

Supporting Information

Improved MALDI imaging MS analysis of phospholipids using graphene oxide as new matrix

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ESI-QqQ MS/MS parameters

ESI-parameters	Positive mode	Negative mode
CUR	20.00	10.00
IS	5500.00	-4500.00
GS1	10.00	10.00

Lipid class	Ion mode	Scan mode	Collision energy (eV)
PC&SM	+	parents (184)	40
PE	+	NL (141)	35
PS	-	NL (87)	40

Supplementary

Fig. S1. SEM image of graphene oxide provided by the manufacturer.

Fig. S2. TEM image of graphene oxide provided by manufacturer.

Fig. S3. AFM image of graphene oxide provided by manufacturer.

Fig. S4. FT-IR absorption spectra of graphene oxide provided by manufacturer.

Fig. S5. Digital photographs of co-crystal of four standard phospholipid species with (a) DHB and (b) GO. For each spot, 1 μ L of phospholipid mixture and 1 μ L of matrix solution were mixed together and 1 μ L of the mixture was spotted on the MALDI plate by the pipette.

Fig. S6. Comparison of shot-to-shot stability of individual phospholipid solution with DHB (black circle) and GO (blue square). Each sample spot was prepared by applying 1 μ L of phospholipid solution with 1 μ L of DHB or 1 μ L of GO to the MALDI plate. For each shot, the mass spectrum was acquired from random locations in one spot by applying 200 laser shots and 50 sub-spectra pass acceptance.

Fig. S7. Comparison of spot-to-spot stability of individual phospholipid solution with DHB (black circle) and GO (blue square). Each sample spot was prepared by applying 1 μ L of phospholipid solution with 1 μ L of DHB or 1 μ L of GO to the MALDI plate. For each spot, the mass spectrum was acquired from random locations by applying 200 laser shots and 50 sub-spectra pass acceptance.

Fig. S8. Further confirmation of molecular peak assignment in MALDI-IMS by ESI QqQ-MS/MS for (a) PC (+ parents 184); (b) PE (+ NL 141) and (c) PS (- NL 87).

Table S1. Lipids detected from mouse brain tissue section by MALDI-TOF MS in positive mode using GO.

Table S2. Lipids detected from mouse brain tissue section by MALDI-TOF MS in positive mode using DHB

Fig. S1.

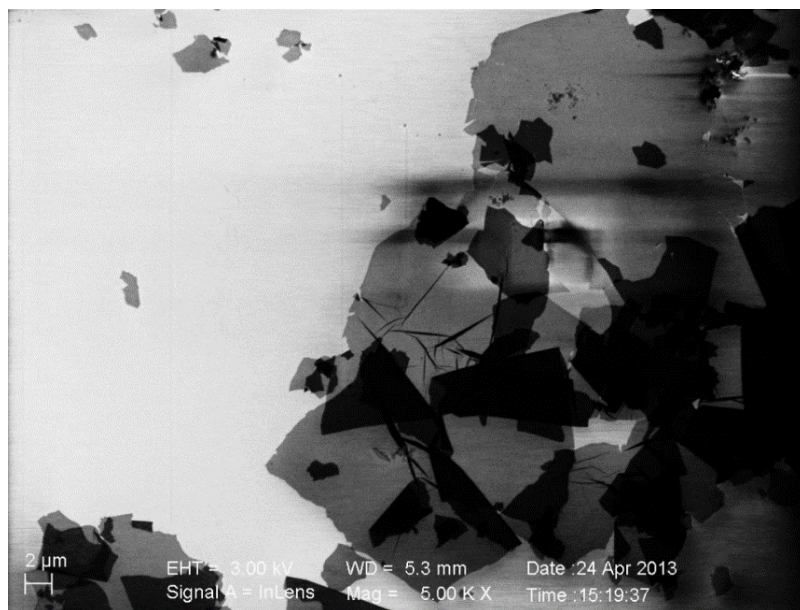


Fig. S2.

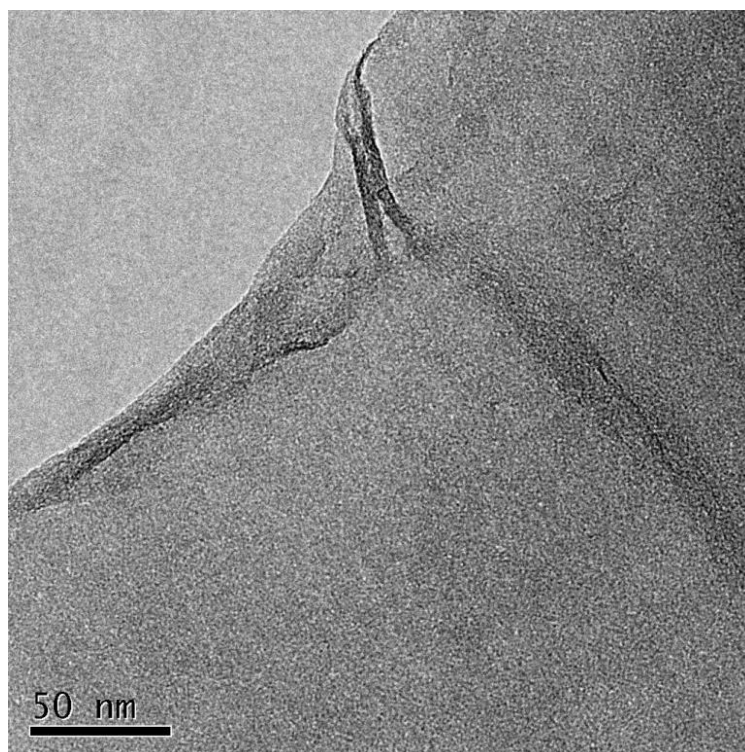


Fig. S3.

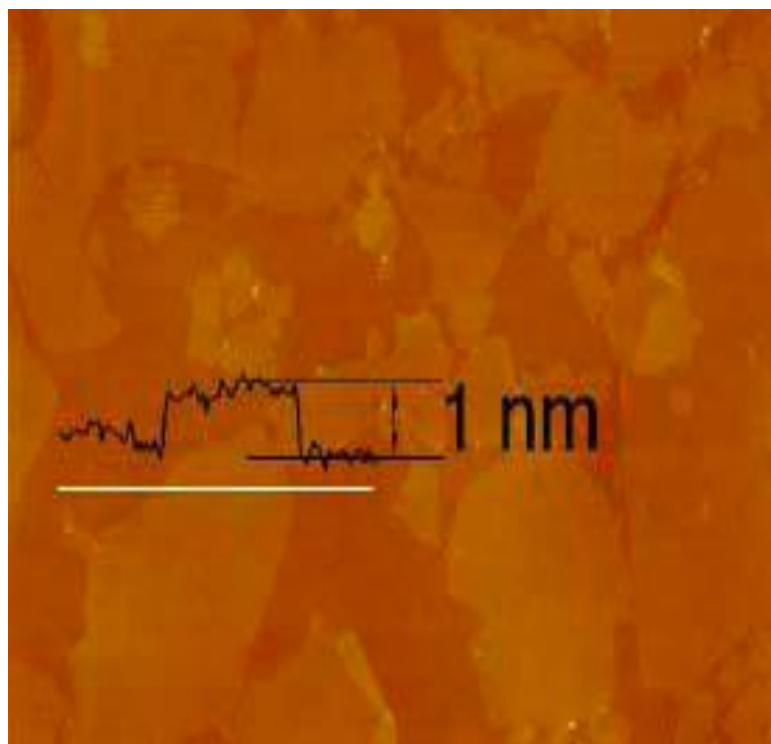


Fig. S4.

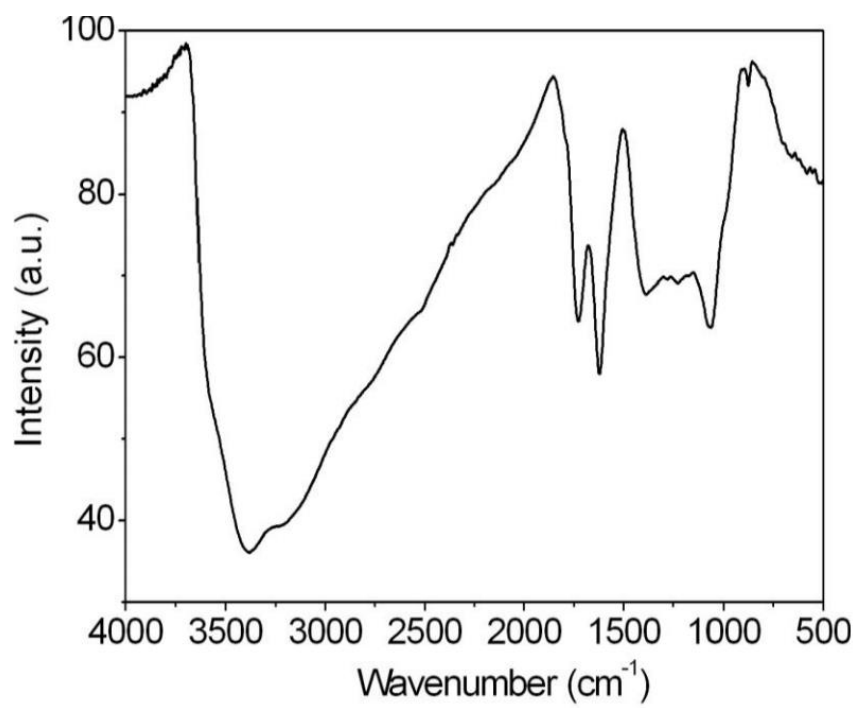


Fig. S5.

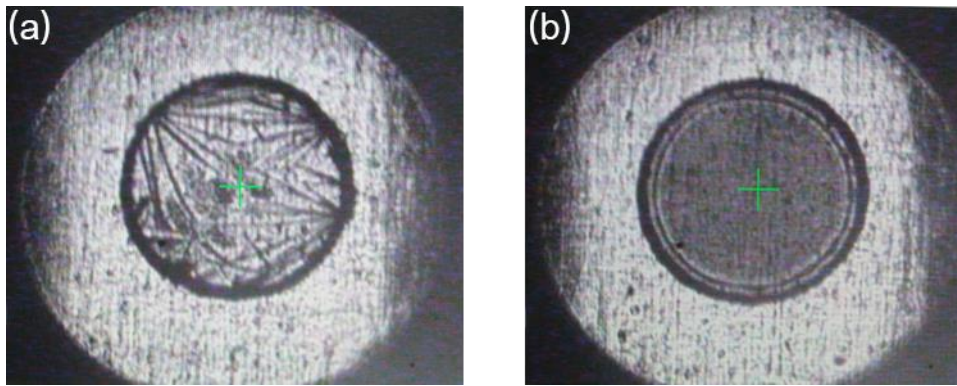


Fig. S6.

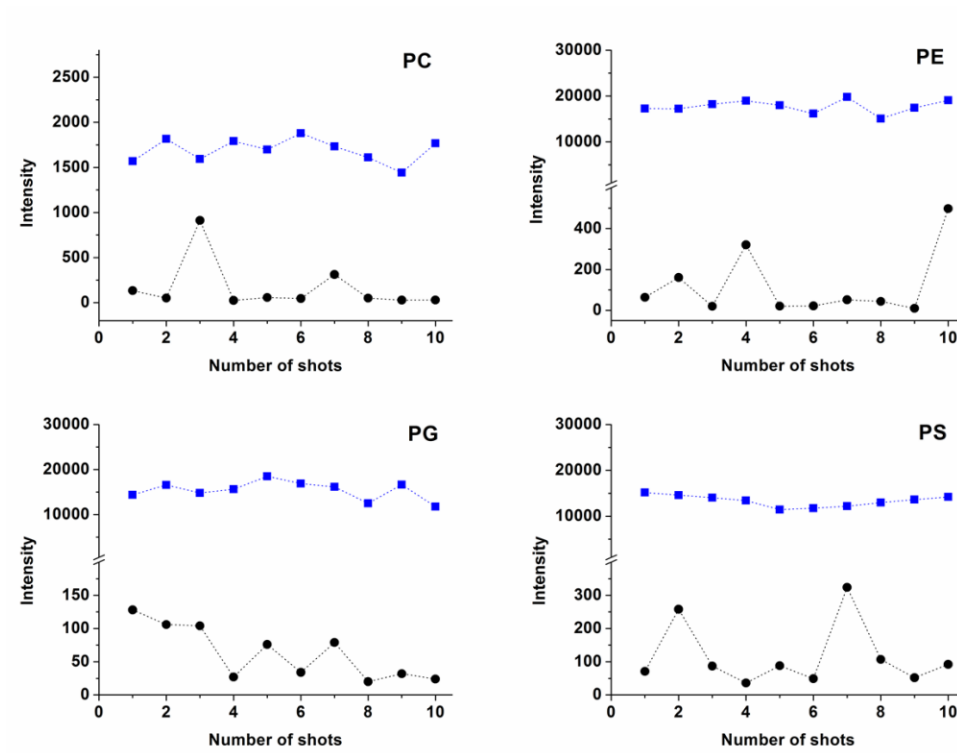


Fig. S7.

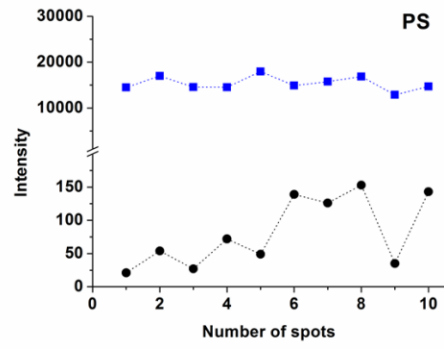
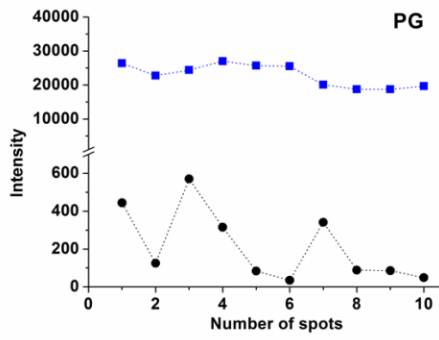
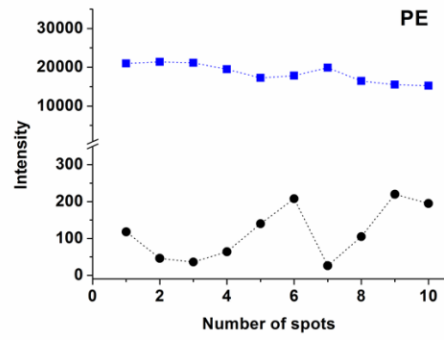
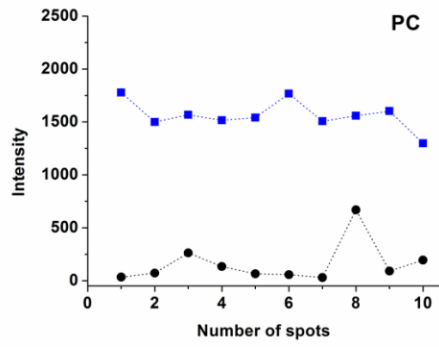


Fig. S8.

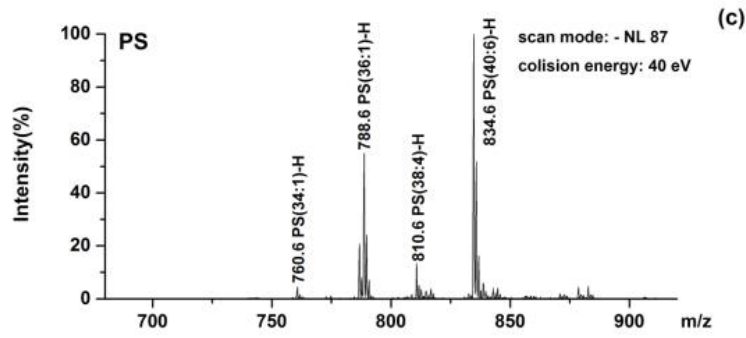
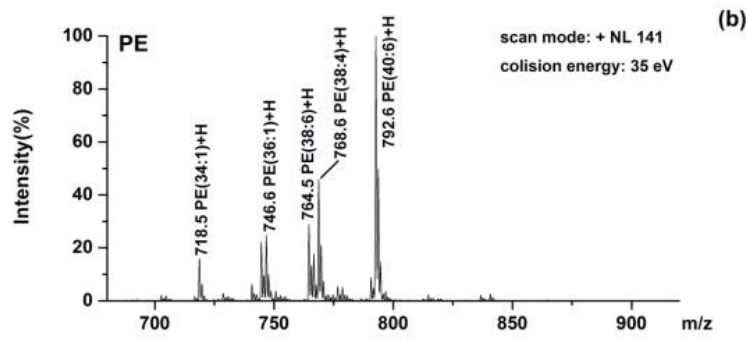
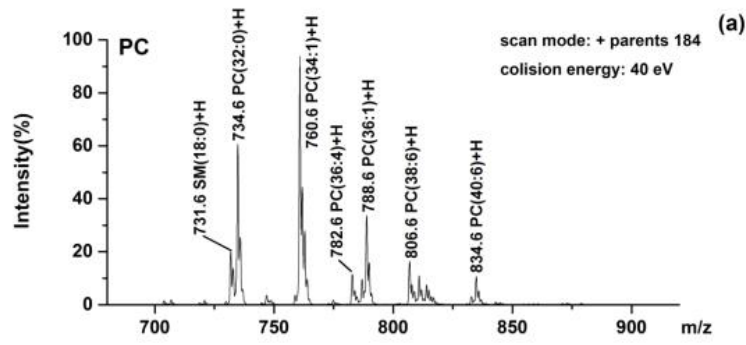


Table S1.

experimental mass (m/z)	theoretical mass (m/z)	assignment
711.37	770.51	PC(32:1)+K-59
713.38	772.52	PC(32:0)+K-59
735.37	794.51	PC(34:3)+K-59
737.37	796.52	PC(34:2)+K-59
739.39	798.54	PC(34:1)+K-59
741.40	800.56	PC(34:0)+K-59
759.38	818.51	PC(36:5)+K-59
761.37	820.52	PC(36:4)+K-59
763.39	822.54	PC(36:3)+K-59
765.41	824.56	PC(36:2)+K-59
767.47	826.57	PC(36:1)+K-59
769.44	828.59	PC(36:0)+K-59
785.40	844.52	PC(38:6)+K-59
787.38	846.54	PC(38:5)+K-59
789.40	848.56	PC(38:4)+K-59
791.42	850.57	PC(38:3)+K-59
793.44	852.59	PC(38:2)+K-59
795.47	854.60	PC(38:1)+K-59
797.46	856.62	PC(38:0)+K-59
813.42	872.56	PC(40:6)+K-59
815.42	874.57	PC(40:5)+K-59
817.42	876.59	PC(40:4)+K-59
821.46	880.62	PC(40:2)+K-59
823.53	882.64	PC(40:1)+K-59
738.40	738.48	PE(34:2p)+K
740.40	740.46	PE(34:1p)+K
754.40	754.48	PE(34:2)+K
756.41	756.49	PE(34:1)+K
758.42	758.51	PE(34:0)+K
762.39	762.48	PE(36:4p)+K
764.43	764.50	PE(36:3p)+K

experimental mass (m/z)	theoretical mass (m/z)	assignment
766.48	766.52	PE(36:2p)+K
768.47	768.53	PE(36:1p)+K
778.40	778.48	PE(36:4)+K
780.43	780.49	PE(36:3)+K
782.47	782.51	PE(36:2)+K
784.46	784.53	PE(36:1)+K
786.40	786.48	PE(38:6p)+K
788.40	788.50	PE(38:5p)+K
790.42	790.52	PE(38:4p)+K
792.43	792.53	PE(38:3p)+K
794.48	794.55	PE(38:2p)+K
796.46	796.56	PE(38:1p)+K
802.39	802.48	PE(38:6)+K
804.41	804.49	PE(38:5)+K
806.42	806.51	PE(38:4)+K
808.43	808.52	PE(38:3)+K
810.49	810.54	PE(38:2)+K
814.42	814.52	PE(40:6p)+K
820.48	820.56	PE(40:3p)+K
830.42	830.51	PE(40:6)+K
832.43	832.52	PE(40:5)+K
834.45	834.54	PE(40:4)+K
800.40	800.48	PS(34:1)+K
826.42	826.50	PS(36:2)+K
828.43	828.52	PS(36:1)+K
852.51	852.52	PS(38:3)+K
854.47	854.53	PS(38:2)+K
872.43	872.48	PS(40:7)+K
874.40	874.50	PS(40:6)+K
878.48	878.53	PS(40:4)+K
710.40	731.61	SM(18:0)+K-59
822.53	822.62	GalCer/GluCer(d18:1/22:0)+K
848.55	848.64	GalCer/GluCer(d18:1/24:1)+K
850.56	850.65	GalCer/GluCer(d18:1/24:0)+K

Table S2.

experimental mass (m/z)	theoretical mass (m/z)	assignment
731.61	731.61	SM(18:0)+H
734.57	734.57	PC(32:0)+H
756.55	756.55	PC(32:0)+Na
760.57	760.58	PC(34:1)+H
762.60	762.60	PC(34:0)+H
772.53	772.53	PC(32:0)+K
782.57	782.57	PC(34:1)+Na/PC(36:4)+H
784.58	784.58	PC(34:0)+Na
786.59	786.60	PC(36:2)+H
788.62	788.62	PC(36:1)+H
798.55	798.54	PC(34:1)+K
800.56	800.56	PC(34:0)+K
804.55	804.55	PC(36:4)+Na
806.57	806.57	PC(38:6)+H
808.59	808.58	PC(36:2)+Na/PC(38:5)+H
810.60	810.60	PC(36:1)+Na/PC(38:4)+H
820.54	820.52	PC(36:4)+K
824.57	824.56	PC(36:2)+K
826.58	826.57	PC(36:1)+K
828.56	828.55	PC(38:6)+Na
834.62	834.60	PC(40:6)+H
836.62	836.61	PC(40:5)+H
838.64	838.63	PC(40:4)+H
844.53	844.52	PC(38:6)+K
846.55	846.54	PC(38:4)+K
856.69	856.58	PC(40:6)+Na
872.67	872.56	PC(40:6)+K