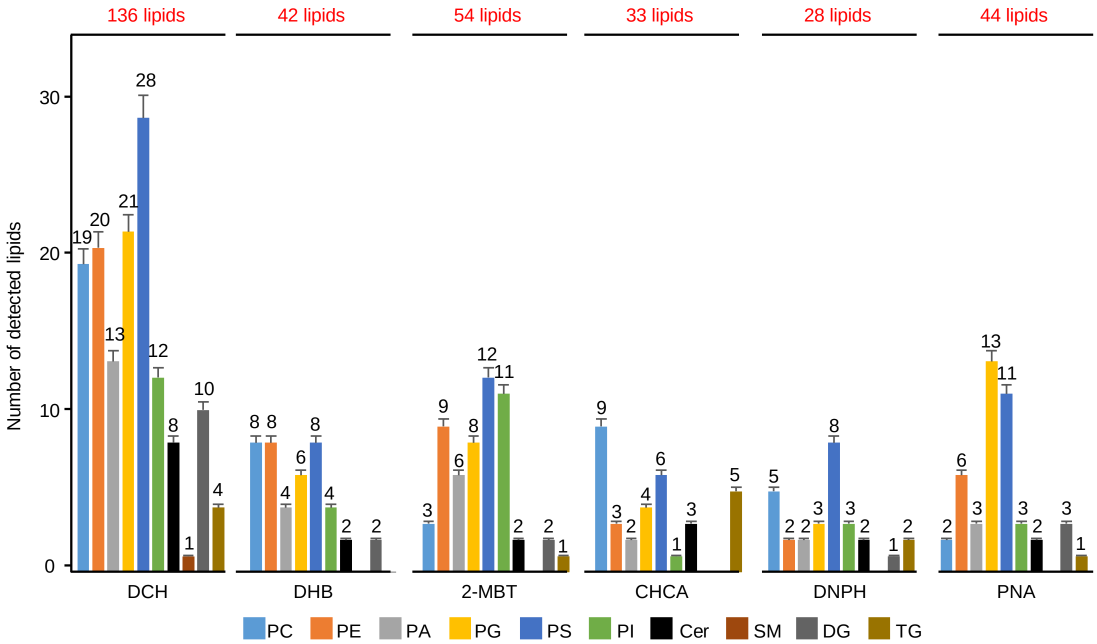


Fig. S5 Bar graphs showing the number of lipid species detected from the rat liver tissue sections by MALDI-TOF MS in the positive-ion mode using DCH, DHB, 2-MBT, CHCA, DNPH, and PNA as the matrices.

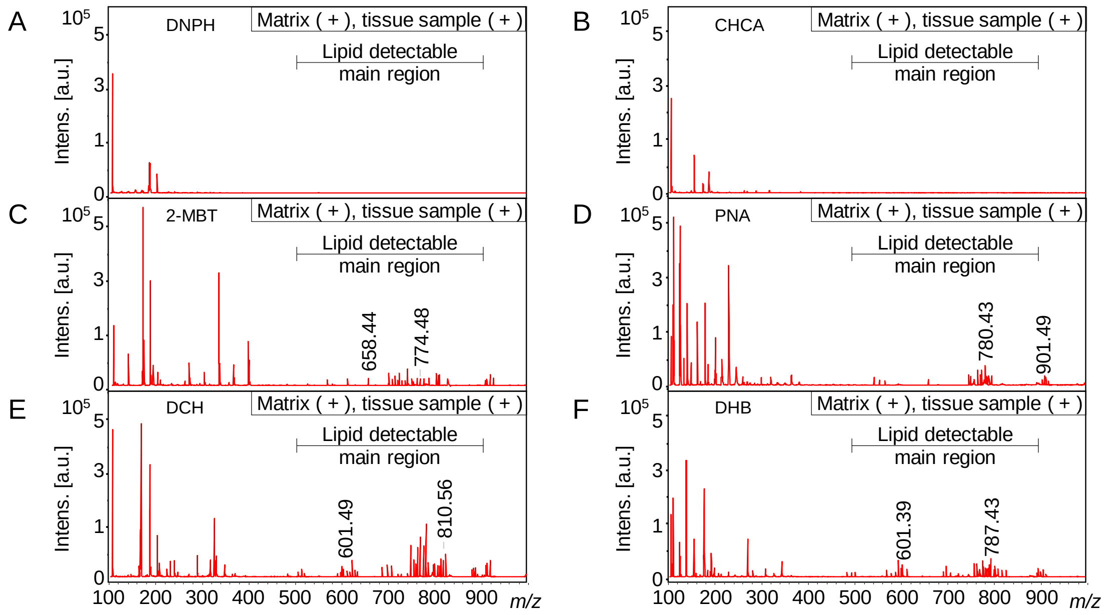


Fig. S6 Comparison of mass spectra acquired using DNPH (A), CHCA (B), 2-MBT (C), PNA (D), DCH (E), and DHB (F) as the matrices from laser irradiation of serial 12-μm tissue sections of the same camelina seed by MALDI-TOF/TOF MS.

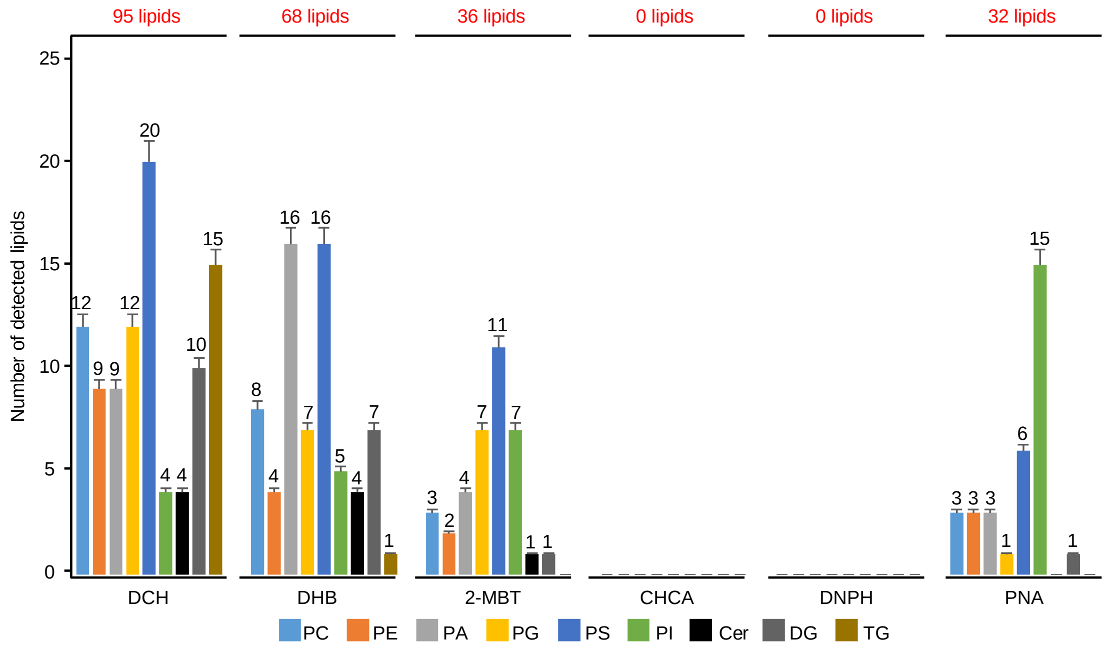


Fig. S7 Bar graphs showing the number of lipid species detected from the camelina seed tissue sections by MALDI-TOF MS in the positive-ion mode using DCH, DHB, 2-MBT, CHCA, DNPH, and PNA as the matrices.

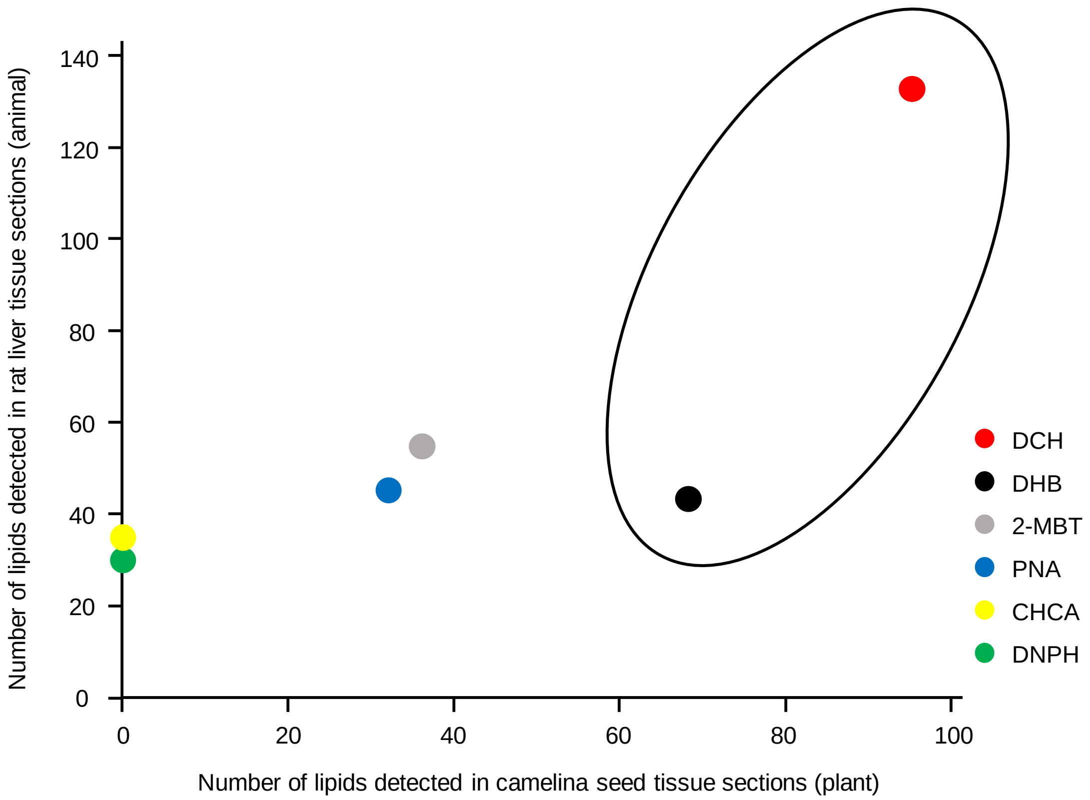


Fig. S8 Scatter diagram showing the total number of lipids detected from the rat liver and camelina seed tissue sections by MALDI-TOF MS in the positive-ion mode using DCH, DHB, 2-MBT, CHCA, DNPH, and PNA as the matrices.

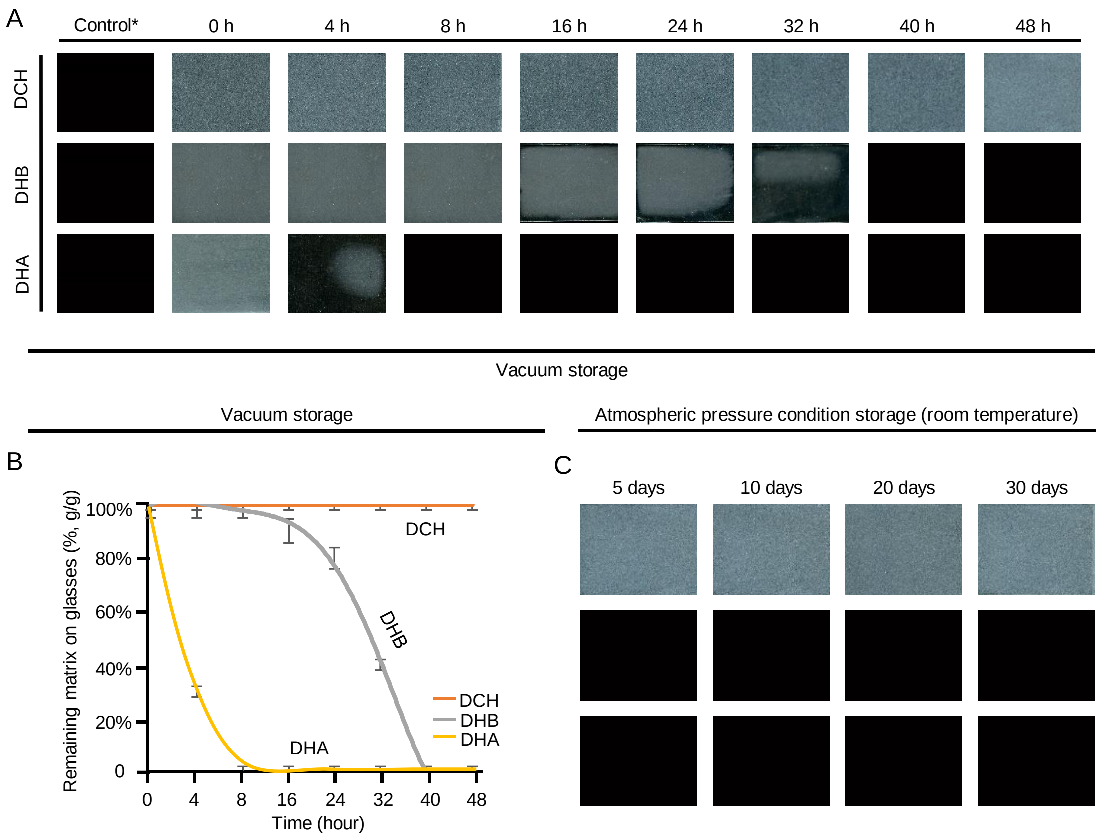


Fig. S9 (A-C) Comparison of chemical stability of three different matrices of DCH, DHB, DHA kept in the high vacuum MALDI ion source (~10^{-7} mbar) and atmospheric pressure condition with different storage times. The optical images of matrix-coated glass slides were captured with an Epson Perfection V550 Photo Scanner. The “control” labeled with asterisk means clean glass without coated matrix.

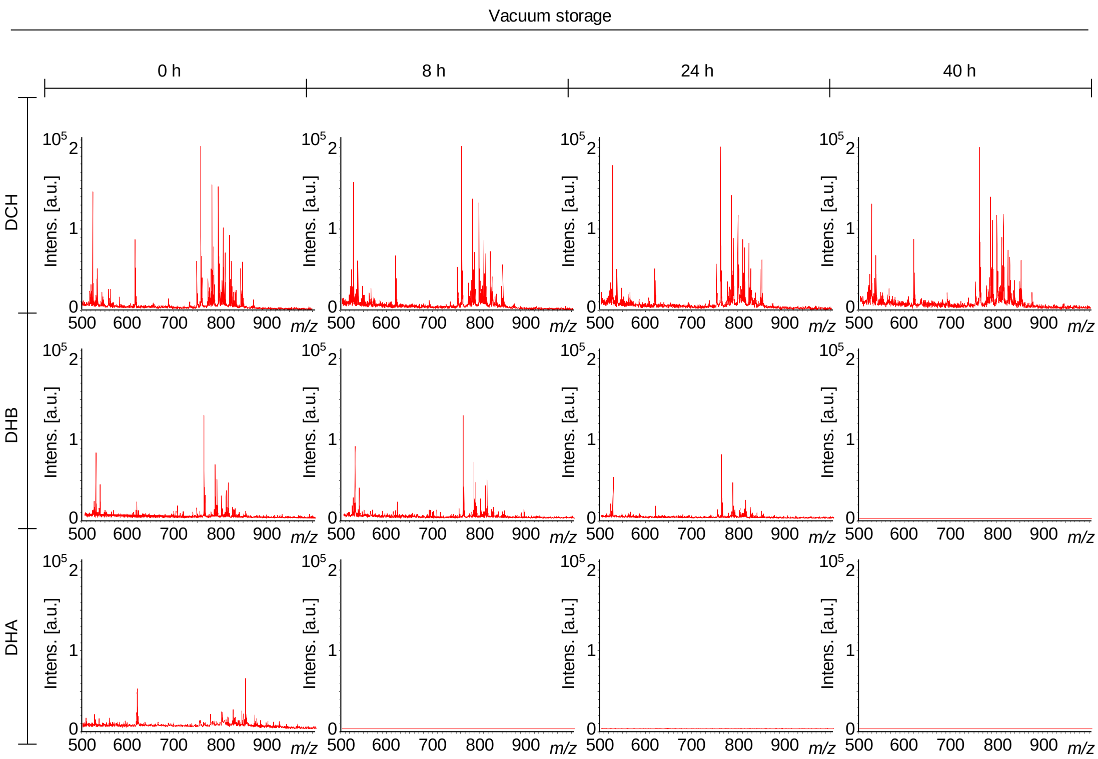


Fig. S10 Comparison of mass spectra of lipids detected in three matrix-coated rat liver tissue sections with different high-vacuum storages (0, 8, 24, and 40 h) by MALDI-TOF MS. DCH, DHB, and DHA were used for rat liver tissue section matrix-coating, respectively.

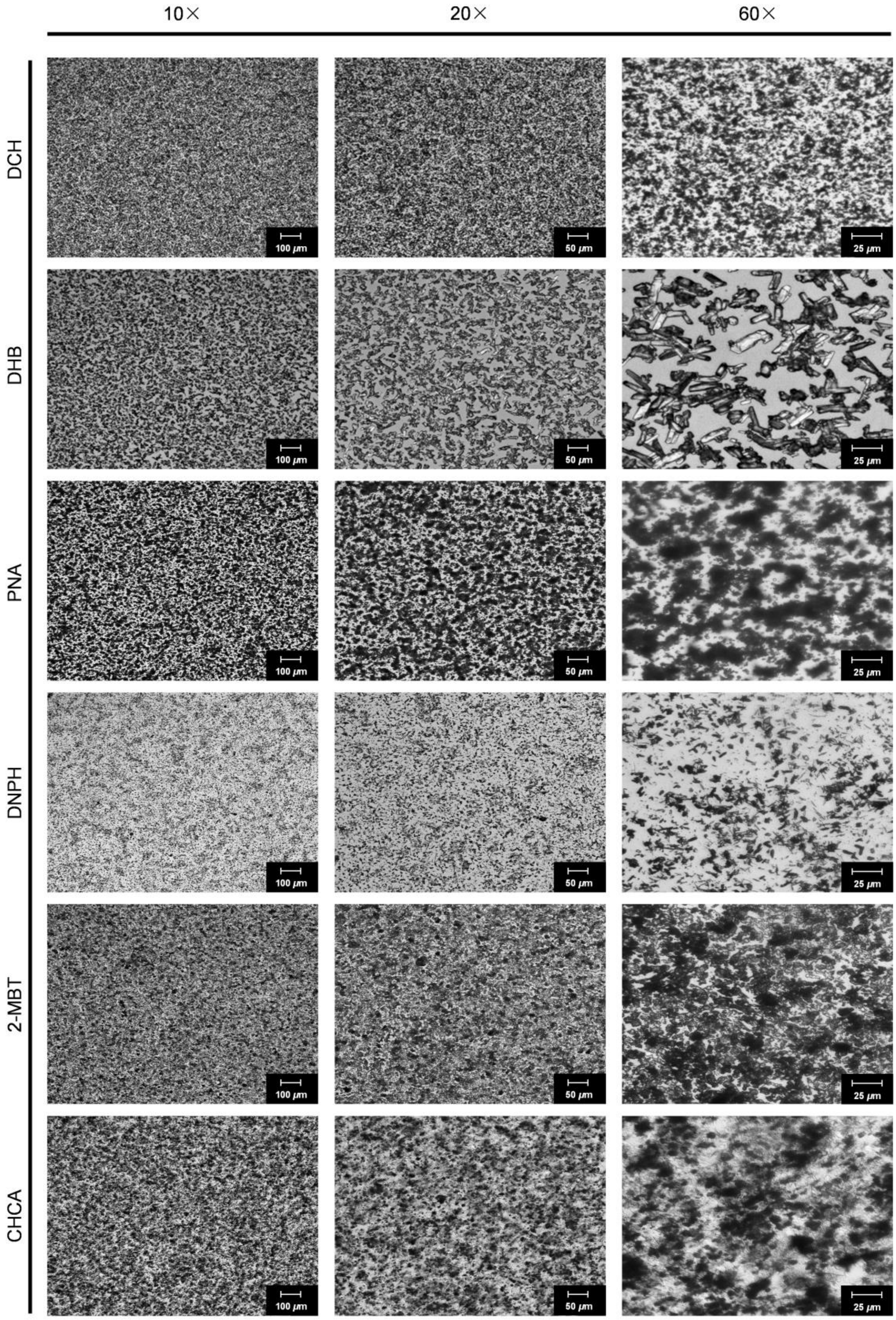


Fig. S11 Comparison of the morphologies of matrix crystals of DCH, DHB, PNA, DNPH, 2-MBT, and CHCA coated on glass slides. A Nikon ECLIPSE Ti2-E inverted microscope was used for microscopic images acquiring under 10×, 20×, 60× magnification.

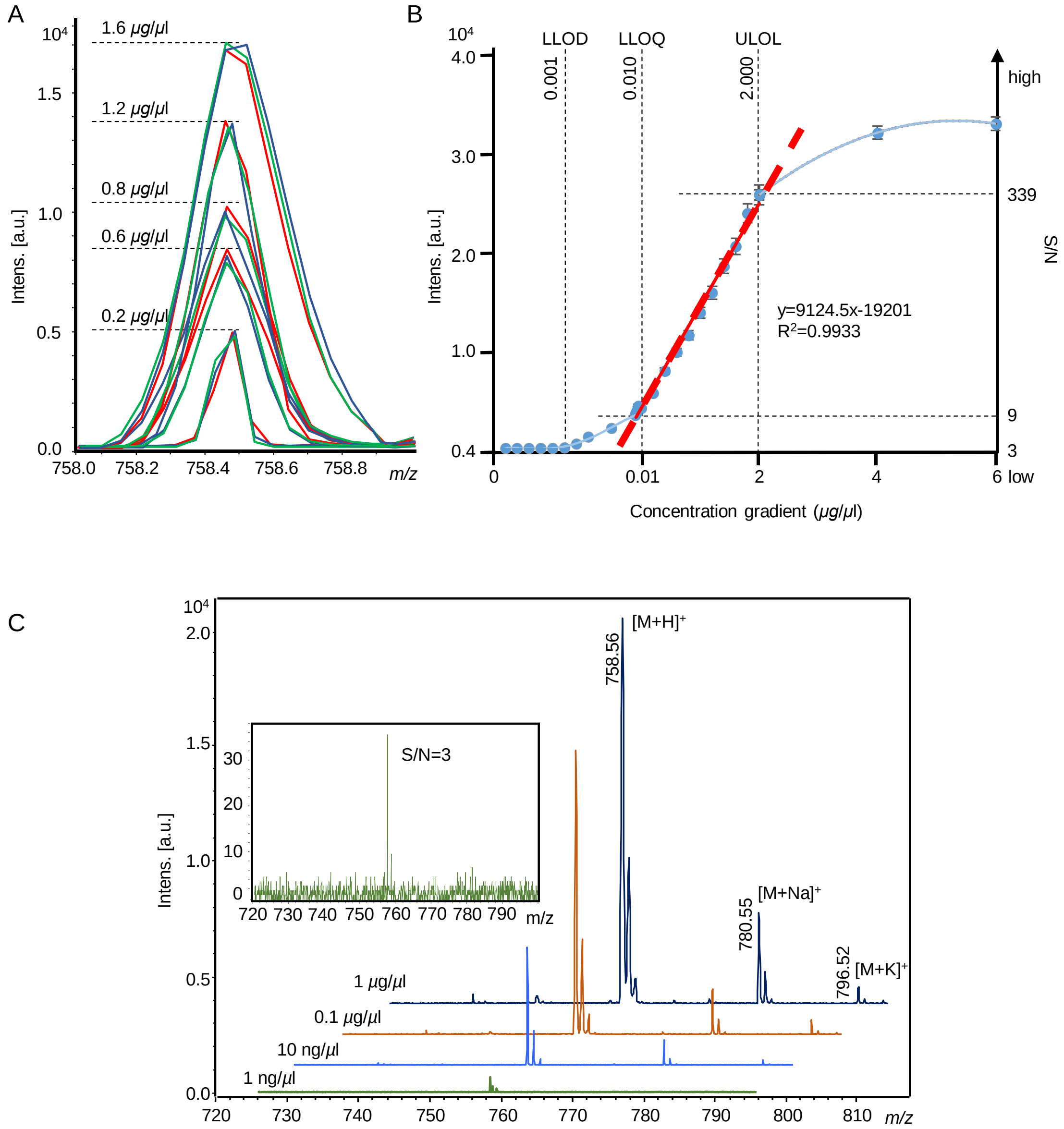


Fig. S12 Quantitative performance of PC(16:0/18:2) standard measured by MALDI-TOF MS using DCH as the matrix in the positive-ion mode. (a) Selected mass spectra showing the quantitative analysis of PC(16:0/18:2) standard with different concentrations by MALDI-TOF MS using DCH as the matrix in positive ion mode. (b) Dynamic range of linearity for detection of PC(16:0/18:2) standard. Three independent experiments and three replicates were carried out (n=3*3) to obtain the generation of quantitative standard curve of PC(16:0/18:2) standard. (c) LLOD of PC(16:0/18:2) standard. Abbreviations: LLOD, lower limit of detection; LLOQ, lower limit of quantitation; ULOL, upper limit of linear response.

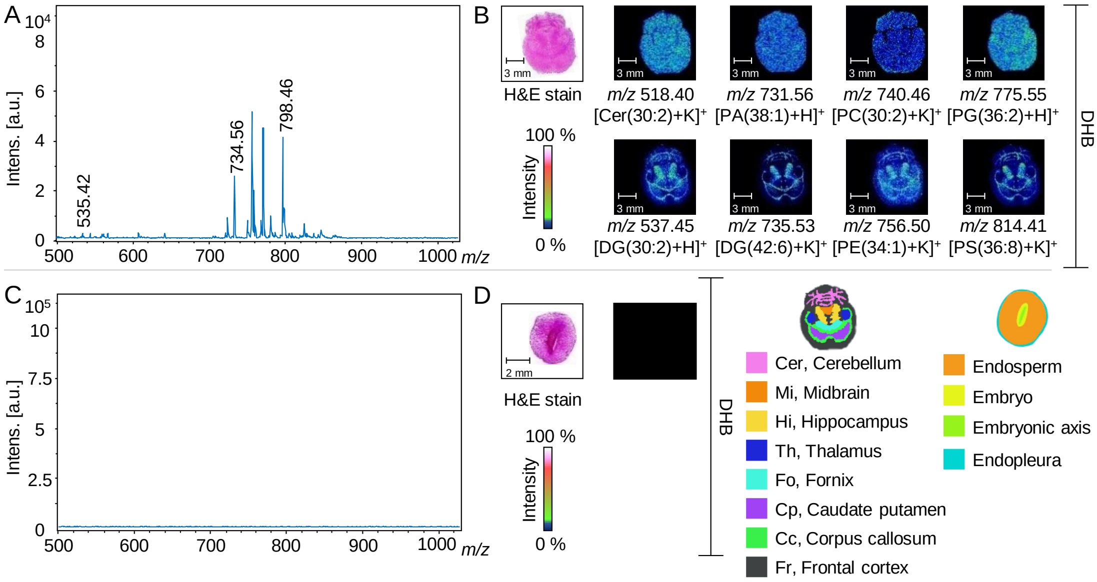


Fig. S13 Mass spectra (A and C) and the selected ion maps of lipids (B and D) detected from mouse brain and germinating Chinese-yew seed tissue sections by MALDI-TOF/TOF MS in the positive-ion mode using DHB as the matrix. The black square represents no lipid ion images were collected by using DHB as a matrix. The H&E stained image was obtained from the same tissue section after MSI. MS imaging was acquired at 100 μm spatial resolution.

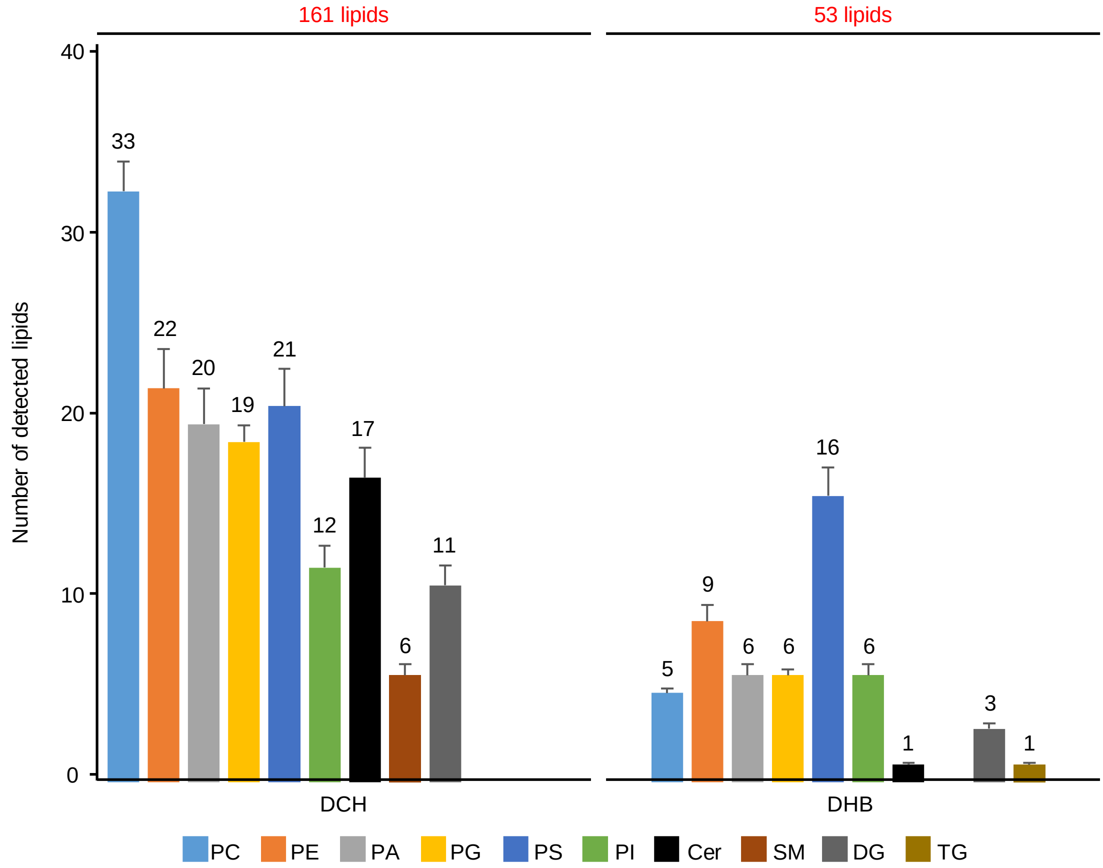


Fig. S14 Comparison of the number of lipid entities detected on the mouse brain tissue sections by MALDI-TOF MS in the positive-ion mode using DCH and DHB as the matrices.

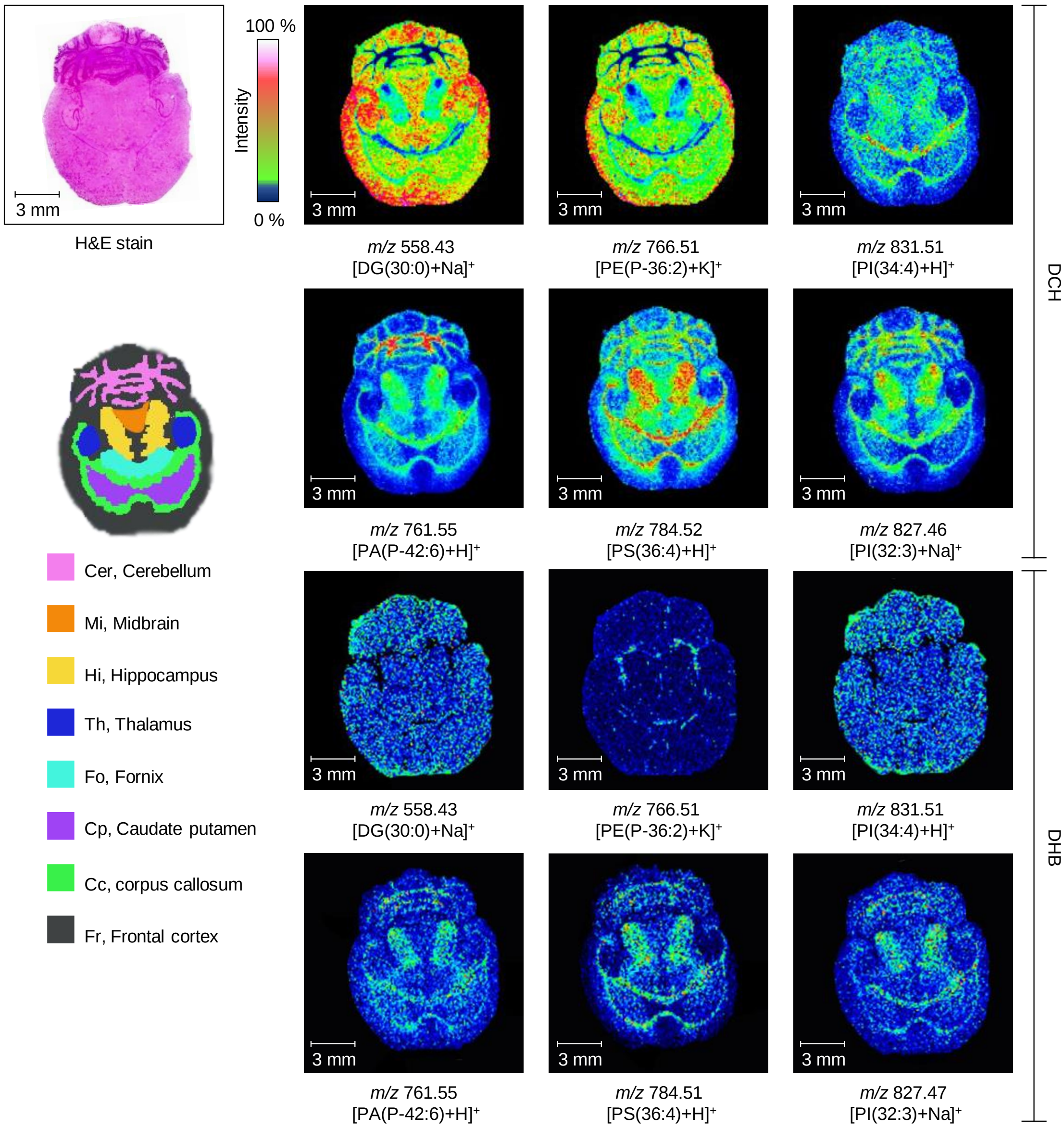


Fig. S15 Comparison of the selected ion maps of lipids detected on a 12 μm mouse brain tissue section by MALDI-TOF MS in the positive-ion mode using DCH and DHB as the matrices. The MS imaging was acquired at 100 μm spatial resolution.

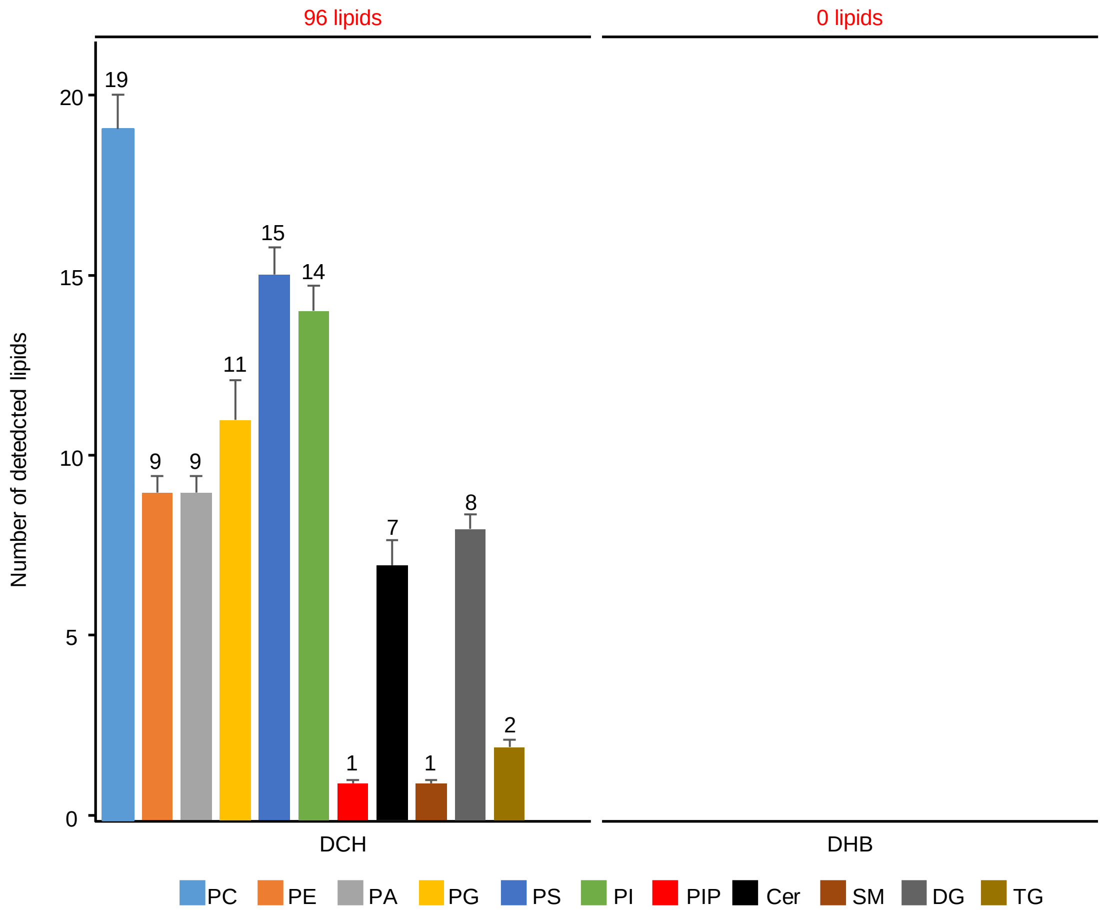


Fig. S16 Comparison of the number of lipid entities detected on the germinating Chinese-yew seed tissue sections by MALDI-TOF MS in the positive-ion mode using DCH and DHB as the matrices.

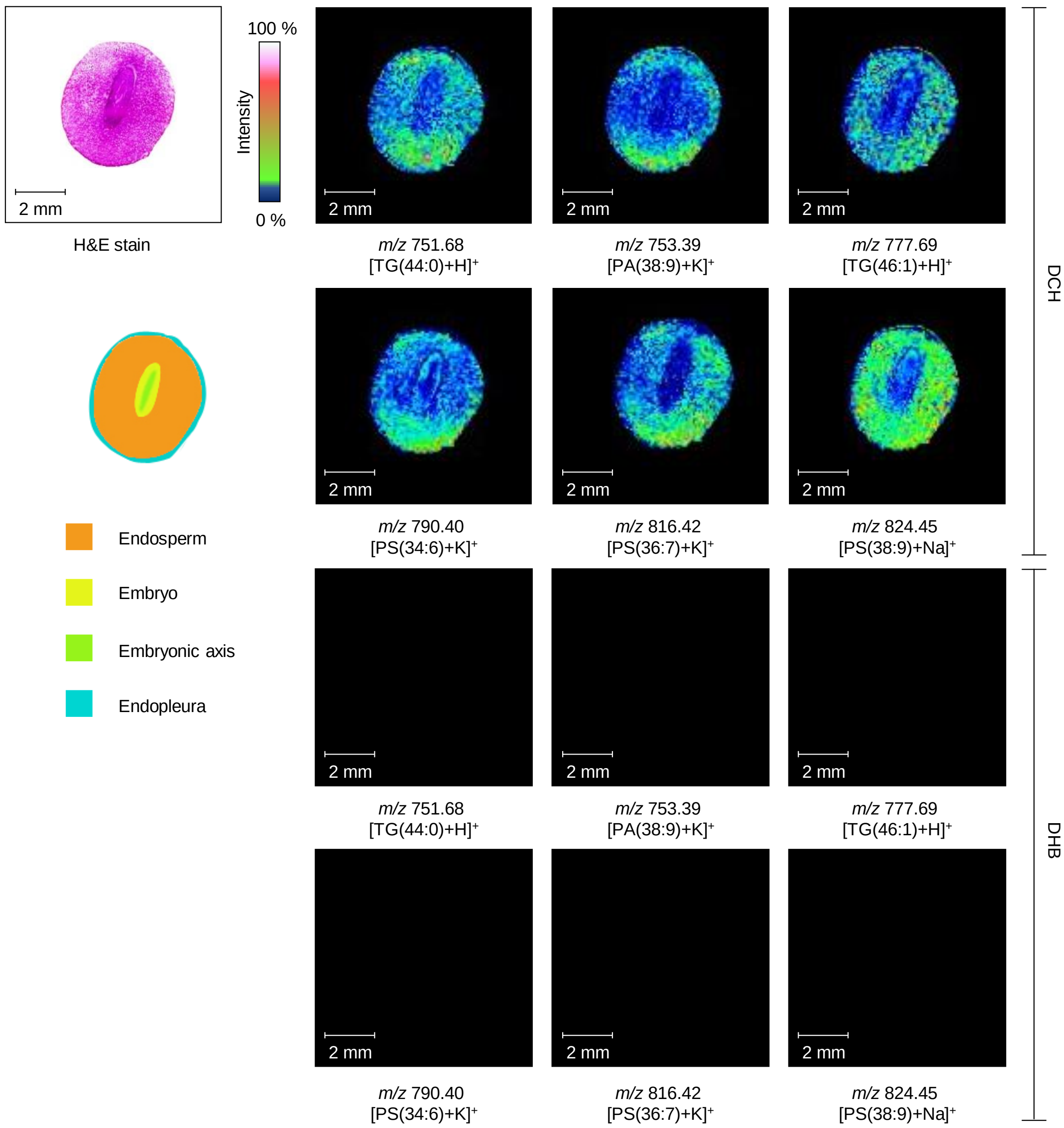


Fig. S17 Comparison of the selected ion maps of the lipids detected on a 12-μm germinating Chinese-yew seed tissue section by MALDI-TOF MS in the positive-ion mode using DCH and DHB as the matrices. The MS imaging was acquired at 100 μm spatial resolution.

Table S1. Lipids detected and identified in the rat liver tissue sections by MALDI-TOF MS in the positive-ion mode using DCH as the matrix.

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment: Ion form	Assignment: Compound	Assignment: Molecular formula	Ref.	Structurally specific CID ions (m/z)a)
1	503.25	503.2534	7	$[M+K]^+$	PA(20:1)	$C_{23}H_{45}O_7P$	[1]	
2	507.25	507.2484	3	$[M+K]^+$	PG(P-16:0)	$C_{22}H_{45}O_8P$	[1]	
3	510.36	510.3554	9	$[M+H]^+$	PE(20:0)	$C_{25}H_{52}NO_7P$	[6]	
4	511.30	511.3030	6	$[M+H]^+$	PG(18:1)	$C_{24}H_{47}O_9P$		493, 475, 419, 283, 155
5	514.23	514.2330	6	$[M+K]^+$	PE(18:3)	$C_{23}H_{42}NO_7P$	[6]	
6	520.28	520.2800	0	$[M+K]^+$	PE(18:0)	$C_{23}H_{48}NO_7P$	[6]	
7	521.32	521.3214	3	$[M+Na]^+$	PG(18:0)	$C_{24}H_{51}O_8P$		
8	522.26	522.2591	2	$[M+Na]^+$	PE(20:5)	$C_{25}H_{42}NO_7P$		
9	524.37	524.3711	2	$[M+H]^+$	PC(18:0)	$C_{26}H_{54}NO_7P$		
10	526.29	526.2928	5	$[M+H]^+$	PE(22:6)	$C_{27}H_{44}NO_7P$	[6]	
11	529.27	529.2691	2	$[M+K]^+$	PA(22:2)	$C_{25}H_{47}O_7P$		
12	531.27	531.2717	3	$[M+H]^+$	PG(20:5)	$C_{26}H_{43}O_9P$		
13	532.30	532.3010	2	$[M+Na]^+$	PC(16:0)	$C_{24}H_{48}NO_8P$		494, 478, 327, 185, 88
14	533.30	533.3004	1	$[M+K]^+$	PA(22:0)	$C_{25}H_{51}O_7P$	[6]	
15	534.32	534.3166	6	$[M+Na]^+$	PS(O-18:0)	$C_{24}H_{50}NO_8P$		
16	535.28	535.2797	1	$[M+K]^+$	PG(P-18:0)	$C_{24}H_{49}O_8P$		
17	536.50	536.5037	7	$[M+H]^+$	Cer(34:2)	$C_{34}H_{65}NO_3$		
18	542.26	542.2643	8	$[M+K]^+$	PE(20:3)	$C_{25}H_{46}NO_7P$	[6]	
19	544.28	544.2800	0	$[M+K]^+$	PE(20:2)	$C_{25}H_{48}NO_7P$	[6]	
20	546.29	546.2956	10	$[M+K]^+$	PE(20:1)	$C_{25}H_{50}NO_7P$	[6]	
21	548.44	548.4440	7	$[M+K]^+$	Cer(d32:1)	$C_{32}H_{63}NO_3$		
22	551.50	551.5034	6	$[M+H]^+$	DG(P-32:1)	$C_{35}H_{66}O_4$	[1]	
23	558.29	558.2956	10	$[M+K]^+$	PC(18:2)	$C_{26}H_{50}NO_7P$	[1]	
24	559.43	559.4333	6	$[M+Na]^+$	DG(30:2)	$C_{33}H_{60}O_5$		
25	560.31	560.3113	2	$[M+K]^+$	PC(18:1)	$C_{26}H_{54}NO_7P$		522, 504, 184, 104
26	563.46	563.4646	8	$[M+Na]^+$	DG(30:0)	$C_{33}H_{64}O_5$		
27	568.28	568.2800	0	$[M+K]^+$	PE(22:4)	$C_{27}H_{48}NO_7P$	[3]	
28	582.29	582.2956	10	$[M+K]^+$	PC(20:4)	$C_{28}H_{50}NO_7P$		544, 526, 184, 104

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (m/z)a)
				Ion form	Compound	Molecular formula		
29	584.41	584.4050	9	$[M+Na]^+$	CerP(d30:1)	$C_{30}H_{60}NO_6P$		
30	594.41	594.4129	5	$[M+H]^+$	PC(22:0)	$C_{30}H_{60}NO_8P$		
31	606.29	606.2956	9	$[M+K]^+$	PC(22:6)	$C_{30}H_{50}NO_7P$	7	
32	607.34	607.3372	5	$[M+K]^+$	PG(22:0)	$C_{28}H_{57}O_9P$		
33	609.45	609.4489	2	$[M+Na]^+$	DG(34:5)	$C_{37}H_{62}O_5$		
34	614.36	614.3582	3	$[M+K]^+$	PC(22:2)	$C_{30}H_{58}NO_7P$		
35	616.37	616.3739	6	$[M+K]^+$	PC(22:1)	$C_{30}H_{60}NO_7P$	3	
36	617.51	617.5115	2	$[M+Na]^+$	DG(34:1)	$C_{37}H_{70}O_5$	2	
37	627.44	627.4385	2	$[M+K]^+$	DG(34:4)	$C_{37}H_{64}O_5$		571, 351, 333, 259, 239, 59
38	631.47	631.4698	0	$[M+K]^+$	DG(34:2)	$C_{37}H_{68}O_5$		
39	637.41	637.4075	4	$[M+H]^+$	PG(26:1)	$C_{32}H_{61}O_{10}P$		
40	638.49	638.4881	3	$[M+Na]^+$	DG(36:2)	$C_{39}H_{67}D_5O_5$	3	
41	646.42	646.4208	1	$[M+K]^+$	PC(24:0)	$C_{32}H_{66}NO_7P$	3	
42	647.56	647.5585	2	$[M+Na]^+$	DG(36:0)	$C_{39}H_{76}O_5$		
43	651.46	651.4595	1	$[M+H]^+$	PG(P-28:0)	$C_{34}H_{67}O_9P$		
44	653.61	653.6079	3	$[M+H]^+$	DG(38:0)	$C_{41}H_{80}O_5$	2	
45	659.51	659.5123	3	$[M+H]^+$	PE-Cer(d24:2)	$C_{36}H_{71}N_2O_6P$		
46	666.47	666.4704	1	$[M+H]^+$	PS(O-28:0)	$C_{34}H_{68}NO_9P$		
47	688.60	688.6004	1	$[M+K]^+$	Cer(d42:1)	$C_{42}H_{83}NO_3$		
48	689.43	689.4364	9	$[M+Na]^+$	PG(28:0)	$C_{34}H_{67}O_{10}P$		
49	694.57	694.5746	7	$[M+K]^+$	Cer(t40:0)	$C_{40}H_{81}NO_5$		
50	703.49	703.4884	2	$[M+Na]^+$	PG(O-30:0)	$C_{36}H_{73}O_9P$		
51	704.43	704.4262	5	$[M+Na]^+$	PE(32:5)	$C_{37}H_{64}NO_8P$		
52	725.49	725.4882	2	$[M+K]^+$	PA(P-36:1)	$C_{39}H_{75}O_7P$		
53	733.62	733.6218	2	$[M+H]^+$	SM(d36:0)	$C_{41}H_{85}N_2O_6P$	8	
54	734.48	734.4755	6	$[M+H]^+$	PE(36:7)	$C_{41}H_{68}NO_8P$		
55	735.53	735.5299	0	$[M+Na]^+$	PA(O-38:3)	$C_{41}H_{77}O_7P$	3	695, 615, 453, 435, 279, 261
56	737.41	737.4153	7	$[M+Na]^+$	PA(38:9)	$C_{41}H_{63}O_8P$		
57	741.45	741.4490	1	$[M+H]^+$	PA(40:10)	$C_{43}H_{65}O_8P$		
58	742.41	742.4056	6	$[M+K]^+$	PS(30:2)	$C_{36}H_{66}NO_{10}P$		

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (m/z)a)
				Ion form	Compound	Molecular formula		
59	749.51	749.5116	2	$[M+H]^+$	PA(40:6)	$C_{43}H_{73}O_8P$		651, 461, 443, 289
60	750.45	750.4471	4	$[M+K]^+$	PE(34:4)	$C_{39}H_{70}NO_8P$	2	
61	751.51	751.5151	7	$[M+K]^+$	PE-Cer(d38:3)	$C_{40}H_{77}N_2O_6P$		
62	752.44	752.4473	2	$[M+Na]^+$	PS(32:3)	$C_{38}H_{68}NO_{10}P$		
63	753.55	753.5517	2	$[M+Na]^+$	PE-Cer(d38:2)	$C_{40}H_{79}N_2O_7P$		
64	754.47	754.4630	9	$[M+Na]^+$	PS(32:2)	$C_{38}H_{70}NO_{10}P$		
65	756.46	756.4576	3	$[M+K]^+$	PS(P-32:1)	$C_{38}H_{72}NO_9P$		
66	757.53	757.5354	7	$[M+Na]^+$	PG(O-34:1)	$C_{40}H_{79}O_9P$		
67	758.49	758.4943	6	$[M+Na]^+$	PS(32:0)	$C_{38}H_{74}NO_{10}P$	9	
68	759.45	759.4573	10	$[M+K]^+$	PG(32:1)	$C_{38}H_{73}O_{10}P$		
69	760.51	760.5123	3	$[M+H]^+$	PS(34:2)	$C_{40}H_{74}NO_{10}P$		714, 504, 263, 239, 88
70	761.55	761.5456	6	$[M+Na]^+$	PA(O-40:4)	$C_{43}H_{79}O_7P$		
71	762.45	762.4471	4	$[M+K]^+$	PC(32:5)	$C_{40}H_{70}NO_8P$		
72	765.45	765.4549	6	$[M+H]^+$	PI(29:2)	$C_{38}H_{69}O_{13}P$		
73	772.49	772.4888	1	$[M+Na]^+$	PC(34:6)	$C_{42}H_{72}NO_8P$		732, 285, 88
74	773.66	773.6630	4	$[M+Na]^+$	TG(44:0)	$C_{47}H_{90}O_6$	10	
75	774.60	774.6007	0	$[M+H]^+$	PE(38:1)	$C_{43}H_{84}NO_8P$	1	
76	775.68	775.6810	1	$[M+H]^+$	TG(46:2)	$C_{49}H_{90}O_6$		757, 519, 197
77	777.43	777.4315	2	$[M+K]^+$	PI(P-28:0)	$C_{37}H_{71}O_{12}P$	2	
78	778.44	778.4420	3	$[M+K]^+$	PS(P-34:4)	$C_{40}H_{70}NO_9P$		
79	779.44	779.4471	9	$[M+K]^+$	PI(O-28:0)	$C_{37}H_{73}O_{12}P$		
80	780.46	780.4575	3	$[M+Na]^+$	PE(38:9)	$C_{43}H_{68}NO_8P$		
81	781.48	781.4862	8	$[M+H]^+$	PI(30:1)	$C_{39}H_{73}O_{13}P$		
82	782.48	782.4733	9	$[M+K]^+$	PS(O-34:3)	$C_{40}H_{74}NO_9P$		
83	784.51	784.5099	2	$[M+Na]^+$	PS(34:1)	$C_{40}H_{76}NO_{10}P$		716, 478, 285, 267, 237
84	785.54	785.5456	7	$[M+Na]^+$	PA(O-42:6)	$C_{45}H_{79}O_7P$		
85	786.51	786.5068	4	$[M+H]^+$	PE(40:9)	$C_{45}H_{72}NO_8P$		
86	787.49	787.4885	2	$[M+K]^+$	PG(34:1)	$C_{40}H_{77}O_{10}P$		
87	788.52	788.5201	0	$[M+Na]^+$	PE(38:5)	$C_{43}H_{76}NO_8P$	11	
88	789.49	789.4888	2	$[M+Na]^+$	PI(P-30:0)	$C_{39}H_{75}O_{12}P$		

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (m/z)a)
				Ion form	Compound	Molecular formula		
89	790.40	790.4056	7	$[M+K]^+$	PS(34:6)	$C_{40}H_{66}NO_{10}P$		
90	791.50	791.4988	2	$[M+K]^+$	PA(40:4)	$C_{43}H_{77}O_8P$		
91	794.43	794.4369	9	$[M+K]^+$	PS(34:4)	$C_{40}H_{70}NO_{10}P$		710, 500, 259
92	796.45	796.4525	3	$[M+K]^+$	PS(34:3)	$C_{40}H_{72}NO_{10}P$		712, 478, 281
93	797.51	797.5093	1	$[M+K]^+$	PG(O-36:3)	$C_{42}H_{79}O_9P$		
94	798.56	798.5619	2	$[M+Na]^+$	PS(O-36:1)	$C_{42}H_{82}NO_9P$		
95	799.52	799.5248	6	$[M+Na]^+$	PA(42:6)	$C_{45}H_{77}O_8P$		
96	800.46	800.4627	3	$[M+K]^+$	PE(38:7)	$C_{43}H_{72}NO_8P$	12	
97	801.70	801.6967	4	$[M+H]^+$	TG(48:3)	$C_{51}H_{92}O_6$	13	
98	802.53	802.5357	7	$[M+Na]^+$	PC(36:5)	$C_{44}H_{78}NO_8P$		
99	804.45	804.4576	9	$[M+K]^+$	PS(P-36:5)	$C_{42}H_{72}NO_9P$		
100	805.73	805.7280	2	$[M+H]^+$	TG(48:1)	$C_{51}H_{96}O_6$	14	
101	806.47	806.4733	4	$[M+K]^+$	PS(P-36:4)	$C_{42}H_{74}NO_9P$		
102	808.51	808.5123	3	$[M+H]^+$	PS(38:6)	$C_{44}H_{74}NO_{10}P$	15	721, 623, 285, 88
103	810.53	810.5256	5	$[M+Na]^+$	PS(36:2)	$C_{42}H_{78}NO_{10}P$		742, 603, 450, 321
104	813.49	813.4831	8	$[M+K]^+$	PA(42:7)	$C_{45}H_{75}O_8P$		
105	814.53	814.5357	7	$[M+Na]^+$	PE(40:6)	$C_{45}H_{78}NO_8P$	6	
106	815.48	815.4858	7	$[M+H]^+$	PG(40:10)	$C_{46}H_{71}O_{10}P$		
107	818.51	818.5097	0	$[M+K]^+$	PC(36:5)	$C_{44}H_{78}NO_8P$	2	
108	820.46	820.4525	9	$[M+K]^+$	PS(36:5)	$C_{42}H_{72}NO_{10}P$	16	764, 597, 502, 261
109	822.47	822.4682	2	$[M+K]^+$	PS(36:4)	$C_{42}H_{74}NO_{10}P$		784, 738, 697, 599, 289
110	823.52	823.5250	6	$[M+K]^+$	PG(P-38:3)	$C_{44}H_{81}O_9P$		
111	824.48	824.4838	5	$[M+K]^+$	PS(36:3)	$C_{42}H_{76}NO_{10}P$	15	740, 504, 263
112	825.54	825.5406	1	$[M+K]^+$	PG(P-38:2)	$C_{44}H_{83}O_9P$		
113	826.53	826.5357	7	$[M+Na]^+$	PC(38:7)	$C_{46}H_{78}NO_8P$	17	786, 528, 289
114	827.55	827.5563	8	$[M+K]^+$	PG(O-38:2)	$C_{44}H_{85}O_9P$		
115	829.44	829.4416	2	$[M+K]^+$	PG(38:8)	$C_{44}H_{71}O_{10}P$		
116	830.47	830.4733	4	$[M+K]^+$	PS(P-38:6)	$C_{44}H_{74}NO_9P$		
117	831.45	831.4573	9	$[M+K]^+$	PG(38:7)	$C_{44}H_{73}O_{10}P$		
118	832.53	832.5253	6	$[M+K]^+$	PE(40:5)	$C_{45}H_{80}NO_8P$	15	751, 653, 482

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (m/z)a)
				Ion form	Compound	Molecular formula		
119	833.51	833.5175	9	$[M+H]^+$	PI(34:3)	$C_{43}H_{77}O_{13}P$		
120	834.53	834.5256	5	$[M+Na]^+$	PS(38:4)	$C_{44}H_{78}NO_{10}P$	[18]	725, 627, 261
121	835.53	835.5331	4	$[M+H]^+$	PI(34:2)	$C_{43}H_{79}O_{13}P$	[19]	
122	840.50	840.4940	7	$[M+K]^+$	PC(38:8)	$C_{46}H_{76}NO_8P$		
123	842.51	842.5097	0	$[M+K]^+$	PC(38:7)	$C_{46}H_{78}NO_8P$	[1]	
124	848.52	848.5201	0	$[M+Na]^+$	PC(40:10)	$C_{48}H_{76}NO_8P$	[20]	713, 701, 603, 450, 337, 319, 211, 89
125	850.60	850.6086	10	$[M+K]^+$	PE(42:2)	$C_{47}H_{90}NO_7P$	[3]	
126	851.55	851.5563	7	$[M+K]^+$	PG(O-40:4)	$C_{46}H_{85}O_9P$		
127	852.55	852.5514	2	$[M+Na]^+$	PC(40:8)	$C_{48}H_{80}NO_8P$		
128	868.45	868.4525	3	$[M+K]^+$	PS(40:9)	$C_{46}H_{72}NO_{10}P$		
129	872.49	872.4838	7	$[M+K]^+$	PS(40:7)	$C_{46}H_{76}NO_{10}P$		788, 526, 285, 486, 289, 88
130	925.48	925.4837	4	$[M+Na]^+$	PI(40:10)	$C_{49}H_{75}O_{13}P$		
131	828.47	828.4786	10	$[M+Na]^+$	PS(38:7)	$C_{44}H_{72}NO_{10}P$	[21]	528, 287, 261, 88
	844.45	844.4525	3	$[M+K]^+$				
132	812.54	812.5436	4	$[M+H]^+$	PS(38:4)	$C_{44}H_{78}NO_{10}P$	[18]	766, 502, 261
	846.46	846.4682	10	$[M+K]^+$				
133	783.50	783.5018	2	$[M+H]^+$	PI(30:0)	$C_{39}H_{75}O_{13}P$		765, 559, 541, 225
134	807.50	807.5018	2	$[M+H]^+$	PI(32:2)	$C_{41}H_{75}O_{13}P$	[15]	789, 581, 265
	845.46	845.4577	3	$[M+K]^+$				
135	809.52	809.5175	3	$[M+H]^+$	PI(32:1)	$C_{41}H_{77}O_{13}P$	[15]	791, 567, 251
	847.47	847.4733	4	$[M+K]^+$				
136	811.54	811.5330	9	$[M+H]^+$	PI(32:0)	$C_{41}H_{79}O_{13}P$	[16, 22]	551, 421, 313
	849.49	849.4889	1	$[M+K]^+$				

a) Structurally specific CID ions of lipids were detected by LC-MS/MS using CID. Fragment ions shown in blue were detected by *in situ* MALDI-MS/MS. Abbreviations: PC, phosphatidylcholine; PE, phosphatidylethanolamine; PA, phosphatidic acid; PG, phosphatidylglycerol; PS, phosphatidylserine; PI, phosphatidylinositol; Cer, ceramide; CerP, ceramide 1-phosphate; PE-Cer, phosphatidylethanolamine-ceramide; SM, sphingomyelin; DG, diacylglycerol; TG, triglyceride. Highlighted lipids were also detected using DCH matrix without optimization (8 mg/mL DCH, prepared in 70% aqueous ACN solution containing 0.1% TFA).

Table S2. Comparison of ion signals of lipids detected in the rat liver tissue sections by MALDI-TOF MS in the positive-ion mode using DCH, DHB, 2-MBT, CHCA, DNPH, and PNA as the matrices.

Number	Lipids ion signals detected in rat liver tissue sections					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
1	503.25					
2					506.31	
3				506.36		
4	507.25					
5		510.31				
6	510.36					
7	511.30					
8	514.23					
9	520.28					
10	521.32					
11	522.26					
12			524.27			
13	524.37					
14	526.29					
15	529.27					
16	531.27					
17	532.30					
18	533.30					
19					534.24	
20	534.32					
21						534.48
22	535.28					
23	536.50					
24	542.26					
25	544.28					
26	546.29					
27	548.44					
28	551.50					
29		554.51				
30		557.41				
31	558.29					
32	559.43					
33	560.31					
34					562.32	
35	563.46					
36	568.28					
37			569.51			
38					569.52	
39						575.47

Number	Lipids ion signals detected in rat liver tissue sections					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
40	582.29					
41	584.41					
42	594.41					
43	606.29					
44	607.34					
45	609.45					
46		614.35				
47	614.36					
48	616.37					
49		616.40				
50	617.51					
51		623.41				
52						627.40
53	627.44					
54		627.45				
55	631.47					
56	637.41					
57	638.49					
58	646.42					
59	647.56					
60	651.46					
61	653.61					
62						657.55
63	659.51					
64	666.47					
65				688.39		
66	688.60					
67	689.43					
68	694.57					
69						703.44
70	703.49					
71	704.43					
72						714.46
73	725.49					
74	733.62					
75						734.45
76	734.48					
77		734.50				
78	735.53					
79	737.41					
80	741.45					
81			741.46			

Number	Lipids ion signals detected in rat liver tissue sections					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
82						742.40
83	742.41					
84				749.49		
85		749.50				
86	749.51					
87			749.56			749.56
88	750.45					
89						750.58
90			750.63		750.63	
91	751.51					
92						751.62
93			751.63			
94					751.68	
95	752.44					
96	753.55					
97	754.47					
98						756.42
99	756.46					
100	757.53					
101			758.47			
102	758.49					
103		758.51				
104			759.43			
105	759.45					
106		759.52				
107						760.43
108			760.46			
109	760.51	760.51				
110		761.54				
111	761.55					
112	762.45					
113						762.48
114	765.45					
115						769.43
116			772.48			
117	772.49					
118				773.51		
119						773.53
120			773.64			
121	773.66					
122					773.67	
123						774.53

Number	Lipids ion signals detected in rat liver tissue sections					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
124		774.54				
125	774.60					
126	775.68					
127				777.42		
128	777.43					
129		777.44				
130			777.60			
131						777.61
132	778.44					
133						778.59
134			778.67			
135	779.44					
136			780.42			780.42
137	780.46					
138		780.48				
139						781.45
140	781.48					
141		781.49				
142						782.47
143	782.48		782.48			
144		782.51				
145			783.43			
146	783.50					
147		783.53				
148			784.45			
149						784.50
150	784.51					
151		784.54				
152			785.47			
153	785.54					
154			786.48			
155	786.51					
156		786.57				
157			787.47			
158	787.49					
159		787.59				
160	788.52		788.52			
161			789.39			
162	789.49					
163	790.40					
164	791.50					
165	794.43					

Number	Lipids ion signals detected in rat liver tissue sections					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
166	796.45					
167		796.46				
168			796.48			
169					796.53	
170				796.58		
171			797.41			
172		797.50				
173	797.51					
174					797.55	
175			798.43			
176					798.50	
177		798.51				
178	798.56					
179				798.64		
180			799.49			
181	799.52					
182		799.53				
183					799.56	
184	800.46					
185			800.59			
186				801.41		
187						801.57
188			801.59			
189	801.70				801.70	
190				802.46	802.46	
191	802.53					
192						802.57
193			802.59			
194					802.66	
195						803.59
196			803.66	803.66		
197			804.41			
198	804.45					
199		804.50				
200				804.69		
201	805.73					
202	806.47		806.47			
203		806.52			806.52	
204			807.43			
205	807.50					
206		807.51				
207			808.45			

Number	Lipids ion signals detected in rat liver tissue sections					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
208	808.51					
209		808.55				
210			809.48			
211	809.52					
212			810.50			
213	810.53					
214		810.55				
215					810.60	
216				810.69		
217			811.47			
218	811.54					
219		811.58				
220			812.48			
221	812.54					
222						813.47
223	813.49					
224	814.53					
225	815.48					
226	818.51					
227	820.46	820.46				
228					820.51	
229				820.61		
230			821.43			
231		821.50				
232					821.53	
233				821.67		
234			822.44			
235	822.47					
236		822.48				
237					822.53	
238			823.48			
239						823.49
240	823.52					
241	824.48					
242		824.52				
243			824.53			
244					824.57	
245				824.65		
246			825.46			
247	825.54					
248		825.55				
249					825.57	

Number	Lipids ion signals detected in rat liver tissue sections					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
250				825.70		
251			826.47			
252						826.49
253	826.53					
254					826.59	
255			827.47			
256						827.49
257	827.55					
258	828.47					
259		828.49				
260			828.54			
261				828.65		
262	829.44					
263	830.47					
264	831.45					
265			832.49			
266	832.53					
267	833.51					
268			834.51			
269		834.52				
270	834.53					
271					834.61	
272						835.46
273			835.48			
274	835.53					
275						837.46
276						839.47
277	840.50					
278				840.59		
279	842.51					
280	844.45					
281		844.46				
282				844.58		
283			845.45			
284	845.46					
285		845.47				
286					845.50	
287				845.60		
288	846.46					846.46
289					846.50	
290				846.59		
291	847.47					

Number	Lipids ion signals detected in rat liver tissue sections					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
292					847.56	
293		848.51				
294	848.52					
295					848.54	
296				848.67		
297			849.45			
298		849.48				
299	849.49					849.49
300					849.59	
301				849.69		
302			850.46			
303						850.51
304		850.54				
305	850.60					
306				850.63		
307			851.48			
308						851.52
309	851.55					
310	852.55					852.55
311			853.58			
312						853.60
313						854.57
314						856.44
315	868.45					
316				868.54		
317	872.49					
318					872.57	
319				872.63		
320			873.48			873.48
321					873.59	
322				873.64		
323			874.47			
324						874.51
325						895.62
326			921.49			
327	925.48					
328				963.60		
329				964.62		
Total number of detected lipids	**136**	**42**	**54**	**33**	**28**	**44**

Table S3. Lipids detected and identified in the camelina seed tissue sections by MALDI-TOF MS in the positive-ion mode using DCH as the matrix.

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a)]
				Ion form	Compound	Molecular formula		
1	504.44	504.4387	3	$[M+Na]^+$	Cer(d30:1)	$C_{30}H_{59}NO_3$	23	
2	522.45	522.4517	3	$[M+H]^+$	Cer(d32:3)	$C_{32}H_{59}NO_4$		
3	527.47	527.4670	6	$[M+H]^+$	DG(29:0)	$C_{32}H_{62}O_5$		509, 239, 197, 155, 75
4	544.47	544.4700	0	$[M+Na]^+$	Cer(d33:2)	$C_{33}H_{63}NO_3$	24	
5	547.43	547.4333	6	$[M+Na]^+$	DG(29:1)	$C_{32}H_{60}O_5$	25	
6	577.42	577.4229	5	$[M+K]^+$	DG(30:1)	$C_{33}H_{62}O_5$	26	
7	595.43	595.4333	6	$[M+Na]^+$	DG(33:5)	$C_{36}H_{60}O_5$		555, 285, 197, 169, 75
8	597.39	597.3916	3	$[M+K]^+$	DG(32:5)	$C_{35}H_{58}O_5$	27	
9	598.38	598.3843	7	$[M+Na]^+$	PC(22:2)	$C_{30}H_{58}NO_7P$	28	
10	599.47	599.4670	5	$[M+H]^+$	DG(35:6)	$C_{38}H_{62}O_5$		
11	601.48	601.4827	4	$[M+H]^+$	DG(35:5)	$C_{38}H_{64}O_5$		
12	603.50	603.4959	7	$[M+Na]^+$	DG(33:1)	$C_{36}H_{68}O_5$	29	
13	605.42	605.4177	4	$[M+H]^+$	PA(29:1)	$C_{32}H_{61}O_8P$		587, 225, 209, 197, 98
14	637.39	637.3840	9	$[M+Na]^+$	PA(30:3)	$C_{33}H_{59}O_8P$		
15	639.43	639.4360	9	$[M+Na]^+$	PA(P-31:1)	$C_{34}H_{65}O_7P$		
16	642.45	642.4469	5	$[M+Na]^+$	PE(P-28:0)	$C_{33}H_{66}NO_7P$		
17	644.50	644.5015	2	$[M+K]^+$	Cer(d38:3)	$C_{38}H_{71}NO_4$		
18	650.44	650.4391	1	$[M+H]^+$	PC(25:0)	$C_{33}H_{64}NO_9P$	27	
19	651.44	651.4385	2	$[M+K]^+$	DG(36:6)	$C_{39}H_{64}O_5$		
20	660.48	660.4748	8	$[M+H]^+$	DG(40:8)	$C_{43}H_{63}D_5O_5$		
21	662.47	662.4755	8	$[M+H]^+$	PE(30:1)	$C_{35}H_{6}8NO_8P$	30	
22	712.45	712.4524	3	$[M+Na]^+$	PS(P-30:1)	$C_{36}H_{68}NO_9P$		
23	714.44	714.4341	8	$[M+H]^+$	PS(31:4)	$C_{37}H_{64}NO_{10}P$		
24	749.45	749.4518	2	$[M+K]^+$	PA(37:4)	$C_{40}H_{71}O_8P$	31	435, 281, 259, 231, 98
25	751.55	751.5484	2	$[M+H]^+$	PG(34:0)	$C_{40}H_{79}O_{10}P$	32, 33	
26	754.41	754.4056	6	$[M+K]^+$	PS(31:3)	$C_{37}H_{66}NO_{10}P$		
27	756.49	756.4940	5	$[M+K]^+$	PE(34:1)	$C_{39}H_{76}NO_8P$		
28	758.49	758.4943	6	$[M+Na]^+$	PS(32:0)	$C_{38}H_{74}NO_{10}P$		295, 183, 88

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a]
				Ion form	Compound	Molecular formula		
29	759.49	759.4935	5	$[M+Na]^+$	PA(39:5)	$C_{42}H_{73}O_8P$		
30	760.49	760.4912	2	$[M+H]^+$	PE(38:8)	$C_{43}H_{70}NO_8P$		
31	761.51	761.5116	2	$[M+H]^+$	PA(41:7)	$C_{44}H_{73}O_8P$		743, 433, 311, 98
32	762.53	762.5280	3	$[M+H]^+$	PS(34:1)	$C_{40}H_{76}NO_{10}P$		
32	800.49	800.4838	8	$[M+K]^+$	PS(34:1)	$C_{40}H_{76}NO_{10}P$		
33	771.49	771.4935	5	$[M+Na]^+$	PA(40:6)	$C_{43}H_{73}O_8P$	30	731, 447, 311, 285, 98
34	773.67	773.6654	6	$[M+H]^+$	TG(46:3)	$C_{49}H_{88}O_6$		
35	774.51	774.5068	4	$[M+H]^+$	PE(39:8)	$C_{44}H_{72}NO_8P$		
36	775.68	775.6810	1	$[M+H]^+$	TG(46:2)	$C_{49}H_{90}O_6$	29	
37	776.66	776.6528	9	$[M+H]^+$	PC(O-36:0)	$C_{44}H_{90}NO_7P$	28	
38	777.70	777.6967	4	$[M+H]^+$	TG(46:1)	$C_{49}H_{92}O_6$		759, 521, 251, 239, 197
39	778.47	778.4654	6	$[M+H]^+$	PS(36:7)	$C_{42}H_{68}NO_{10}P$	34	
40	779.45	779.4471	4	$[M+K]^+$	PI(O-28:0)	$C_{37}H_{73}O_{12}P$		
41	780.48 796.45	780.4786 796.4525	2 3	$[M+Na]^+$ $[M+K]^+$	PS(34:3)	$C_{40}H_{72}NO_{10}P$	35	
42	781.50	781.5014	2	$[M+H]^+$	PG(37:6)	$C_{43}H_{73}O_{10}P$	36	763, 609, 285, 75
43	782.50	782.4967	4	$[M+H]^+$	PS(36:5)	$C_{42}H_{72}NO_{10}P$	15	
44	783.51 799.49	783.5147 799.4886	6 2	$[M+Na]^+$ $[M+K]^+$	PG(35:2)	$C_{41}H_{77}O_{10}P$	36	
45	784.53	784.5253	6	$[M+K]^+$	PC(33:1)	$C_{41}H_{80}NO_8P$		
46	785.54	785.5457	7	$[M+K]^+$	PA(39:0)	$C_{42}H_{83}O_8P$		729, 477, 253, 98
47	786.56	786.5619	2	$[M+Na]^+$	PS(O-35:0)	$C_{41}H_{82}NO_9P$		
48	787.58	787.5823	3	$[M+Na]^+$	PG(O-36:0)	$C_{42}H_{85}O_9P$	37	
49	788.58	788.5800	0	$[M+H]^+$	PS(O-37:2)	$C_{43}H_{82}NO_9P$		
50	789.54	789.5406	1	$[M+K]^+$	PG(O-35:0)	$C_{41}H_{83}O_9P$		733, 579, 281, 225
51	794.49	794.4943	5	$[M+Na]^+$	PS(35:3)	$C_{41}H_{74}NO_{10}P$	31	
52	797.47	797.4729	4	$[M+K]^+$	PG(35:3)	$C_{41}H_{75}O_{10}P$		
53	798.50	798.5046	6	$[M+K]^+$	PS(O-35:2)	$C_{41}H_{78}NO_9P$	38	
54	802.52	802.5147	7	$[M+K]^+$	PC(P-36:5)	$C_{44}H_{78}NO_7P$	25	581, 285, 223,

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (m/z)[a]
				Ion form	Compound	Molecular formula		
55	804.50	804.4940	7	$[M+K]^+$	PE(38:5)	$C_{43}H_{76}NO_8P$		
56	805.53	805.5354	7	$[M+Na]^+$	PG(P-38:4)	$C_{44}H_{79}O_9P$		
57	806.51	806.5097	0	$[M+K]^+$	PE(38:4)	$C_{43}H_{78}NO_8P$		295, 259, 44, 27
58	807.51	807.5147	6	$[M+Na]^+$	PG(37:4)	$C_{43}H_{77}O_{10}P$		
59	808.54	808.5463	8	$[M+Na]^+$	PS(P-37:2)	$C_{43}H_{80}NO_9P$	38	
60	810.56	810.5619	2	$[M+Na]^+$	PS(P-37:1)	$C_{43}H_{82}NO_9P$	38	603, 279, 251, 88, 42
61	818.43	818.4369	8	$[M+K]^+$	PS(36:6)	$C_{42}H_{70}NO_{10}P$		
62	819.45	819.4420	10	$[M+K]^+$	PI(30:1)	$C_{39}H_{73}O_{13}P$		
63	820.51	820.5099	0	$[M+Na]^+$	PS(37:4)	$C_{43}H_{76}NO_{10}P$		
64	821.47	821.4729	4	$[M+K]^+$	PG(37:5)	$C_{43}H_{75}O_{10}P$		611, 477, 289, 75
65	822.47	822.4682	2	$[M+K]^+$	PS(36:4)	$C_{42}H_{74}NO_{10}P$		
66	823.52	823.5250	6	$[M+K]^+$	PG(O-38:4)	$C_{44}H_{81}O_9P$		
67	824.49	824.4838	8	$[M+K]^+$	PS(36:3)	$C_{42}H_{76}NO_{10}P$	39	
68	825.54	825.5405	1	$[M+Na]^+$	PA(44:7)	$C_{47}H_{79}O_8P$		475, 321, 293, 98
69	826.53	826.5357	7	$[M+Na]^+$	PC(38:7)	$C_{46}H_{78}NO_8P$	40	
70	830.67	830.6633	8	$[M+H]^+$	PC(39:1)	$C_{47}H_{92}NO_8P$	41	
71	856.52	856.5253	6	$[M+K]^+$	PE(42:7)	$C_{47}H_{80}NO_8P$		
72	873.66	873.6579	2	$[M+H]^+$	PG(43:2)	$C_{49}H_{93}O_{10}P$		701, 547, 319, 75
73	874.67	874.6660	5	$[M+Na]^+$	PC(O-42:4)	$C_{50}H_{94}NO_7P$	28	
74	875.71	875.7099	0	$[M+Na]^+$	TG(52:5)	$C_{55}H_{96}O_6$		
75	876.52	876.5151	6	$[M+K]^+$	PS(40:5)	$C_{46}H_{80}NO_{10}P$	42	
76	877.72	877.7256	6	$[M+Na]^+$	TG(52:4)	$C_{55}H_{98}O_6$		837, 655, 543, 295, 183
77	878.70	878.6973	3	$[M+Na]^+$	PC(O-42:2)	$C_{52}H_{96}NO_7P$		
78	879.75 901.72	879.7436 901.7256	7 6	$[M+H]^+$ $[M+Na]^+$	TG(54:6)	$C_{57}H_{98}O_6$		
79	881.75	881.7569	8	$[M+Na]^+$	TG(52:2)	$C_{55}H_{102}O_6$		
80	889.67	889.6682	2	$[M+K]^+$	TG(52:6)	$C_{55}H_{94}O_6$		833, 597, 315, 237, 209
81	891.64	891.6473	8	$[M+Na]^+$	TG(54:11)	$C_{57}H_{88}O_6$		

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a)]
				Ion form	Compound	Molecular formula		
82	893.66	893.6630	3	$[M+Na]^+$	TG(54:10)	$C_{57}H_{90}O_6$		
83	895.67	895.6634	7	$[M+H]^+$	PI(O-39:0)	$C_{48}H_{95}O_{12}P$		
84	896.68	896.6869	8	$[M+K]^+$	PC(P-42:0)	$C_{50}H_{100}NO_7P$		675, 518, 323, 279, 88
85	898.67	898.6661	4	$[M+K]^+$	PE(44:0)	$C_{49}H_{98}NO_8P$		
86	899.71	899.7099	0	$[M+Na]^+$	TG(54:7)	$C_{57}H_{96}O_6$		
	915.68	915.6838	4	$[M+K]^+$				
87	900.69	900.6817	9	$[M+Na]^+$	PC(O-44:5)	$C_{52}H_{96}NO_7P$	28	
88	903.74	903.7412	1	$[M+Na]^+$	TG(54:5)	$C_{57}H_{100}O_6$	43	
	919.71	919.7151	6	$[M+K]^+$				
89	905.75	905.7569	8	$[M+Na]^+$	TG(54:4)	$C_{57}H_{102}O_6$		617, 599, 333, 267
90	907.77	907.7725	3	$[M+Na]^+$	TG(54:3)	$C_{57}H_{104}O_6$	44	
91	911.66	911.6525	8	$[M+K]^+$	TG(54:9)	$C_{57}H_{92}O_6$		
92	912.61	912.6090	1	$[M+K]^+$	PS(42:1)	$C_{48}H_{92}NO_{10}P$		689, 321, 295
93	913.63	913.6294	1	$[M+K]^+$	PG(43:1)	$C_{49}H_{95}O_{10}P$		
94	918.63	918.6349	5	$[M+K]^+$	PC(43:4)	$C_{51}H_{94}NO_8P$		715, 548, 315, 88
95	981.58	981.5829	3	$[M+K]^+$	PI(42:4)	$C_{51}H_{91}O_{13}P$		

a) Structurally specific CID ions of lipids were detected by LC-MS/MS using CID. Fragment ions shown in blue were detected by *in situ* MALDI-MS/MS. Abbreviations: PC, phosphatidylcholine; PE, phosphatidylethanolamine; PA, phosphatidic acid; PG, phosphatidylglycerol; PS, phosphatidylserine; PI, phosphatidylinositol; Cer, ceramide; DG, diacylglycerol; TG, triglyceride.

Table S4. Comparison of ion signals of lipids detected in the camelina seed tissue sections by MALDI-TOF MS in the positive-ion mode using DCH, DHB, 2-MBT, CHCA, DNPH, and PNA as the matrices.

Number	Lipids ion signals detected in Camelina seed tissue section					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
1			502.42			
2			504.30			
3		504.34				
4	504.44					
5			507.21			
6	522.45					
7		524.30				
8	527.47	527.47				
9		528.43				
10	544.47					
11	547.43					
12		553.49				
13		558.49				
14						573.39
15		573.42				
16		574.42				
17		575.41				
18		576.40				
19	577.42					
20			582.22			
21		587.44				
22			593.28			
23						595.29
24	595.43					
25						596.28
26			597.30			
27	597.39					
28	598.38					
29						599.33
30	599.47					
31						600.33
32						601.34
33		601.39				
34	601.48					
35	603.50					
36	605.42					
37			629.46			
38			630.45			

Number	Lipids ion signals detected in Camelina seed tissue section					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
39			631.38			
40		634.46				
41		636.62				
42	637.39					
43			639.42			
44	639.43					
45	642.45					
46	644.50					
47		645.55				
48	650.44					
49	651.44					
50		653.42				
51			658.44			
52		660.40				
53	660.48					
54	662.47					
55			674.42			
56			675.41			
57			676.35			
58		680.49				
59		681.47				
60						682.45
61			699.41			
62		700.41				
63		701.41				
64			702.43			
65		710.51				
66		711.40				
67	712.45					
68		713.42				
69		714.39				
70	714.44					
71		727.40				
72		729.38				
73		739.44				
74		740.44				
75		742.45				
76		743.65				
77		744.63				
78		745.46				
79		746.60				
80		747.50				

Number	Lipids ion signals detected in Camelina seed tissue section					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
81		748.42				
82	749.45					
83		749.50				
84		750.50				
85		751.48				
86	751.55					
87		752.46				
88		753.47				
89	754.41					
90		754.49				
91		755.50				
92			756.43			
93	756.49					
94		756.63				
95		757.42				
96			758.43			
97		758.44				
98	758.49					
99			759.43			
100	759.49					759.49
101		759.51				
102			760.44			
103	760.49					
104		760.53				
105						761.42
106		761.50				
107	761.51					
108		762.42				
109	762.53					
110		763.47				
111		765.44				
112		766.50				
113		771.46				
114	771.49					
115		772.48				
116		773.46				
117	773.67					
118			774.48			
119	774.51					
120			775.59			
121	775.68					
122	776.66					

Number	Lipids ion signals detected in Camelina seed tissue section					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
123			777.55			
124	777.70					
125	778.47					
126		779.44				
127	779.45					
128						780.43
129		780.45				
130	780.48					
131		781.45				
132	781.50					
133		782.43				
134			782.44			
135	782.50					
136						783.43
137	783.51					
138	784.53					
139						785.44
140			785.45			
141	785.54					
142	786.56					
143		787.43				787.43
144	787.58					
145			788.45			
146	788.58					
147						789.39
148	789.54					
149	794.49					
150						795.45
151		795.46				
152	796.45					
153	797.47					
154						798.45
155	798.50	798.50				
156		799.46				
157	799.49					
158		800.44				
159	800.49					
160		801.45				
161		802.47				
162	802.52					
163	804.50					
164	805.53					

Number	Lipids ion signals detected in Camelina seed tissue section					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
165	806.51					
166	807.51					
167	808.54					
168	810.56					
169						816.42
170	818.43					
171	819.45					819.45
172	820.51					
173						821.45
174	821.47					
175	822.47					
176	823.52					
177						824.47
178	824.49					
179						825.46
180	825.54					
181	826.53					
182		829.42				
183	830.67					
184	856.52					
185						873.45
186			873.51			
187	873.66					
188	874.67					
189						875.47
190			875.50			
191	875.71					
192	876.52					
193						877.49
194	877.72					
195	878.70					
196						879.45
197	879.75					
198	881.75					
199						889.42
200	889.67					
201	891.64					
202	893.66					
203						894.46
204			895.47			
205	895.67					
206			896.48			896.48

Number	Lipids ion signals detected in Camelina seed tissue section					
	DCH	DHB	2-MBT	CHCA	DNPH	PNA
207	896.68					
208			897.48			
209			898.51			
210	898.67					
211						899.46
212			899.47			
213	899.71					
214	900.69					
215			901.48			
216						901.49
217	901.72					
218		902.49				902.49
219			902.53			
220			903.49			903.49
221	903.74					
222						905.45
223	905.75					
224	907.77					
225	911.66					
226	912.61					
227	913.63					
228						915.45
229	915.68					
230						917.45
231			917.47			
232	918.63					
233	919.71					
234						920.56
235						961.53
236	981.58					
Total number of detected lipids	**95**	**68**	**36**	**0**	**0**	**32**

Table S5. Lipids detected and identified in the mouse brain tissue sections by MALDI-TOF MS in the positive-ion mode using DCH as the matrix.

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a)]
				Ion form	Compound	Molecular formula		
1	502.42	502.4231	6	$[M+Na]^+$	Cer(d30:2)	$C_{30}H_{57}NO_3$	6	
2	504.34	504.3424	5	$[M+Na]^+$	PC(O-16:0)	$C_{24}H_{52}NO_6P$	6	
3	506.32	506.3241	8	$[M+H]^+$	PE(20:2)	$C_{25}H_{48}NO_7P$	6	
4	507.40	507.4020	4	$[M+Na]^+$	DG(26:0)	$C_{29}H_{56}O_5$		
5	509.42	509.4201	0	$[M+H]^+$	DG(28:2)	$C_{31}H_{56}O_5$		
6	518.40	518.3970	6	$[M+K]^+$	Cer(30:2)	$C_{30}H_{57}NO_3$		444, 224, 137
7	519.25	519.2483	3	$[M+K]^+$	PA(20:0)	$C_{23}H_{45}O_8P$		463, 383, 309, 173, 155
8	520.41	520.4127	5	$[M+K]^+$	Cer(d30:1)	$C_{30}H_{59}NO_3$		
9	522.28	522.2826	5	$[M+H]^+$	PS(18:2)	$C_{24}H_{44}NO_9P$		
10	524.37	524.3711	2	$[M+H]^+$	PC(18:0)	$C_{26}H_{54}NO_7P$	45	506, 184, 104, 88
11	534.29	534.2956	10	$[M+K]^+$	PC(16:0)	$C_{24}H_{50}NO_7P$	6	
12	537.45	537.4514	3	$[M+H]^+$	DG(30:2)	$C_{33}H_{60}O_5$		293, 209, 181
13	540.25	540.2487	2	$[M+K]^+$	PE(20:4)	$C_{25}H_{44}NO_7P$	1	
14	546.45	546.4493	1	$[M+Na]^+$	Cer(d32:2)	$C_{32}H_{61}NO_4$		
15	548.44	548.4440	7	$[M+K]^+$	Cer(d32:1)	$C_{32}H_{63}NO_3$		
16	552.50	552.4986	3	$[M+H]^+$	Cer(d34:2)	$C_{34}H_{65}NO_4$		
17	558.43	558.4255	8	$[M+Na]^+$	DG(30:0)	$C_{33}H_{59}D_5O_5$		299, 243, 225, 197, 183
18	560.33	560.3323	4	$[M+Na]^+$	PS(P-20:0)	$C_{26}H_{52}NO_8P$	6	
19	561.45	561.4514	2	$[M+H]^+$	DG(32:4)	$C_{35}H_{60}O_5$	6	
20	562.52	562.5194	1	$[M+H]^+$	Cer(d36:3)	$C_{36}H_{67}NO_3$		
21	563.37	563.3707	1	$[M+H]^+$	PA(26:1)	$C_{29}H_{55}O_8P$		
22	564.54	564.5350	9	$[M+H]^+$	Cer(d36:2)	$C_{36}H_{69}NO_3$	6	
23	565.46	565.4591	2	$[M+H]^+$	PA(O-28:0)	$C_{31}H_{65}O_6P$		
24	566.46	566.4544	10	$[M+H]^+$	PC(O-22:0)	$C_{30}H_{64}NO_6P$		
25	576.48	576.4753	8	$[M+K]^+$	Cer(d34:1)	$C_{34}H_{67}NO_3$		
26	578.49	578.4909	2	$[M+K]^+$	Cer(d34:0)	$C_{34}H_{69}NO_3$		
27	580.4	580.3972	5	$[M+H]^+$	PE(24:0)	$C_{29}H_{58}NO_8P$		
28	602.32	602.3219	3	$[M+K]^+$	PC(20:1)	$C_{28}H_{54}NO_8P$	6	

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment: Ion form	Assignment: Compound	Assignment: Molecular formula	Ref.	Structurally specific CID ions (m/z)[a]
29	609.45	609.4489	2	$[M+K]^+$	DG(34:5)	$C_{37}H_{62}O_5$		
30	611.39	611.3918	3	$[M+H]^+$	PG(24:0)	$C_{30}H_{59}O_{10}P$		
31	651.46	651.4595	1	$[M+H]^+$	PG(P-28:0)	$C_{34}H_{67}O_9P$		
32	706.42	706.4182	3	$[M+K]^+$	PG(28:0)	$C_{34}H_{68}O_{10}P$		
33	707.65	707.6548	7	$[M+H]^+$	DG(42:1)	$C_{45}H_{86}O_5$		
34	709.42	709.4205	1	$[M+K]^+$	PA(34:3)	$C_{37}H_{67}O_8P$	6	
35	710.5	710.4968	5	$[M+K]^+$	GlcCer(d32:1)	$C_{38}H_{73}NO_8$	6	
36	711.53	711.5299	0	$[M+Na]^+$	PA(O-36:1)	$C_{39}H_{77}O_7P$	6	
37	712.43	712.4314	2	$[M+K]^+$	PC(28:2)	$C_{36}H_{68}NO_8P$		
38	713.41	713.4153	7	$[M+Na]^+$	PA(36:7)	$C_{39}H_{63}O_8P$	2	
39	714.5	714.5044	6	$[M+Na]^+$	PE(32:0)	$C_{37}H_{74}NO_8P$		
40	720.55	720.5538	5	$[M+H]^+$	PE(34:0)	$C_{39}H_{78}NO_8P$	46	267, 44, 27
41	722.4	722.4004	1	$[M+Na]^+$	PS(30:4)	$C_{36}H_{62}NO_{10}P$		
42	724.57	724.5697	0	$[M+Na]^+$	GlcCer(d34:0)	$C_{40}H_{79}NO_8$		
43	725.56	725.5568	4	$[M+Na]^+$	SM(d34:1)	$C_{39}H_{79}N_2O_6P$	7	703, 184
44	726.59	726.5878	3	$[M+H]^+$	GlcCer(d36:2)	$C_{42}H_{79}NO_8$		
45	727.47	727.4698	0	$[M+K]^+$	DG(42:10)	$C_{45}H_{68}O_5$	6	
46	731.56	731.5585	2	$[M+H]^+$	PA(38:1)	$C_{41}H_{79}O_8P$	1	447, 293, 239
47	732.48	732.4810	1	$[M+H]^+$	PS(32:2)	$C_{38}H_{70}NO_{10}P$		
48	734.50	734.4967	4	$[M+H]^+$	PS(32:1)	$C_{38}H_{72}NO_{10}P$		
49	735.53	735.5324	3	$[M+K]^+$	DG(42:6)	$C_{45}H_{76}O_5$		385, 311, 283
50	736.54	736.5334	9	$[M+Na]^+$	GlcCer(d34:2)	$C_{40}H_{75}NO_9$		
51	737.54	737.5456	8	$[M+Na]^+$	PA(O-38:2)	$C_{41}H_{79}O_7P$		
52	738.44	738.4471	10	$[M+K]^+$	PC(30:3)	C38H70NO8P		
53	739.43	739.4309	1	$[M+Na]^+$	PA(38:8)	$C_{41}H_{65}O_8P$		
54	740.46	740.4627	4	$[M+K]^+$	PC(30:2)	$C_{38}H_{72}NO_8P$	47	436, 249, 88
55	741.47	741.4677	3	$[M+Na]^+$	PG(32:2)	$C_{38}H_{71}O_{10}P$	48	
56	742.51	742.5147	6	$[M+K]^+$	PE(P-34:0)	$C_{39}H_{78}NO_7P$	3	
57	746.54	746.5330	9	$[M+H]^+$	PS(P-34:1)	$C_{40}H_{76}NO_9P$		
58	750.51	750.5068	4	$[M+H]^+$	PC(34:6)	$C_{42}H_{72}NO_8P$		311, 283, 88
59	752.44	752.4473	10	$[M+Na]^+$	PS(32:3)	$C_{38}H_{68}NO_{10}P$		
60	753.55	753.5429	9	$[M+H]^+$	PA(40:4)	$C_{43}H_{77}O_8P$	2	

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a]
				Ion form	Compound	Molecular formula		
61	754.57	754.5721	3	$[M+Na]^+$	PE(P-36:0)	$C_{41}H_{82}NO_7P$	49	
62	755.56	755.5674	10	$[M+Na]^+$	PE-Cer(d38:1)	$C_{40}H_{81}N_2O_7P$		
63	756.50	756.494	8	$[M+K]^+$	PE(34:1)	$C_{39}H_{76}NO_8P$	1	265, 44, 27
64	757.42	757.4205	1	$[M+K]^+$	PA(38:7)	$C_{41}H_{67}O_8P$		
65	758.48	758.4733	9	$[M+K]^+$	PS(O-32:1)	$C_{38}H_{74}NO_9P$		
66	759.46	759.4573	4	$[M+K]^+$	PG(32:1)	$C_{38}H_{73}O_{10}P$	50	
67	760.49	760.4889	1	$[M+K]^+$	PS(O-32:0)	$C_{38}H_{76}NO_9P$		
68	761.55	761.5480	3	$[M+H]^+$	PA(P-42:6)	$C_{45}H_{77}O_7P$		433, 311, 279, 98
69	762.54	762.5408	1	$[M+Na]^+$	PC(O-34:4)	$C_{42}H_{78}NO_7P$	51	
70	763.58	763.5847	6	$[M+H]^+$	PG(P-36:0)	$C_{42}H_{83}O_9P$		
71	764.55	764.5565	9	$[M+Na]^+$	PC(P-34:2)	$C_{42}H_{80}NO_7P$		
72	765.49	765.4912	2	$[M+H]^+$	PI(P-30:1)	$C_{39}H_{73}O_{12}P$		
73	766.51	766.5147	6	$[M+K]^+$	PE(P-36:2)	$C_{41}H_{78}NO_7P$	49	283, 44, 27
74	767.54	767.5464	8	$[M+K]^+$	SM(d36:2)	$C_{41}H_{81}N_2O_6P$	52	
75	768.5	768.4940	8	$[M+K]^+$	PC(32:2)	$C_{40}H_{76}NO_8P$	53	
76	769.53	769.5256	6	$[M+K]^+$	PE-Cer(d38:2)	$C_{40}H_{79}N_2O_7P$		
77	770.51	770.5095	1	$[M+Na]^+$	PE(P-38:6)	$C_{43}H_{74}NO_7P$	54	
78	771.52	771.5171	4	$[M+H]^+$	PG(36:4)	$C_{42}H_{75}O_{10}P$	1, 55	
79	772.53	772.5253	6	$[M+K]^+$	PC(32:0)	$C_{40}H_{80}NO_8P$	7, 56, 57	
80	773.53	773.5303	0	$[M+Na]^+$	PG(34:0)	$C_{40}H_{79}O_{10}P$		
81	774.54	774.5408	1	$[M+Na]^+$	PE(38:4)	$C_{43}H_{78}NO_7P$	1	
82	775.55	775.5484	2	$[M+H]^+$	PG(36:2)	$C_{42}H_{79}O_{10}P$	50, 58	603, 293, 251, 75
83	778.51	778.5147	6	$[M+K]^+$	PC(P-34:3)	$C_{42}H_{78}NO_7P$		
84	779.47	779.4705	1	$[M+H]^+$	PI(30:2)	$C_{39}H_{71}O_{13}P$	2	
85	780.5	780.4940	8	$[M+K]^+$	PE(36:3)	$C_{41}H_{76}NO_8P$	2	619, 267, 44
86	782.54	782.5460	8	$[M+K]^+$	PC(P-34:1)	$C_{42}H_{82}NO_7P$	59	
87	783.55	783.5510	1	$[M+Na]^+$	PG(P-36:1)	$C_{42}H_{81}O_9P$		
88	784.52	784.5123	10	$[M+H]^+$	PS(36:4)	$C_{42}H_{74}NO_{10}P$		287, 88, 42
89	785.54	785.5456	7	$[M+Na]^+$	PA(O-42:6)	$C_{45}H_{79}O_7P$		
90	786.54	786.5409	1	$[M+K]^+$	PE(36:0)	$C_{41}H_{82}NO_8P$	1	
91	787.67	787.6688	2	$[M+H]^+$	SM(d40:1)	$C_{45}H_{91}N_2O_6P$		702, 604, 586,

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (m/z)[a]
				Ion form	Compound	Molecular formula		
92	788.55	788.5436	8	$[M+H]^+$	PS(36:2)	$C_{42}H_{78}NO_{10}P$		
93	789.57	789.5769	9	$[M+Na]^+$	PA(O-42:4)	$C_{45}H_{83}O_7P$		
94	790.56	790.5593	1	$[M+H]^+$	PS(36:1)	$C_{42}H_{80}NO_{10}P$	60	703, 446, 299, 281
95	791.59	791.5925	3	$[M+Na]^+$	PA(P-42:2)	$C_{45}H_{85}O_7P$		
96	794.53	794.5306	1	$[M+Na]^+$	PS(O-36:3)	$C_{42}H_{78}NO_9P$		
97	795.49	795.4935	4	$[M+Na]^+$	PA(42:8)	$C_{45}H_{73}O_8P$		
98	796.52	796.5253	7	$[M+K]^+$	PC(34:2)	$C_{42}H_{80}NO_8P$	7, 61, 62	740, 184
99	797.54	797.5457	7	$[M+K]^+$	PA(40:1)	$C_{43}H_{83}O_8P$		
100	798.54	798.5410	1	$[M+K]^+$	PC(34:1)	$C_{42}H_{82}NO_8P$	61, 63, 64	742, 184, 88
101	799.61	799.6090	1	$[M+K]^+$	SM(d38:0)	$C_{43}H_{89}N_2O_6P$		
102	800.55	800.5565	8	$[M+Na]^+$	PE(P-40:5)	$C_{45}H_{80}NO_7P$	1	
103	801.57	801.5616	10	$[M+Na]^+$	PG(36:0)	$C_{42}H_{83}O_{10}P$	65	
104	802.52	802.5147	7	$[M+K]^+$	PC(P-36:5)	$C_{44}H_{78}NO_7P$		
105	803.56	803.5585	2	$[M+H]^+$	PA(44:7)	$C_{47}H_{79}O_8P$		
106	804.61	804.6113	2	$[M+H]^+$	PS(P-38:0)	$C_{44}H_{86}NO_9P$		
107	806.55	806.5460	5	$[M+K]^+$	PC(O-36:4)	$C_{44}H_{82}NO_7P$	16, 59	
108	807.55	807.5510	1	$[M+Na]^+$	PG(O-38:4)	$C_{44}H_{81}O_9P$		
109	808.56	808.5617	2	$[M+K]^+$	PC(P-36:2)	$C_{44}H_{84}NO_7P$	59	
110	809.6	809.6031	4	$[M+Na]^+$	PA(42:1)	$C_{45}H_{87}O_8P$		
111	810.6	810.6007	1	$[M+H]^+$	PC(38:4)	$C_{46}H_{84}NO_8P$	61, 66	792, 751, 627, 184
112	811.58	811.5823	3	$[M+Na]^+$	PG(O-38:2)	$C_{44}H_{85}O_9P$		
113	812.54	812.5436	4	$[M+H]^+$	PS(38:4)	$C_{44}H_{78}NO_{10}P$	18	725, 436, 315, 287
114	814.41	814.4056	5	$[M+K]^+$	PS(36:8)	$C_{42}H_{66}NO_{10}P$		456, 259, 88
115	816.57	816.5749	6	$[M+H]^+$	PS(38:2)	$C_{44}H_{82}NO_{10}P$		337, 88
116	820.56	820.5617	2	$[M+K]^+$	PE(P-40:3)	$C_{45}H_{84}NO_7P$	67	
117	821.59	821.5933	4	$[M+K]^+$	SM(d40:3)	$C_{45}H_{87}N_2O_6P$		
118	822.56	822.5619	2	$[M+Na]^+$	PS(P-38:2)	$C_{44}H_{82}NO_9P$		
119	823.57	823.5695	1	$[M+H]^+$	PI(O-34:1)	$C_{43}H_{83}O_{12}P$		
120	824.55	824.5566	8	$[M+K]^+$	PC(36:2)	$C_{44}H_{84}NO_8P$	7, 63	621, 603, 560, 448, 339, 321, 209, 88

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a]
				Ion form	Compound	Molecular formula		
121	825.45	825.4524	3	$[M+Na]^+$	PI(32:4)	$C_{41}H_{71}O_{13}P$		
122	826.58	826.5804	0	$[M+H]^+$	PI-Cer(t36:0)	$C_{42}H_{84}NO_{12}P$		
123	827.46	827.4681	10	$[M+Na]^+$	PI(32:3)	$C_{41}H_{73}O_{13}P$		539, 249, 223, 163
124	828.56	828.5538	7	$[M+H]^+$	PC(40:9)	$C_{48}H_{78}NO_8P$	7	
125	829.53	829.5354	7	$[M+Na]^+$	PG(P-40:6)	$C_{46}H_{79}O_9P$		
126	830.5	830.4943	7	$[M+Na]^+$	PS(38:6)	$C_{44}H_{74}NO_{10}P$	15	721, 641, 623, 462, 285
127	831.51	831.5018	10	$[M+H]^+$	PI(34:4)	$C_{43}H_{75}O_{13}P$		577, 261, 237, 181
128	832.62	832.6191	1	$[M+Na]^+$	PE(O-42:4)	$C_{47}H_{8}8NO_7P$		
129	833.6	833.6031	4	$[M+Na]^+$	PA(44:3)	$C_{47}H_{87}O_8P$		
130	834.6	834.6007	1	$[M+H]^+$	PC(40:6)	$C_{48}H_{84}NO_8P$	7, 57, 66	
131	835.58	835.5823	3	$[M+Na]^+$	PG(P-40:3)	$C_{46}H_{85}O_9P$		
132	836.54	836.5412	1	[M+Na]+	PS(38:3)	$C_{44}H_{80}NO_{10}P$	17	727, 508, 279
133	838.61	838.6086	2	$[M+K]^+$	PC(O-38:2)	$C_{46}H_{90}NO_7P$	68	
134	839.61	839.6136	4	$[M+Na]^+$	PG(O-40:2)	$C_{46}H_{89}O_9P$		
135	840.62	840.6243	5	$[M+K]^+$	PC(O-38:1)	$C_{46}H_{92}NO_7P$		
136	844.52	844.5253	6	$[M+K]^+$	PC(38:6)	$C_{46}H_{80}NO_8P$	7, 56, 66	
137	845.53	845.5303	0	$[M+Na]^+$	PG(40:6)	$C_{46}H_{79}O_{10}P$	60, 69	
138	846.51	846.5046	6	$[M+K]^+$	PE(40:6)	$C_{45}H_{78}NO_9P$		327, 267, 239, 44
139	848.61	848.6140	5	$[M+Na]^+$	PE(42:3)	$C_{47}H_{88}NO_8P$	55	
140	849.62	849.6246	5	$[M+K]^+$	SM(d42:3)	$C_{47}H_{91}N_2O_6P$	70, 71	
141	850.64	850.6320	9	$[M+H]^+$	PE(44:5)	$C_{49}H_{88}NO_8P$	72	
142	851.60	851.6008	1	$[M+H]^+$	PI(O-36:1)	$C_{45}H_{87}O_{12}P$		
143	852.62	852.6243	5	$[M+K]^+$	PE(P-42:1)	$C_{47}H_{92}NO_7P$		
144	852.59	852.5879	2	$[M+K]^+$	PC(38:2)	$C_{46}H_{88}NO_8P$	59	
145	853.57	853.5719	2	$[M+K]^+$	PG(P-40:2)	$C_{46}H_{87}O_9P$		
146	854.55	854.5460	5	$[M+K]^+$	PC(P-40:7)	$C_{48}H_{82}NO_7P$		
147	855.50	855.5018	2	$[M+H]^+$	PI(36:6)	$C_{45}H_{75}O_{13}P$		
148	856.51	856.5099	0	$[M+Na]^+$	PS(40:7)	$C_{46}H_{76}NO_{10}P$		747, 528, 287, 88
149	864.62	864.6243	5	$[M+K]^+$	PC(P-40:2)	$C_{48}H_{92}NO_7P$		

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (m/z)[a]
				Ion form	Compound	Molecular formula		
150	865.58	865.5801	0	$[M+H]^+$	PI(36:1)	$C_{45}H_{85}O_{13}P$	3	
151	866.61	866.6036	7	$[M+K]^+$	PE(42:2)	$C_{47}H_{90}NO_8P$	1	
152	867.56	867.5512	10	$[M+K]^+$	PG(40:3)	$C_{46}H_{85}O_{10}P$		519, 311
153	868.52	868.5253	6	$[M+K]^+$	PC(40:8)	$C_{48}H_{80}NO_8P$	73	
154	869.55	869.5514	2	$[M+Na]^+$	PI(O-36:3)	$C_{45}H_{83}O_{12}P$		
155	870.54	870.5410	1	$[M+K]^+$	PC(40:7)	$C_{48}H_{82}NO_8P$		649, 287, 88
156	871.48	871.4733	8	$[M+K]^+$	PI(34:3)	C43H77O13P		
157	872.55	872.5566	8	$[M+K]^+$	PC(40:6)	$C_{48}H_{84}NO_8P$		
158	873.48	873.4890	10	$[M+K]^+$	PI(34:2)	$C_{43}H_{79}O_{13}P$		
159	874.48	874.4783	2	$[M+K]^+$	PE(44:12)	$C_{49}H_{74}NO_8P$	74	
160	508.41	508.4122	4	$[M+H]^+$	DG(28:0)	$C_{31}H_{55}D_5O_5$	75	
	530.39	530.3942	8	$[M+Na]^+$		$C_{31}H_{55}D_5O_5$		
161	533.42	533.4176	4	$[M+Na]^+$	DG(28:1)	$C_{31}H_{58}O_5$		
	549.39	549.3916	3	$[M+K]^+$				

a) Structurally specific CID ions of lipids were detected by LC-MS/MS using CID. Fragment ions shown in blue were detected by *in situ* MALDI-MS/MS. Abbreviations: PC, phosphatidylcholine; PE, phosphatidylethanolamine; PA, phosphatidic acid; PG, phosphatidylglycerol; PS, phosphatidylserine; PI, phosphatidylinositol; Cer, ceramide; GlcCer, glycosylceramide; PE-Cer, phosphatidylethanolamine-ceramide; PI-Cer, phosphatidylinositol-ceramide; SM, sphingomyelin; DG, diacylglycerol.

Table S6. Lipids detected and identified in the mouse brain tissue sections by MALDI-TOF MS in the positive-ion mode using DHB as the matrix.

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a)]
				Ion form	Compound	Molecular formula		
1	535.43	535.4333	6	$[M+Na]^+$	DG(28:0)	$C_{31}H_{60}O_5$		
2	537.45	537.4514	3	$[M+H]^+$	DG(30:2)	$C_{33}H_{60}O_5$		311, 237, 181
3	706.47	706.4654	7	$[M+H]^+$	PS(30:1)	$C_{36}H_{68}NO_{10}P$		
4	723.47	723.4725	3	$[M+K]^+$	PA(P-36:2)	$C_{39}H_{73}O_7P$		
5	731.57	731.5698	0	$[M+H]^+$	PE-Cer(d38:2)	$C_{40}H_{79}N_2O_7P$		
6	734.57	734.5694	1	$[M+H]^+$	PC(32:0)	$C_{40}H_{80}NO_8P$		
7	735.53	735.5324	3	$[M+K]^+$	DG(42:6)	$C_{45}H_{76}O_5$		385, 313, 285
8	736.49	736.4888	2	$[M+Na]^+$	PE(34:3)	$C_{39}H_{72}NO_8P$		
9	751.39	751.3947	6	$[M+K]^+$	PG(32:5)	$C_{38}H_{65}O_{10}P$		
10	753.52	753.5195	1	$[M+K]^+$	PA(P-38:1)	$C_{41}H_{79}O_7P$		
11	754.51	754.5147	6	$[M+K]^+$	PC(P-32:1)	$C_{40}H_{78}NO_7P$	[67]	
12	756.50	756.4940	8	$[M+K]^+$	PE(34:1)	$C_{39}H_{76}NO_8P$	[1, 59]	265, 44, 27
13	758.47	758.4733	4	$[M+K]^+$	PS(P-32:0)	$C_{38}H_{74}NO_9P$		
14	759.46	759.4573	4	$[M+K]^+$	PG(32:1)	$C_{38}H_{73}O_{10}P$		
15	760.49	760.4889	1	[M+K]+	PS(O-32:0)	$C_{38}H_{76}NO_9P$		
16	761.55	761.5480	3	$[M+H]^+$	PA(P-42:6)	$C_{45}H_{77}O_7P$		433, 311, 279, 98
17	762.51	762.5068	4	$[M+H]^+$	PE(38:7)	$C_{43}H_{72}NO_8P$	[72, 76]	
18	763.48	763.4732	9	$[M+Na]^+$	PI(O-28:0)	$C_{37}H_{73}O_{12}P$		
19	766.50	766.4993	1	$[M+Na]^+$	PS(P-34:2)	$C_{40}H_{74}NO_9P$		
20	770.43	770.4369	9	$[M+K]^+$	PS(32:2)	$C_{38}H_{70}NO_{10}P$	[77]	
21	771.48	771.4725	10	$[M+K]^+$	PA(P-40:6)	$C_{43}H_{73}O_7P$		
22	772.45	772.4525	3	$[M+K]^+$	PS(32:1)	$C_{38}H_{72}NO_{10}P$	[48]	
23	773.49	773.4882	2	$[M+K]^+$	PA(O-40:6)	$C_{43}H_{75}O_7P$		
24	774.47	774.4682	2	$[M+K]^+$	PS(32:0)	$C_{38}H_{74}NO_{10}P$	[9]	
25	775.47	775.4675	3	$[M+K]^+$	PA(39:5)	$C_{42}H_{73}O_8P$	[78]	
26	779.72	779.7123	10	$[M+H]^+$	TG(46:0)	$C_{49}H_{94}O_6$	[79]	
27	782.47	782.4731	4	$[M+Na]^+$	PE(38:8)	$C_{43}H_{70}NO_8P$		
28	783.50	783.5018	2	$[M+H]^+$	PI(30:0)	$C_{39}H_{75}O_{13}P$		765, 559, 541, 225
29	784.51	784.5123	3	$[M+H]^+$	PS(36:4)	$C_{42}H_{74}NO_{10}P$		289, 88, 42

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a]
				Ion form	Compound	Molecular formula		
30	786.48	786.4834	4	$[M+K]^+$	PE(P-38:6)	$C_{43}H_{74}NO_7P$	1, 59	
31	788.50	788.4991	1	$[M+K]^+$	PE(P-38:5)	$C_{43}H_{74}NO_7P$	1	
32	789.50	789.5042	5	$[M+K]^+$	PG(34:0)	$C_{40}H_{79}O_{10}P$	80	
33	796.43	796.4314	2	$[M+K]^+$	PE(38:9)	$C_{43}H_{68}NO_8P$		
34	798.46	798.4682	10	$[M+K]^+$	PS(34:2)	$C_{40}H_{74}NO_{10}P$		
35	799.44	799.4368	4	$[M+Na]^+$	PI(30:3)	$C_{39}H_{69}O_{13}P$		
36	800.44	800.4473	9	$[M+Na]^+$	PS(36:7)	$C_{42}H_{68}NO_{10}P$		
37	801.45	801.4524	3	$[M+Na]^+$	PI(30:2)	$C_{39}H_{71}O_{13}P$	81	
38	802.48	802.4784	2	$[M+K]^+$	PE(38:6)	$C_{43}H_{74}NO_8P$	1	287, 44
39	806.49	806.4967	8	$[M+H]^+$	PS(38:7)	$C_{44}H_{72}NO_{10}P$		
40	810.50	810.5046	6	$[M+K]^+$	PS(O-36:3)	$C_{42}H_{78}NO_9P$		
41	811.49	811.4886	2	$[M+K]^+$	PG(36:3)	$C_{42}H_{77}O_{10}P$	82	
42	814.41	814.4056	5	$[M+K]^+$	PS(36:8)	$C_{42}H_{66}NO_{10}P$		456, 259, 88
43	824.44	824.4473	9	$[M+Na]^+$	PS(38:9)	$C_{44}H_{68}NO_{10}P$		
44	827.47	827.4681	2	$[M+Na]^+$	PI(32:3)	$C_{41}H_{73}O_{13}P$		539, 249, 223, 163
45	832.49	832.4888	1	$[M+Na]^+$	PE(42:11)	$C_{47}H_{72}NO_8P$		
46	839.48	839.4834	4	$[M+Na]^+$	PG(40:9)	$C_{46}H_{73}O_{10}P$		
47	848.49	848.4838	7	$[M+K]^+$	PS(38:5)	$C_{44}H_{76}NO_{10}P$	83	723, 500, 287
48	849.49	849.4890	1	$[M+K]^+$	PI(32:0)	$C_{41}H_{79}O_{13}P$		793, 569, 253, 181
49	850.50	850.4995	1	$[M+K]^+$	PS(38:4)	$C_{44}H_{78}NO_{10}P$	18	795, 490, 261, 88
50	864.49	864.4940	5	$[M+K]^+$	PC(40:10)	$C_{48}H_{76}NO_8P$	84	
51	866.51	866.5097	0	$[M+K]^+$	PC(40:9)	$C_{48}H_{78}NO_8P$	7	
52	822.51	822.5044	7	$[M+Na]^+$	PC(38:9)	$C_{46}H_{74}NO_8P$		
	838.48	838.4784	2	$[M+K]^+$				
53	769.50	769.5014	2	$[M+H]^+$	PG(36:5)	$C_{42}H_{73}O_{10}P$		
	807.46	807.4573	3	$[M+K]^+$				

a) Structurally specific CID ions of lipids were detected by LC-MS/MS using CID. Fragment ions shown in blue were detected by *in situ* MALDI-MS/MS. Abbreviations: PC, phosphatidylcholine; PE, phosphatidylethanolamine; PA, phosphatidic acid; PG, phosphatidylglycerol; PS, phosphatidylserine; PI, phosphatidylinositol; PE-Cer, phosphatidylethanolamine-ceramide; DG, diacylglycerol; TG, triglyceride.

Table S7. Lipids detected and identified in the germinating Chinese-yew seed tissue sections by MALDI-TOF MS in the positive-ion mode using DCH as the matrix.

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a)]
				Ion form	Compound	Molecular formula		
1	506.45	506.4544	9	$[M+Na]^+$	Cer(d30:0)	$C_{30}H_{61}NO_3$		
2	518.40	518.3970	6	$[M+K]^+$	Cer(d30:2)	$C_{30}H_{57}NO_3$		
3	520.38	520.3762	7	$[M+H]^+$	PC(P-19:1)	$C_{27}H_{54}NO_6P$		
4	523.38	523.3759	8	$[M+K]^+$	DG(26:0)	$C_{29}H_{56}O_5$		
5	524.41	524.4075	5	$[M+H]^+$	PC(O-19:0)	$C_{27}H_{58}NO_6P$		
6	525.45	525.4514	3	$[M+H]^+$	DG(29:1)	$C_{32}H_{60}O_5$		
7	526.52	526.5194	1	$[M+H]^+$	Cer(d33:0)	$C_{33}H_{67}NO_3$		
8	533.3	533.3004	1	$[M+K]^+$	PA(22:0)	$C_{25}H_{51}O_7P$	85	
9	535.44	535.4357	8	$[M+H]^+$	DG(30:3)	$C_{33}H_{58}O_5$		
10	539.47	539.4670	6	$[M+H]^+$	DG(30:1)	$C_{33}H_{62}O_5$		521, 339, 257, 183, 59
11	544.37	544.3737	7	$[M+Na]^+$	PC(O-19:1)	$C_{27}H_{56}NO_6P$		
12	545.42	545.4176	4	$[M+Na]^+$	DG(29:2)	$C_{32}H_{58}O_5$		
13	548.44	548.4440	7	$[M+K]^+$	Cer(32:1)	$C_{32}H_{63}NO_3$		492, 267
14	552.44	552.4388	2	$[M+H]^+$	PC(O-21:0)	$C_{29}H_{62}NO_6P$		
15	556.47	556.4700	0	$[M+Na]^+$	Cer(d34:3)	$C_{34}H_{63}NO_3$		
16	558.39	558.3894	1	$[M+Na]^+$	PC(P-20:0)	$C_{28}H_{58}NO_6P$		
17	560.40	560.4050	9	$[M+Na]^+$	PC(O-20:0)	$C_{28}H_{60}NO_6P$		
18	561.45	561.4514	2	$[M+H]^+$	DG(32:4)	$C_{35}H_{60}O_5$		543, 333, 259, 169
19	564.40	564.4024	4	$[M+H]^+$	LysoPE(24:1)	$C_{29}H_{58}NO_7P$		
20	584.50	584.5013	2	$[M+Na]^+$	Cer(d36:3)	$C_{36}H_{67}NO_3$		
21	615.43	615.4360	10	$[M+Na]^+$	PA(O-29:0)	$C_{32}H_{65}O_7P$		
22	629.42	629.4177	4	$[M+H]^+$	PA(31:3)	$C_{34}H_{61}O_8P$		415, 215, 169
23	631.47	631.4698	0	$[M+K]^+$	DG(34:2)	$C_{37}H_{68}O_5$		355, 295, 211
24	642.41	642.4105	1	$[M+Na]^+$	PE(27:1)	$C_{32}H_{62}NO_8P$		
25	660.40	660.4001	0	$[M+K]^+$	PE(27:0)	$C_{32}H_{64}NO_8P$		225, 44, 27
26	661.41	661.4051	7	$[M+Na]^+$	PG(26:0)	$C_{32}H_{63}O_{10}P$		
27	701.45	701.4517	2	$[M+Na]^+$	PA(P-36:5)	$C_{39}H_{67}O_7P$	82	377, 285, 223
28	739.46	739.4675	10	$[M+K]^+$	PA(36:2)	$C_{39}H_{73}O_8P$		475, 321, 209
29	749.51	749.5116	2	$[M+H]^+$	PA(40:6)	$C_{43}H_{73}O_8P$		651, 465, 435

No.	Measured m/z	Calculated m/z	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (m/z)[a]
				Ion form	Compound	Molecular formula		
30	750.44	750.4471	9	$[M+K]^+$	PE(34:4)	$C_{39}H_{70}NO_8P$		289, 44
31	751.68	751.6810	1	$[M+H]^+$	TG(44:0)	$C_{47}H_{90}O_6$		509, 225, 183, 127
32	752.43	752.4320	3	$[M+Na]^+$	PI(25:0)	$C_{34}H_{68}NO_{13}P$		
33	753.39	753.3892	1	$[M+K]^+$	PA(38:9)	$C_{41}H_{63}O_8P$		439, 285, 259, 98
34	756.55	756.5514	2	$[M+Na]^+$	PC(32:0)	$C_{40}H_{80}NO_8P$		716, 535, 309, 224, 169, 88
35	757.42	757.4205	1	$[M+K]^+$	PA(38:7)	$C_{41}H_{67}O_8P$		
36	758.44	758.4369	4	$[M+K]^+$	PS(31:1)	$C_{37}H_{70}NO_{10}P$		251, 88, 42
37	759.45	759.4573	10	$[M+K]^+$	PG(32:1)	$C_{38}H_{73}O_{10}P$		
38	760.58	760.5851	7	$[M+H]^+$	PC(34:1)	$C_{42}H_{82}NO_8P$		742, 577, 184, 88
39	761.47	761.4729	4	$[M+K]^+$	PG(32:0)	$C_{38}H_{75}O_{10}P$		
40	762.47	762.4680	3	$[M+Na]^+$	PS(P-34:4)	$C_{40}H_{70}NO_9P$		259, 88, 42
41	778.51	778.5147	6	$[M+K]^+$	PC(P-34:3)	$C_{42}H_{78}NO_7P$		
42	773.54	773.5327	9	$[M+H]^+$	PG(36:3)	$C_{42}H_{77}O_{10}P$	[82]	601, 263, 75
43	774.59	774.5854	6	$[M+Na]^+$	GlcCer(d38:3)	$C_{44}H_{81}NO_8$		
44	775.65	775.6576	10	$[M+K]^+$	DG(44:0)	$C_{45}H_{91}O_7P$		
45	777.69	777.6967	9	$[M+H]^+$	TG(46:1)	$C_{49}H_{92}O_6$	[86]	339, 265, 223, 197, 155
46	779.41	779.4107	1	$[M+K]^+$	PI(27:0)	$C_{36}H_{69}O_{13}P$		
47	780.48	780.4810	1	$[M+H]^+$	PS(36:6)	$C_{42}H_{70}NO_{10}P$		311, 88
48	781.44	781.4416	2	$[M+K]^+$	PG(34:4)	$C_{40}H_{71}O_{10}P$		
49	782.43	782.4369	9	$[M+K]^+$	PS(33:3)	$C_{39}H_{70}NO_{10}P$		559, 235, 88, 42
50	784.59	784.5827	9	$[M+Na]^+$	PC(34:0)	$C_{42}H_{84}NO_8P$		744, 184, 166
51	785.51	785.5093	1	$[M+K]^+$	PG(O-35:2)	$C_{41}H_{79}O_9P$		
52	786.48	786.4834	4	$[M+K]^+$	PE(P-38:6)	$C_{43}H_{74}NO_7P$	[59]	
53	787.67	787.6688	2	$[M+H]^+$	SM(d40:1)	$C_{45}H_{91}N_2O_6P$		751, 604, 447, 323, 88
54	788.52	788.5201	0	$[M+Na]^+$	PE(38:5)	$C_{43}H_{76}NO_8P$		
55	789.5	789.5042	5	$[M+K]^+$	PG(34:0)	$C_{40}H_{79}O_{10}P$		
56	790.4	790.4056	7	$[M+K]^+$	PS(34:6)	$C_{40}H_{66}NO_{10}P$	[87]	303, 181, 88,
57	791.43	791.4260	5	$[M+K]^+$	PG(35:6)	$C_{41}H_{69}O_{10}P$		

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a]
				Ion form	Compound	Molecular formula		
58	793.43	793.4264	5	$[M+K]^+$	PI(28:0)	$C_{37}H_{71}O_{13}P$		
59	795.45	795.4573	9	$[M+K]^+$	PG(35:4)	$C_{41}H_{73}O_{10}P$		
60	796.52	796.5253	7	$[M+K]^+$	PC(34:2)	$C_{42}H_{80}NO_8P$		740, 184
61	797.42	797.4211	1	$[M+Na]^+$	PI(30:4)	$C_{39}H_{67}O_{13}P$		
62	798.43	798.4317	2	$[M+Na]^+$	PS(36:8)	$C_{42}H_{66}NO_{10}P$		
63	799.44	799.4368	4	$[M+Na]^+$	PI(30:3)	$C_{39}H_{69}O_{13}P$		
64	800.53	800.5225	9	$[M+H]^+$	PC(38:9)	$C_{46}H_{74}NO_8P$		635, 285, 88
65	801.46	801.4549	6	$[M+H]^+$	PI(32:5)	$C_{41}H_{69}O_{13}P$		
	823.44	823.4368	4	$[M+Na]^+$				
66	806.44	806.4369	4	$[M+K]^+$	PS(35:5)	$C_{41}H_{70}NO_{10}P$		
67	808.45	808.4525	3	$[M+K]^+$	PS(35:4)	$C_{41}H_{72}NO_{10}P$		
68	810.57	810.5773	9	$[M+K]^+$	PC(P-36:1)	$C_{44}H_{86}NO_7P$		754, 184
69	812.47	812.4627	9	$[M+K]^+$	PC(36:8)	$C_{44}H_{72}NO_8P$		
70	813.45	813.4524	3	$[M+Na]^+$	PI(31:3)	$C_{40}H_{71}O_{13}P$		
71	814.51	814.5147	6	$[M+K]^+$	PE(P-40:6)	$C_{45}H_{78}NO_7P$		313, 44
72	815.46	815.4622	3	$[M+Na]^+$	PA(44:12)	$C_{47}H_{69}O_8P$		
73	816.42	816.4212	1	$[M+K]^+$	PS(36:7)	$C_{42}H_{68}NO_{10}P$		456, 259, 88, 42
74	817.46	817.4628	3	$[M+K]^+$	PI(P-31:1)	$C_{40}H_{75}O_{12}P$		
75	818.51	818.5097	0	$[M+K]^+$	PC(36:5)	$C_{44}H_{78}NO_8P$	2	
76	821.45	821.4577	9	$[M+K]^+$	PI(30:0)	$C_{39}H_{75}O_{13}P$		765, 583, 541, 225
77	822.44	822.4471	9	$[M+K]^+$	PS(36:10)	$C_{45}H_{70}NO_8P$		
78	824.45	824.4473	3	$[M+Na]^+$	PS(38:9)	$C_{44}H_{68}NO_{10}P$		617, 285, 88, 42
79	825.50	825.5042	5	$[M+K]^+$	PG(37:3)	$C_{43}H_{79}O_{10}P$		
80	826.48	826.4784	2	$[M+K]^+$	PE(40:8)	$C_{45}H_{74}NO_8P$		
81	827.49	827.4834	8	$[M+Na]^+$	PG(39:8)	$C_{45}H_{73}O_{10}P$		
82	828.48	828.4810	1	$[M+H]^+$	PS(40:10)	$C_{46}H_{70}NO_{10}P$		741, 526, 285
83	830.47	830.4733	4	$[M+K]^+$	PS(P-38:6)	$C_{44}H_{74}NO_9P$		775, 607, 436, 311, 223, 88
84	834.46	834.4682	10	$[M+K]^+$	PS(37:5)	$C_{43}H_{74}NO_{10}P$		
85	838.48	838.4784	2	$[M+K]^+$	PC(38:9)	$C_{46}H_{74}NO_8P$		635, 285, 88
86	846.47	846.4682	2	$[M+K]^+$	PS(38:6)	$C_{44}H_{74}NO_{10}P$		

No.	Measured *m/z*	Calculated *m/z*	Error |ppm|	Assignment			Ref.	Structurally specific CID ions (*m/z*)[a]
				Ion form	Compound	Molecular formula		
87	848.52	848.5201	0	$[M+Na]^+$	PC(40:10)	$C_{48}H_{76}NO_8P$	88	550, 311, 259, 88
88	851.47	851.4705	1	$[M+H]^+$	PI(36:8)	$C_{45}H_{71}O_{13}P$		
89	852.49	852.4940	5	$[M+K]^+$	PE(42:9)	$C_{47}H_{76}NO_8P$		315, 44
90	853.48	853.4837	4	$[M+Na]^+$	PI(34:4)	$C_{43}H_{75}O_{13}P$		
91	855.48	855.4784	2	$[M+K]^+$	PI(P-34:3)	$C_{43}H_{77}O_{12}P$		
92	870.54	870.5410	1	$[M+K]^+$	PC(40:7)	$C_{48}H_{82}NO_8P$		649, 269, 88
93	872.55	872.5566	8	$[M+K]^+$	PC(40:6)	$C_{48}H_{84}NO_8P$		816, 761, 184, 88
94	919.57	919.5672	3	$[M+K]^+$	PI(37:0)	$C_{46}H_{89}O_{13}P$		
95	921.59	921.5827	8	$[M+Na]^+$	PI(O-40:5)	$C_{49}H_{87}O_{12}P$		
96	979.48	979.4710	9	$[M+K]^+$	PIP(36:3)	$C_{45}H_{82}O_{16}P_2$		

a) Structurally specific CID ions of lipids were detected by LC-MS/MS using CID. Fragment ions shown in blue were detected by *in situ* MALDI-MS/MS. Abbreviations: PC, phosphatidylcholine; PE, phosphatidylethanolamine; lysoPE, lysophosphatidylethanolamine; PA, phosphatidic acid; PG, phosphatidylglycerol; PS, phosphatidylserine; PI, phosphatidylinositol; PIP, Phosphatidylinositol monophosphate; Cer, ceramide; GlcCer, glycosylceramide; SM, sphingomyelin; DG, diacylglycerol; TG, triglyceride.

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