Supporting Information I

1 Purity determination of Neurons

To observe the purity of neurons 7 d after incubation, cortical neurons in culture plates were fixed by 4% paraformaldehyde for 20 min, blocked in antibody buffer with 20% goat serum, permeabilized with 0.2 % Triton X-100™and incubated in mouse anti-MAP2 antibody(Ab11267; 1:200; Abcam, Cambridge, UK) for 24 h at 4 ℃, incubated with FITC-labeled goat anti-rabbit IgG for 1.5 h at room temperature. Sections were washed in PBS after each step and finally visualized by laser scanning confocal microscopy (CLSM, Tokyo, Japan)

2 Oxygen-glucose deprivation (OGD)

After washing twice, control group were immersed in controlled salt solution (CSS, 120 mMNaCl, 5.4 mMKCl, 0.8 mM $MgCl_2$×6 H_2O, 1.8 mM $CaCl_2$×2 H_2O, 25 Mm Tris, 15 mM D-glucose, PH=7.2) and incubated at 37 °C in an incubator supplemented with 5 % CO2 for 3 h, 6 h, 9 h, 12 h. OGD group were immersed in deoxygenated controlled salt solution (CSSO, prepare for CSS, but substitute 15 mM D-glucose. Bubble the amount of solution needed for each experiment with N_2 for at least 10 min in the anaerobic chamber) and incubated at oxygen-free N2/CO2 (95%/5%) gas at 37 ℃ for 3 h, 6 h, 9 h, 12 h. Percentage of cell death was determined by LDH assay. A time interval, at which 50 % of cell mortality was observed, was utilized for further analysis.

3 Evaluation of edaravone protection effect against OGD

To determine the effect of edaravone, cultured cortical neurons were treated with 1 μM, 0.1 μM, 0.01 μM, 0.001 μM EDA for 6 h of OGD. The cell viability was quantitatively assessed by the measurement of LDH released into the bathing medium.

3 Results

At 7 d after plating, the cultures were used for the experiments. Confirmed by the use of mouse anti-MAP2 staining, the majority of cultured cells showed MAP2 immunoreactivity (Figure S1), which indicated that these cells were neurons and the purity was calculated over 87%. Later on, the cells further showed full of thick and projecting interweaving network. This stage was the best time for testing

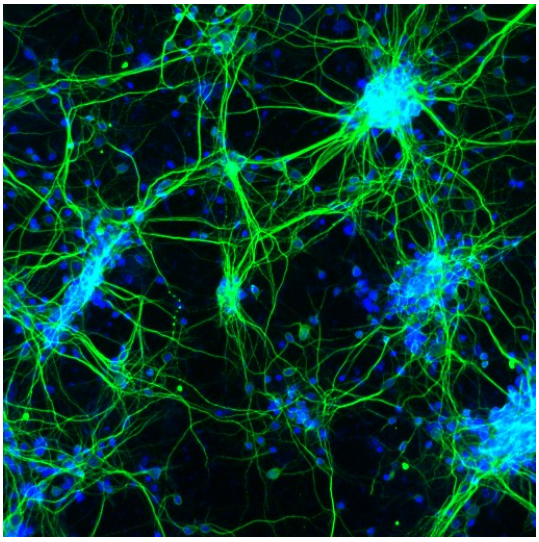

Figure S1. immunofluorescence staining of primary cortical neurons. MAP2 (green) and DAPI (blue). The purity of cortical neurons was calculated as over 87% (×200).

As shown in figure S2, LDH assay has shown time-dependent increase in cell mortality with OGD duration. At 3 and 6 h, 29.6 % and 48.5 % cell deaths, respectively, were observed, whereas at 9 h and 12 h exposure, the cell mortality had increased to 62.0 % and 72.7 %, respectively, in comparison to non-OGD control. Hence, 6 h OGD exposure was carried forward for evaluating neuroprotective efficacy of the molecules.

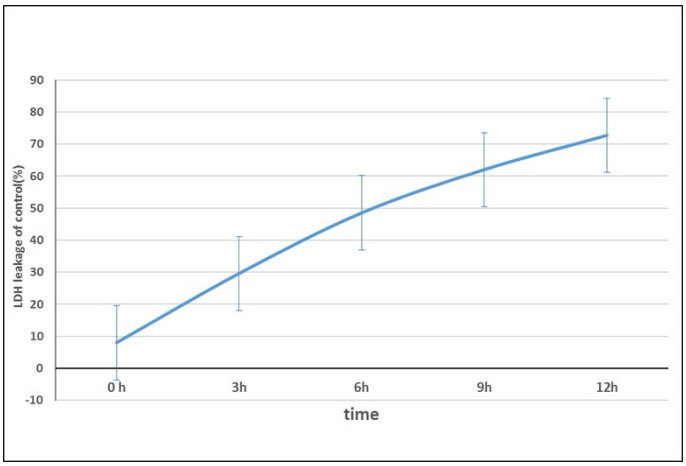

Figure S2. The extent of LDH release of OGD duration. Line chart represent mean, n>3.

As shown in the Figure S3, the leakage rate of LDH has dramatically decreased compared with OGD group which implying the cortical neuron injury after EDA treatment with 0.1 μM, 0.01 μM, 0.001 μM for 6 h of OGD. In addition, in the four doses of EDA-treated OGD groups, the dose of 0.01 μM of EDA had the best neuroprotective efficacy. So, the dose of 0.01 μM was chosen for the further analysis served as positive drugs.

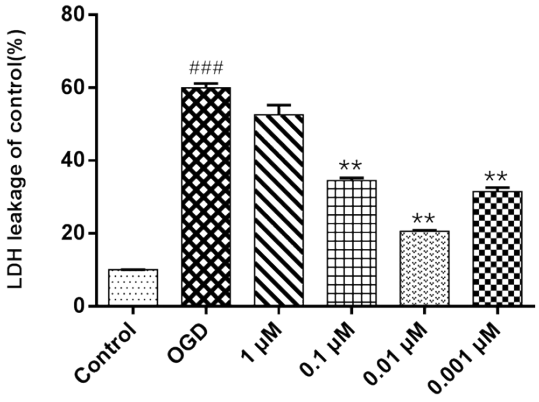

Figure S3. Effects of different concentrations of EDA on cell viability by LDH assay. $^{\#}P<0.05$, $^{\#\#}P<0.01$, $^{\#\#\#}P<0.001$ the OGD group versus the Control group; $^{*}P<0.05$, $^{**}P<0.01$, $^{***}P<0.001$ the DHI group (or positive group) versus the OGD group OGD. Histograms represent mean ± SD, n>3.

Supporting InformationII

In order to get a reliable result and improve the accuracy of lipid analysis, a target database including the accurately indentified98 PCs, 28 SMs and 41 Cers was constructed on the LC-MS platform in advance by the internal standard standards and using the relative data of accurate masses and MS/MS fragments based on the organic samples. The internal standard mixes including PCs, SMs and Cers were purchased from Avanti Polar Lipids. Cer/Sph Mixture I (https://avantilipids.com/product/lm-6002/) PC(12:0/13:0) (https://avantilipids.com/product/lm-1000/).

Results

Separation for relative quantification of PCs, Cers, and SMs was performed by UltiMate™ 3000 Rapid Separation LC (RSLC) system (Thermo Scientific, USA). As stationary phase, an ACQUITY UPLC HSS T3 C18 column (1.8μM, 100x2.1mm, Waters^{TM}, USA) was used suited for polar compound retention. The mobile phase consisted of solvent A (0.1% formic acid-water containing 2 mM ammonium formate) and solvent B (methanol) with a gradient elution (0–2 min, 20-30% B; 2–5 min, 30-45% B; 5-6.5 min, 45-55% B; 6.5–12 min, 55-65% B; 12–14 min, 65-85% B; 14–17.5 min, 85-100% B; 17.5–18 min, 100–100% B). The re-equilibration was 2 minutes with 20% B. The flow rate of the mobile phase was 0.3 mL/min. The column temperature was maintained at 45 °C and the sample manager temperature was set at 4 °C.

A Thermo Scientific™ Q Exactive hybrid quadrupole Orbitrap mass spectrometer equipped with a HESI-II probe was used in the positive electrospray ionization mode. The pos HESI-II spray voltages were 3.7 kV, the heated capillary temperature was 320 °C, the sheath gas pressure was 30 psi, the auxiliary gas setting was 10 psi, and the heated vaporizer temperature was 300 °C. The parameters of the full mass scan were as follows: resolution of 70,000, auto gain control target under 1×10^6, maximum isolation time of 50 ms, and *m/z* range of 150–1500.

Table S1 The information of the identified PCs in the organicsamples for constructing the database on the LC-MS platform

No.	name	LM ID	Formula	Retention Time (min)	Detected ion and m/z
1	PC(0:0/14:0)	LMGP01050073	$C_{22}H_{46}NO_7P$	7.90	[M+H]+, 468.3085
2	PC(0:0/16:0)	LMGP01050074	$C_{24}H_{50}NO_7P$	7.14	[M+H]+, 496.3398
3	PC(0:0/16:1(9Z))	Not recorded in LIPID MAPS	$C_{24}H_{48}NO7P$	6.27	[M+H]+, 494.3241
4	PC(0:0/17:0)	Not recorded in LIPID MAPS	$C_{25}H_{52}NO7P$	8.77	[M+H]+, 510.3554
5	PC(0:0/18:0)	LMGP01050076	$C_{26}H_{54}NO_7P$	7.13	[M+H]+, 524.3711
6	PC(0:0/18:1(9Z))	LMGP01050082	$C_{26}H_{52}NO_7P$	7.41	[M+H]+, 522.3554
7	PC(0:0/18:2(9Z,12Z))	Not recorded in LIPID MAPS	$C_{26}H_{50}NO_7P$	6.73	[M+H]+, 520.3398
8	PC(0:0/19:0)	Not recorded in LIPID MAPS	$C_{27}H_{56}NO_7P$	6.55	[M+H]+, 538.3867
9	PC(0:0/20:2(11Z,14Z))	Not recorded in LIPID MAPS	$C_{28}H_{54}NO_7P$	7.72	[M+H]+, 548.3711
10	PC(0:0/20:3(8Z,11Z,14Z))	Not recorded in LIPID MAPS	$C_{28}H_{52}NO_7P$	6.17	[M+H]+, 546.3554
11	PC(0:0/20:4(5Z,8Z,11Z,14Z))	LMGP01050121	$C_{28}H_{50}NO_7P$	7.74	[M+H]+, 544.3398
12	PC(0:0/20:5(5Z,8Z,11Z,14Z,17Z))	Not recorded in LIPID MAPS	$C_{28}H_{48}NO_7P$	7.12	[M+H]+, 542.3241
13	PC(0:0/22:4(7Z,10Z,13Z,16Z))	Not recorded in LIPID MAPS	$C_{30}H_{54}NO_7P$	8.67	[M+H]+, 572.3711
14	PC(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	Not recorded in LIPID MAPS	$C_{30}H_{50}NO_7P$	8.73	[M+H]+, 568.3398
15	PC(14:0/0:0)	LMGP01050012	$C_{22}H_{46}NO_7P$	8.13	[M+H]+, 468.3085
16	PC(14:0/18:2(9Z,12Z))	LMGP01010496	$C_{40}H_{76}NO_8P$	8.49	[M+H]+, 730.5381
17	PC(16:0/0:0)	LMGP01050018	$C_{24}H_{50}NO_7P$	8.59	[M+H]+, 496.3398
18	PC(16:0/14:0)	LMGP01010560	$C_{38}H_{76}NO_8P$	8.87	[M+H]+, 706.5381
19	PC(16:0/16:0)	LMGP01010564	$C_{40}H_{80}NO_8P$	9.47	[M+H]+, 734.5694
20	PC(16:0/17:1(9Z))	LMGP01010571	$C_{41}H_{80}NO_8P$	9.25	[M+H]+, 746.5694
21	PC(16:0/18:1(9Z))	LMGP01010005	$C_{42}H_{82}NO_8P$	9.56	[M+H]+, 760.5851
22	PC(16:0/20:4(5Z,8Z,11Z,14Z))	LMGP01010007	$C_{44}H_{80}NO_8P$	9.03	[M+H]+, 782.5694
23	PC(16:0/9:0(CHO))	LMGP20010008	$C_{33}H_{64}NO_9P$	6.11	[M+H]+, 650.4391
24	PC(16:1(9Z)/0:0)	LMGP01050022	$C_{24}H_{48}NO_7P$	4.55	[M+H]+, 494.3241
25	PC(16:1(9Z)/14:0)	LMGP01011475	$C_{38}H_{74}NO_8P$	8.45	[M+H]+, 704.5225
26	PC(16:1(9Z)/16:0)	LMGP01011479	$C_{40}H_{78}NO_8P$	8.98	[M+H]+, 732.5538
27	PC(17:0/0:0)	LMGP01050024	$C_{25}H_{52}NO_7P$	6.91	[M+H]+, 510.3554
28	PC(17:1(9Z)/0:0)	LMGP01050126	$C_{25}H_{50}NO_7P$	7.14	[M+H]+, 508.3398
29	PC(18:0/0:0)	LMGP01050026	$C_{26}H_{54}NO_7P$	8.88	[M+H]+, 524.3711
30	PC(18:0/16:0)	LMGP01010742	$C_{42}H_{84}NO_8P$	10.2	[M+H]+, 762.6007
31	PC(18:0/18:0)	LMGP01010006	$C_{44}H_{88}NO_8P$	11.09	[M+H]+, 790.632
32	PC(18:0/18:1(9Z))	LMGP01010761	$C_{44}H_{86}NO_8P$	10.3	[M+H]+, 788.6164
33	PC(18:0/18:2(9Z,12Z))	LMGP01010768	$C_{44}H_{84}NO_8P$	9.75	[M+H]+, 786.6007
34	PC(18:0/20:2(5Z,14Z))	LMGP01010790	$C_{46}H_{88}NO_8P$	10.54	[M+H]+, 814.632
35	PC(18:0/20:3(8Z,11Z,14Z))	LMGP01010799	$C_{46}H_{86}NO_8P$	9.97	[M+H]+, 812.6164
36	PC(18:0/22:5(7Z,10Z,13Z,16Z,19Z))	LMGP01010818	$C_{48}H_{86}NO_8P$	12.06	[M+H]+, 836.6164
37	PC(18:1(9Z)/0:0)	LMGP01050032	$C_{26}H_{52}NO_7P$	7.65	[M+H]+, 522.3554
38	PC(18:1(9Z)/17:0)	LMGP01011600	$C_{43}H_{84}NO_8P$	9.91	[M+H]+, 774.6007
39	PC(18:1(9Z)/19:0)	LMGP01011605	$C_{45}H_{88}NO_8P$	10.75	[M+H]+, 802.632
40	PC(18:2(9Z,12Z)/0:0)	LMGP01050035	$C_{26}H_{50}NO_7P$	8.45	[M+H]+, 520.3398
41	PC(18:2(9Z,12Z)/15:0)	LMGP01011618	$C_{41}H_{78}NO_8P$	8.84	[M+H]+, 744.5538
42	PC(18:2(9Z,12Z)/16:0)	LMGP01010932	$C_{42}H_{80}NO_8P$	9.11	[M+H]+, 758.5694
43	PC(18:2(9Z,12Z)/17:0)	LMGP01011621	$C_{43}H_{82}NO_8P$	9.43	[M+H]+, 772.5851
44	PC(18:2(9Z,12Z)/19:0)	LMGP01011628	$C_{45}H_{86}NO_8P$	10.13	[M+H]+, 800.6164

45	PC(18:3(9Z,12Z,15Z)/0:0)	LMGP01050038	$C_{26}H_{48}NO_7P$	4.16	[M+H]+, 518.3241
46	PC(P-18:0/20:4(5Z,8Z,11Z,14Z))	LMGP01030012	$C_{46}H_{84}NO_7P$	9.5	[M+H]+, 794.6058
47	PC(18:3(9Z,12Z,15Z)/16:0)	LMGP01011677	$C_{42}H_{78}NO_8P$	8.83	[M+H]+, 756.5538
48	PC(19:0/0:0)	LMGP01050041	$C_{27}H_{56}NO_7P$	6.75	[M+H]+, 538.3867
49	PC(19:0/19:0)	LMGP01010976	$C_{46}H_{92}NO_8P$	12.26	[M+H]+, 818.6633
50	PC(20:0/0:0)	LMGP01050045	$C_{28}H_{58}NO_7P$	7.1	[M+H]+, 552.4024
51	PC(20:0/18:1(9Z))	LMGP01011010	$C_{46}H_{90}NO_8P$	11.18	[M+H]+, 816.6477
52	PC(20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	LMGP01011028	$C_{50}H_{88}NO_8P$	10.25	[M+H]+, 862.632
53	PC(20:2(11Z,14Z)/0:0)	LMGP01050132	$C_{28}H_{54}NO_7P$	5.95	[M+H]+, 548.3711
54	PC(20:3(8Z,11Z,14Z)/0:0)	LMGP01050133	$C_{28}H_{52}NO_7P$	5.41	[M+H]+, 546.3554
55	PC(20:3(8Z,11Z,14Z)/16:0)	LMGP01011872	$C_{44}H_{82}NO_8P$	9.2	[M+H]+, 784.5851
56	PC(20:4(5Z,8Z,11Z,14Z)/0:0)	LMGP01050048	$C_{28}H_{50}NO_7P$	4.96	[M+H]+, 544.3398
57	PC(20:4(5Z,8Z,11Z,14Z)/14:0)	LMGP01011899	$C_{42}H_{76}NO_8P$	8.53	[M+H]+, 754.5381
58	PC(20:4(5Z,8Z,11Z,14Z)/15:0)	LMGP01011901	$C_{43}H_{78}NO_8P$	8.87	[M+H]+, 768.5538
59	PC(20:4(5Z,8Z,11Z,14Z)/16:1(9Z))	LMGP01011903	$C_{44}H_{78}NO_8P$	8.82	[M+H]+, 780.5538
60	PC(20:4(5Z,8Z,11Z,14Z)/17:0)	LMGP01011904	$C_{45}H_{82}NO_8P$	9.34	[M+H]+, 796.5851
61	PC(20:4(5Z,8Z,11Z,14Z)/18:0)	LMGP01011907	$C_{46}H_{84}NO_8P$	9.65	[M+H]+, 810.6007
62	PC(20:4(5Z,8Z,11Z,14Z)/18:1(9Z))	LMGP01011908	$C_{46}H_{82}NO_8P$	9.15	[M+H]+, 808.5851
63	PC(20:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	LMGP01011909	$C_{46}H_{80}NO_8P$	8.76	[M+H]+, 806.5694
64	PC(20:4(5Z,8Z,11Z,14Z)/19:0)	LMGP01011913	$C_{47}H_{86}NO_8P$	10.01	[M+H]+, 824.6164
65	PC(20:4(5Z,8Z,11Z,14Z)/20:3(8Z,11Z,14Z))	LMGP01011918	$C_{48}H_{82}NO_8P$	9.03	[M+H]+, 832.5851
66	PC(20:4(5Z,8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	LMGP01011052	$C_{48}H_{80}NO_8P$	8.67	[M+H]+, 830.5694
67	PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	LMGP01050050	$C_{28}H_{48}NO_7P$	8.36	[M+H]+, 542.3241
68	PC(22:0/0:0)	LMGP01050053	$C_{30}H_{62}NO_7P$	7.73	[M+H]+, 580.4337
69	PC(22:4(7Z,10Z,13Z,16Z)/0:0)	LMGP01050124	$C_{30}H_{54}NO_7P$	5.79	[M+H]+, 572.3711
70	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	LMGP01050056	$C_{30}H_{50}NO_7P$	7.95	[M+H]+, 568.3398
71	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/14:0)	LMGP01012099	$C_{44}H_{76}NO_8P$	10..45	[M+H]+, 778.5381
72	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:0)	LMGP01011116	$C_{46}H_{80}NO_8P$	8.94	[M+H]+, 806.5694
73	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/17:0)	LMGP01012104	$C_{47}H_{82}NO_8P$	9.23	[M+H]+, 820.5851
74	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	LMGP01012107	$C_{48}H_{84}NO_8P$	9.52	[M+H]+ 834.6007
75	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	LMGP01011119	$C_{52}H_{80}NO_8P$	8.51	[M+H]+, 878.5694
76	PC(24:0/0:0)	LMGP01050057	$C_{32}H_{66}NO_7P$	8.27	[M+H]+, 608.465
77	PC(O-16:0/0:0)	LMGP01060010	$C_{24}H_{52}NO_6P$	8.84	[M+H]+ 482.3605
78	PC(O-16:0/16:0)	LMGP01020029	$C_{40}H_{82}NO_7P$	9.92	[M+H]+, 720.5902
79	PC(O-16:0/16:1(9Z))	LMGP01020182	$C_{40}H_{80}NO_7P$	9.34	[M+H]+, 718.5745
80	PC(O-16:0/18:1(9Z))	LMGP01020003	$C_{42}H_{84}NO_7P$	10.02	[M+H]+, 746.6058
81	PC(O-16:0/18:2(9Z,12Z))	LMGP01020039	$C_{42}H_{82}NO_7P$	9.5	[M+H]+, 744.5902
82	PC(O-16:0/18:3(9Z,12Z,15Z))	LMGP01020042	$C_{42}H_{80}NO_7P$	9.4	[M+H]+, 742.5745
83	PC(O-16:0/20:4(5Z,8Z,11Z,14Z))	LMGP01020056	$C_{44}H_{82}NO_7P$	9.43	[M+H]+, 768.5902
84	PC(O-16:0/22:4(7Z,10Z,13Z,16Z))	LMGP01020192	$C_{46}H_{86}NO_7P$	9.95	[M+H]+, 796.6215

85	PC(O-18:0/0:0)	LMGP01060014	$C_{26}H_{56}NO_6P$	9.25	[M+H]+, 510.3918
86	PC(O-18:0/16:0)	LMGP01020086	$C_{42}H_{86}NO_7P$	10.75	[M+H]+, 748.6215
87	PC(O-18:0/20:4(5Z,8Z,11Z,14Z))	LMGP01020102	$C_{46}H_{86}NO_7P$	10.13	[M+H]+, 796.6215
88	PC(O-20:0/20:4(5Z,8Z,11Z,14Z))	LMGP01020238	$C_{48}H_{90}NO_7P$	11.03	[M+H]+, 824.6528
89	PC(P-16:0/0:0)	LMGP01070006	$C_{24}H_{50}NO_6P$	8.83	[M+H]+, 480.3449
90	PC(P-16:0/18:1(9Z))	LMGP01030006	$C_{42}H_{82}NO_7P$	9.87	[M+H]+, 744.5902
91	PC(P-16:0/20:0)	LMGP01030036	$C_{44}H_{88}NO_7P$	10.94	[M+H]+, 774.6371
92	PC(P-16:0/20:4(5Z,8Z,11Z,14Z))	LMGP01030010	$C_{44}H_{80}NO_7P$	9.06	[M+H]+, 766.5745
93	PC(P-18:0/20:5(5Z,8Z,11Z,14Z,17Z))	LMGP01030068	$C_{46}H_{82}NO_7P$	9.31	[M+H]+, 792.5902
94	PC(P-18:0/0:0)	LMGP01070009	$C_{26}H_{54}NO_6P$	8.94	[M+H]+, 508.3762
95	PC(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	LMGP01030014	$C_{48}H_{84}NO_7P$	9.39	[M+H]+, 818.6058
96	PC(P-18:0/18:1(9Z))	LMGP01030013	$C_{44}H_{86}NO_7P$	10.26	[M+H]+, 772.6215
97	PC(P-18:0/18:2(9Z,12Z))	LMGP01030058	$C_{44}H_{84}NO_7P$	11.87	[M+H]+, 770.6058
98	PC(20:2/0:0)	Not recorded in LIPID MAPS	$C_{28}H_{54}NO_7P$	8.82	[M+H]+, 548.3711

Table S2 The information of SMs in the organic samples for constructing the database on the LC-MS platform

No	name	LM ID	Formula	Retention time (min)	Detected ion and m/z
1	SM (d18:1/16:0)	LMSP03010003	C39H79N2O6P	8.93	[M+H]+, 703.5749
2	SM (d18:1/18:1(9Z))	LMSP03010029	$C_{41}H_{81}N_2O_6P$	9.04	[M+H]+, 729.5905
3	SM(d16:0/20:0)	LMSP03010053	$C_{41}H_{85}N_2O_6P$	9.71	[M+H]+, 733.6218
4	SM(d16:1/16:0)	LMSP03010035	$C_{37}H_{75}N_2O_6P$	10.27	[M+H]+, 675.5436
5	SM(d16:1/17:0)	LMSP03010037	$C_{38}H_{77}N_2O_6P$	10.56	[M+H]+, 689.5592
6	SM(d16:1/18:0)	LMSP03010042	$C_{39}H_{79}N_2O_6P$	8.83	[M+H]+, 703.5749
7	SM(d16:1/18:1)	LMSP03010040	$C_{39}H_{77}N_2O_6P$	8.42	[M+H]+, 701.5592
8	SM(d16:1/20:1)	LMSP03010048	$C_{41}H_{81}N_2O_6P$	8.96	[M+H]+, 729.5905
9	SM(d16:1/24:1)	LMSP03010071	$C_{45}H_{89}N_2O_6P$	10.31	[M+H]+, 785.6531
10	SM(d17:1/24:0)	LMSP03010077	$C_{46}H_{93}N_2O_6P$	11.61	[M+H]+, 801.6844
11	SM(d18:0/16:0)	LMSP03010004	$C_{39}H_{81}N_2O_6P$	11.08	[M+H]+, 705.5905
12	SM(d18:1/12:0)	LMSP03010002	$C_{35}H_{71}N_2O_6P$	7.81	[M+H]+, 647.5123
13	SM(d18:1/18:0)	LMSP03010001	$C_{41}H_{83}N_2O_6P$	9.43	[M+H]+, 731.6062
14	SM(d18:1/19:0)	LMSP03010055	$C_{42}H_{85}N_2O_6P$	9.78	[M+H]+, 745.6218
15	SM(d18:1/20:0)	LMSP03010005	$C_{43}H_{87}N_2O_6P$	10.16	[M+H]+, 759.6375
16	SM(d18:1/22:0)	LMSP03010006	$C_{45}H_{91}N_2O_6P$	11.06	[M+H]+, 787.6688
17	SM(d18:1/24:0)	LMSP03010008	$C_{47}H_{95}N_2O_6P$	12.21	[M+H]+, 815.7001
18	SM(d18:2/14:0)	LMSP03010034	$C_{37}H_{73}N_2O_6P$	7.93	[M+H]+, 673.5279
19	SM(d18:2/18:1)	LMSP03010047	$C_{41}H_{79}N_2O_6P$	8.56	[M+H]+, 727.5749
20	SM(d18:2/20:0)	LMSP03010060	$C_{43}H_{85}N_2O_6P$	9.55	[M+H]+, 757.6218
21	SM(d18:2/24:0)	LMSP03010081	$C_{47}H_{93}N_2O_6P$	13.45	[M+H]+, 813.6844
22	SM(d18:2/24:1)	LMSP03010080	$C_{47}H_{91}N_2O_6P$	10.38	[M+H]+, 811.6688
23	SM(d19:1/20:0)	LMSP03010068	$C_{44}H_{89}N_2O_6P$	10.57	[M+H]+, 773.6531
24	SM(d20:1/23:0)	LMSP03010087	$C_{48}H_{97}N_2O_6P$	12.96	[M+H]+, 829.7157
25	SM(d18:1/17:0)	LMSP03010044	$C_{40}H_{81}N_2O_6P$	11.14	[M+H]+, 717.5905

26	SM(d17:1/24:1)	LMSP03010074	$C_{46}H_{91}N_2O_6P$	12.92	[M+H]+, 799.6687
27	SM(d18:2/23:0)	LMSP03010075	$C_{46}H_{91}N_2O_6P$	12.93	[M+H]+, 799.6687
28	SM(d18:1/24:1(15Z))	LMSP03010007	C47H93N2O6P	13.45	[M+H]+, 813.6844

Table S3 The information of Cers standards in the constructing database on the LC-MS platform

No	name	LM ID	Formular	Retention time (min)	Detected ion and m/z
1	Cer(d16:1/17:0)	LMSP02010015	$C_{33}H_{65}NO_3$	9.69	[M+H]+, 524.5037
2	Cer(d16:1/23:0)	LMSP02010017	$C_{39}H_{77}NO_3$	11.12	[M+H]+, 608.5976
3	Cer(d18:0/14:0)	LMSP02020016	$C_{32}H_{65}NO_3$	11.54	[M+H]+, 512.5037
4	Cer(d18:0/15:0)	LMSP02010019	$C_{33}H_{67}NO_3$	10.35	[M+H]+, 526.5194
5	Cer(d18:0/16:0)	LMSP02020001	$C_{34}H_{69}NO_3$	9.38	[M+H]+, 540.535
6	Cer(d18:0/18:0)	LMSP02020008	$C_{36}H_{73}NO_3$	15.39	[M+H]+, 568.5663
7	Cer(d18:0/22:0)	LMSP02020010	$C_{40}H_{81}NO_3$	12.13	[M+H]+, 624.6289
8	Cer(d18:0/24:0)	LMSP02020012	$C_{42}H_{85}NO_3$	13.63	[M+H]+, 652.6602
9	Cer(d18:0/24:1(15Z))	LMSP02020011	$C_{42}H_{83}NO_3$	12.22	[M+H]+, 650.6446
10	Cer(d18:0/h24:0)	LMSP02020017	$C_{42}H_{85}NO_4$	11.92	[M+H]+, 668.6551
11	Cer(d18:1/12:0)	LMSP02010002	C30H59NO3	10.04	[M+H]+, 482.4568
12	Cer(d18:1/14:0)	LMSP02010001	C32H63NO3	8.56	[M+H]+, 510.4881
13	Cer(d18:1/16:0)	LMSP02010004	C34H67NO3	9.11	[M+H]+, 538.5194
14	Cer(d18:1/18:0)	LMSP02010006	C36H71NO3	9.82	[M+H]+, 566.5507
15	Cer(d18:1/19:0)	LMSP02010032	C37H73NO3	10.19	[M+H]+, 580.5663
16	Cer(d18:1/20:0)	LMSP02010007	C38H75NO3	10.61	[M+H]+, 594.582
17	Cer(d18:1/22:0)	LMSP02010008	C40H79NO3	11.68	[M+H]+, 622.6133
18	Cer(d18:1/23:0)	LMSP02010021	C41H81NO3	12.04	[M+H]+, 636.6289
19	Cer(d18:1/24:0)	LMSP02010012	C42H83NO3	13	[M+H]+, 650.6446
20	Cer(d18:1/24:0)	LMSP02010012	C42H83NO3	12.73	[M+H]+, 650.6446
21	Cer(d18:1/24:1(15Z))	LMSP02010009	C42H81NO3	11.75	[M+H]+, 648.6289
22	Cer(d18:1/25:0)	LMSP02010013	C43H85NO3	13.52	[M+H]+, 664.6602
23	Cer(d18:1/26:0)	LMSP02010011	C44H87NO3	16.59	[M+H]+, 678.6759
24	Cer(d18:2/22:0)	LMSP02010029	C40H77NO3	10.7	[M+H]+, 620.5976
25	Cer(d18:2/23:0)	LMSP02010030	$C_{41}H_{79}NO_3$	11.23	[M+H]+, 634.6133
26	Cer(t18:0/16:0)	LMSP02030001	$C_{34}H_{69}NO_4$	8.78	[M+H]+, 556.5299
27	Cer(t18:0/24:0)	LMSP02030004	$C_{42}H_{85}NO_4$	12.17	[M+H]+, 668.6551
28	Cer(t18:0/26:0)	LMSP02030005	$C_{44}H_{89}NO_4$	13.63	[M+H]+, 696.6864
29	Cer(t18:0/h24:0)	LMSP02030002	$C_{42}H_{85}NO_5$	11.68	[M+H]+, 684.6501
30	PE-Cer(d14:1/22:0)	LMSP03020008	$C_{38}H_{77}N_2O_6P$	10.53	[M+H]+, 689.5592
31	GlcCer(d18:1/16:0)	LMSP0501AA03	C40H77NO8	8.72	[M+H]+, 700.5722
32	GlcCer(d18:1/18:1(9Z))	LMSP0501AA27	C42H79NO8	16.98	[M+H]+, 726.5878
33	GlcCer(d18:1/20:0)	LMSP0501AA06	C44H85NO8	9.97	[M+H]+, 756.6348
34	GlcCer(d18:1/22:0)	LMSP0501AA07	C46H89NO8	10.82	[M+H]+, 784.6661
35	GlcCer(d18:1/23:0)	LMSP0501AA32	C47H91NO8	11.33	[M+H]+, 798.6817
36	GlcCer(d18:1/24:0)	LMSP0501AA09	C48H93NO8	11.9	[M+H]+, 812.6974
37	GlcCer(d18:1/24:1(15Z))	LMSP0501AA08	C48H91NO8	10.89	[M+H]+, 810.6817

38	GlcCer(d18:2/22:0)	LMSP0501AA37	C46H87NO8	10.03	[M+H]+, 782.6504
39	LacCer(d18:1/16:0)	LMSP0501AB03	C46H87NO13	8.58	[M+H]+, 862.625
40	LacCer(d18:1/24:0)	LMSP0501AB07	C54H103NO13	11.56	[M+H]+, 974.7502
41	LacCer(d18:1/24:1(15Z))	LMSP0501AB09	C54H101NO13	10.6	[M+H]+, 972.7346