

**Monitoring the three-dimensional distribution of endogenous species in the lungs by matrix-assisted laser desorption/ionization mass spectrometry imaging**

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## Supporting information

### Monitoring the three-dimensional distribution of endogenous species in the lungs by MALDI-MSI

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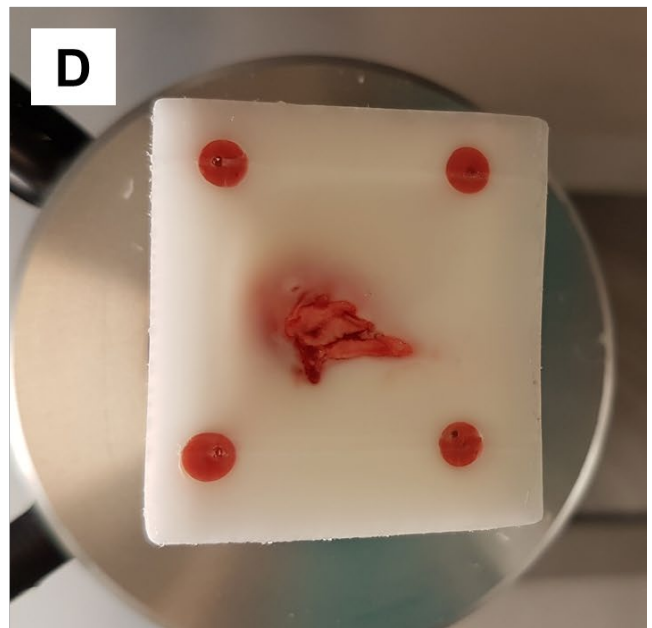
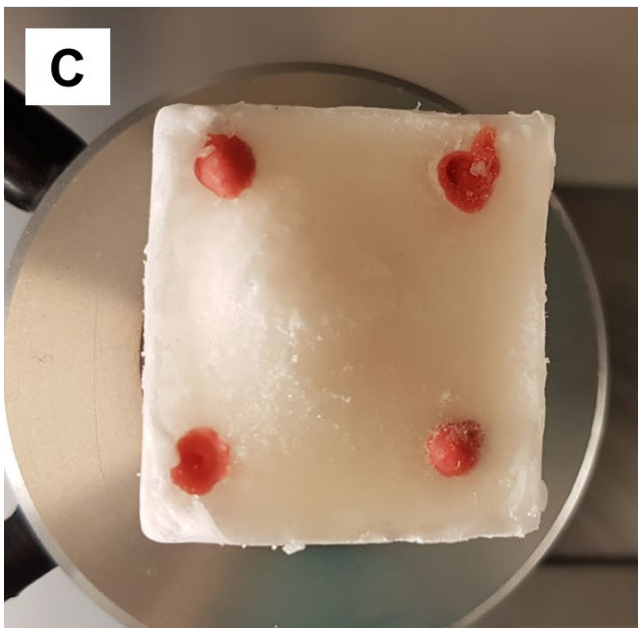
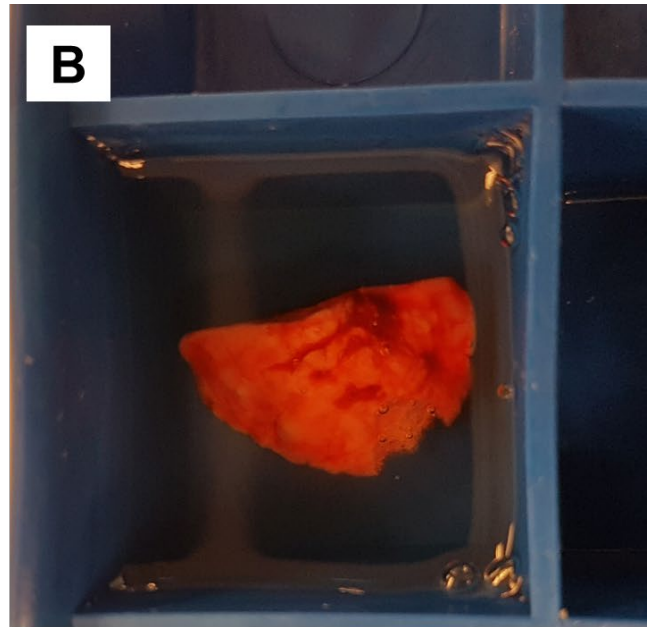
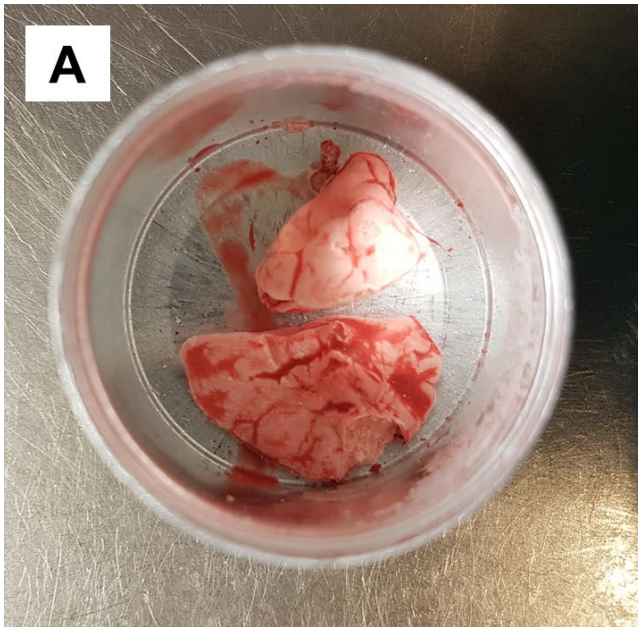
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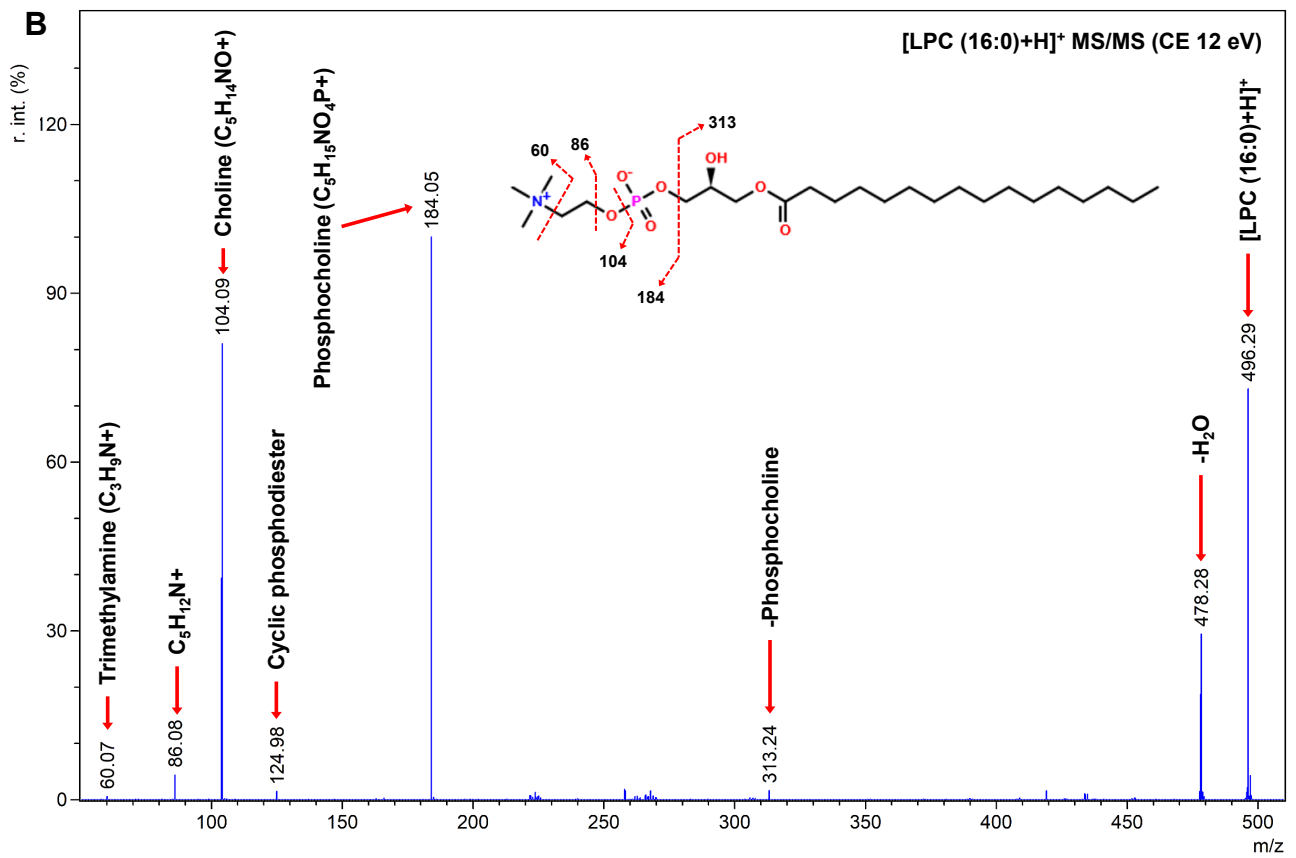
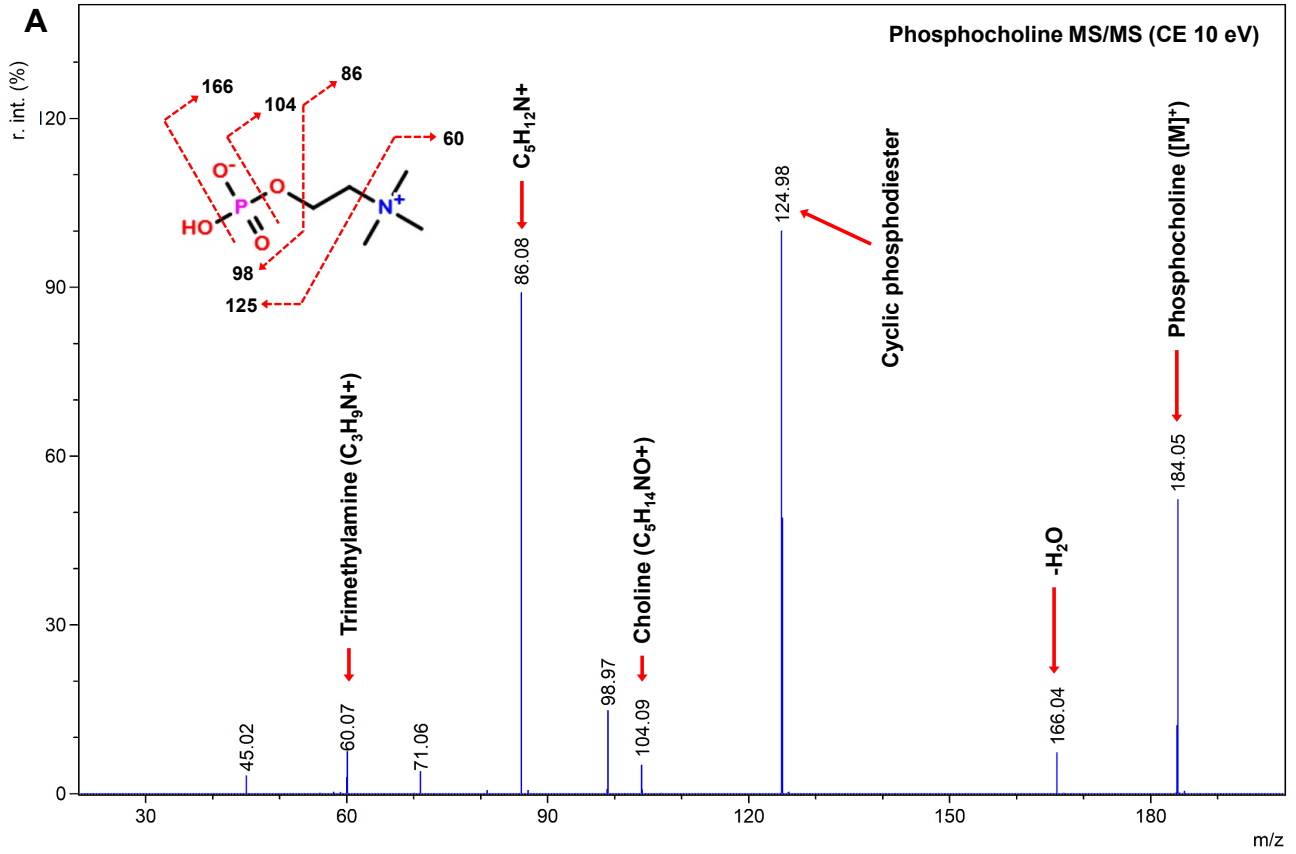
Corresponding author\*: Prof. Malcolm Clench, tel +441142253054, fax +441142253064, email: [m.r.clench@shu.ac.uk](mailto:m.r.clench@shu.ac.uk)

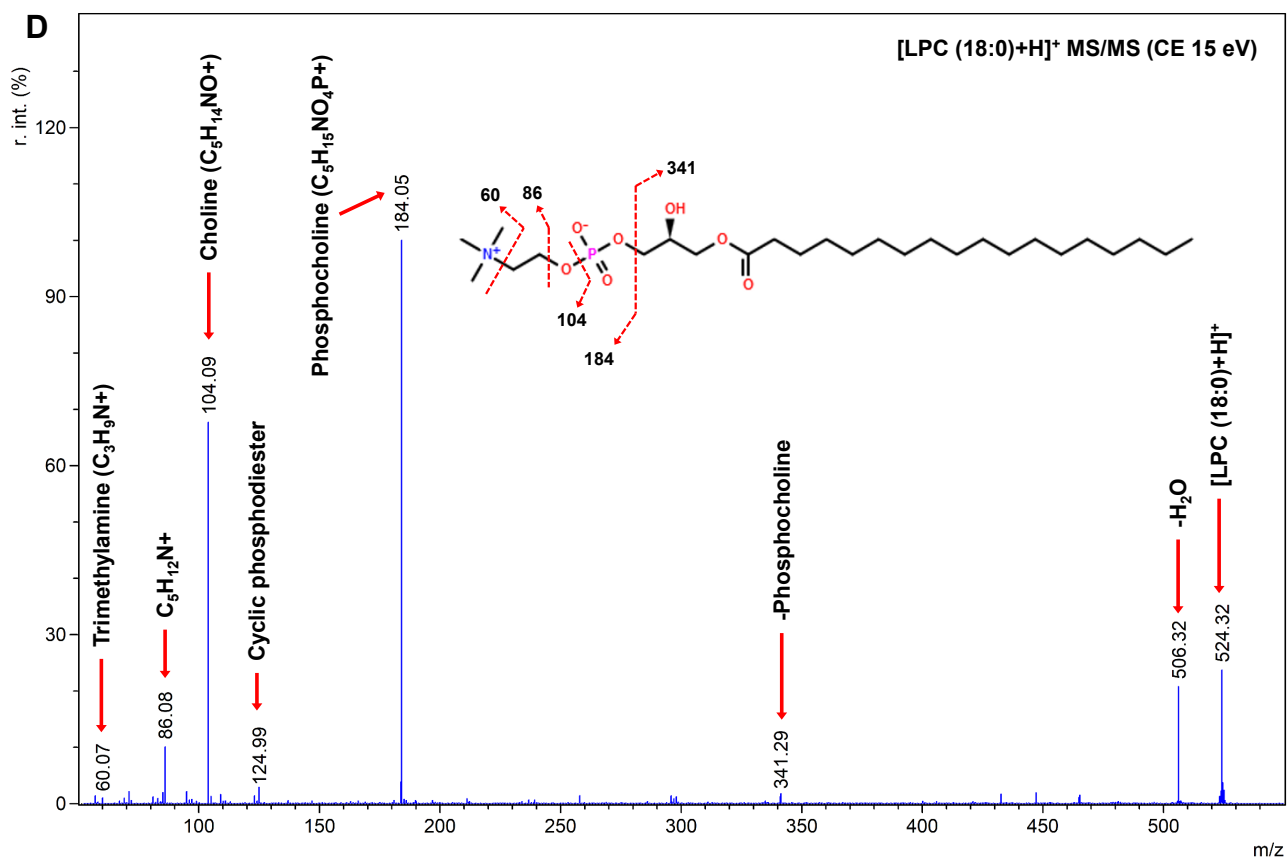
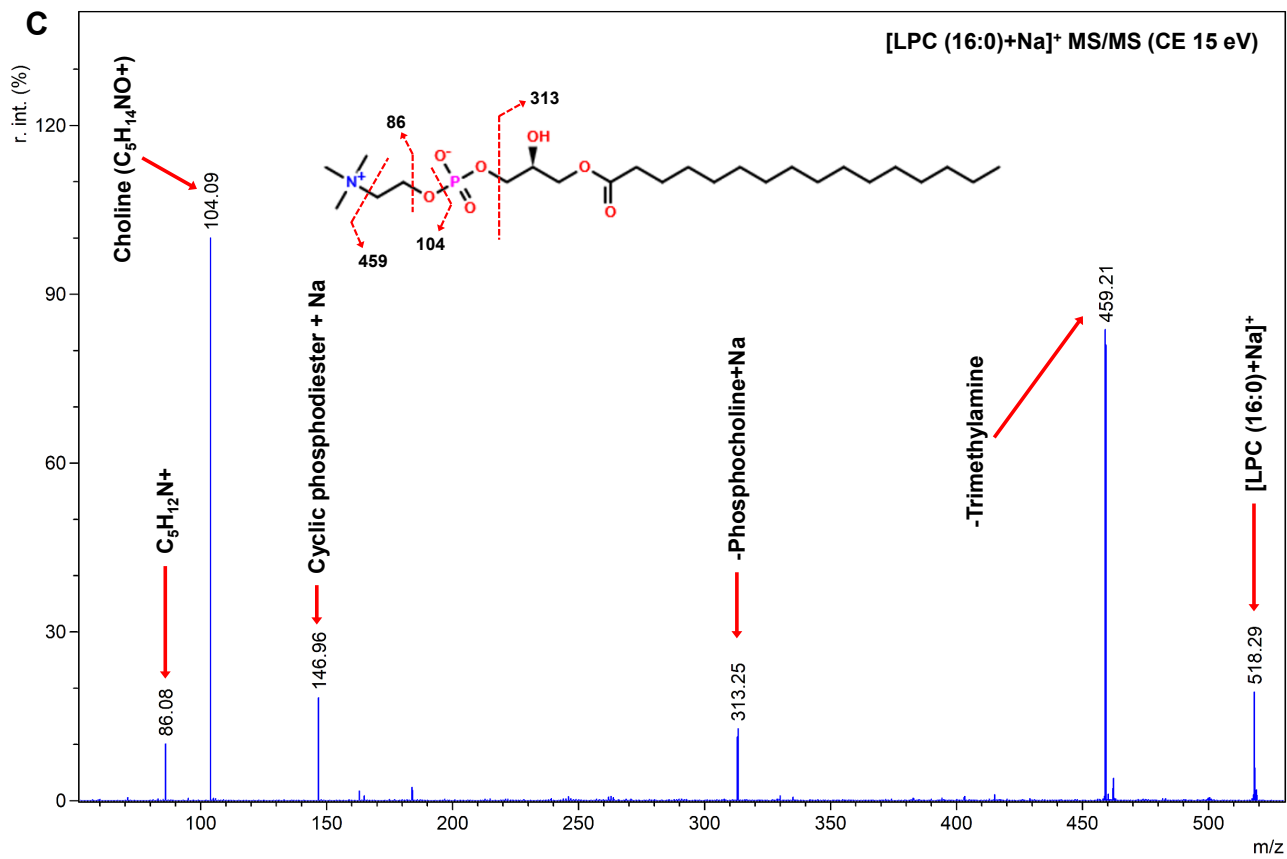
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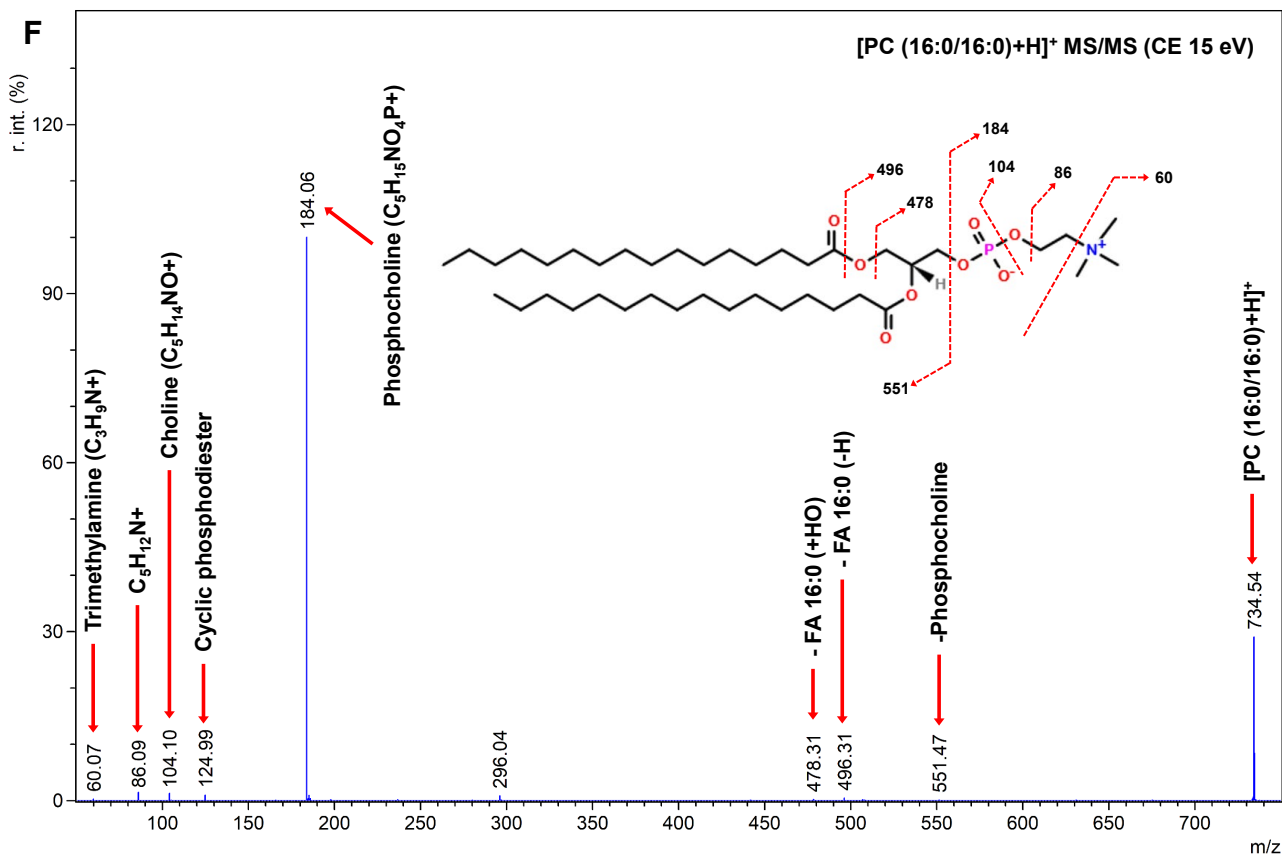
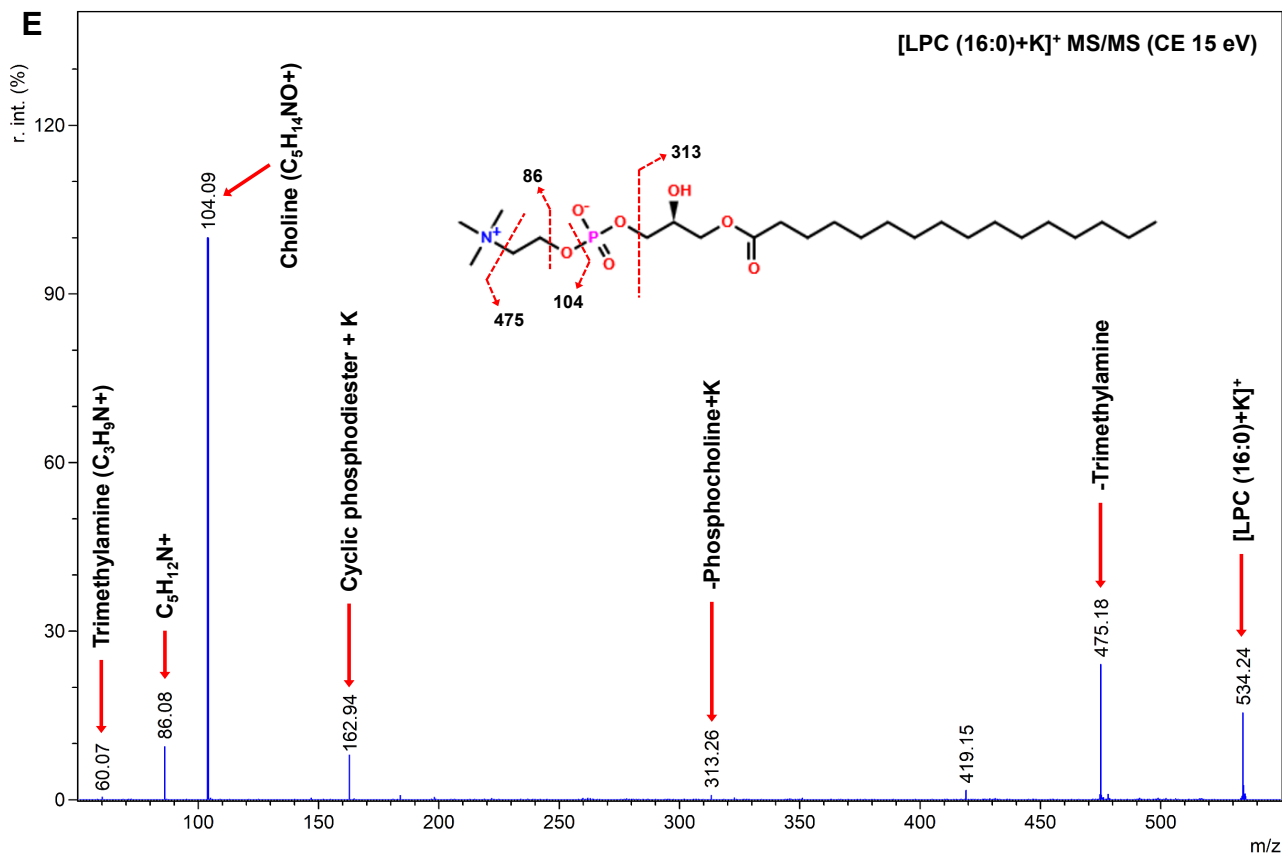
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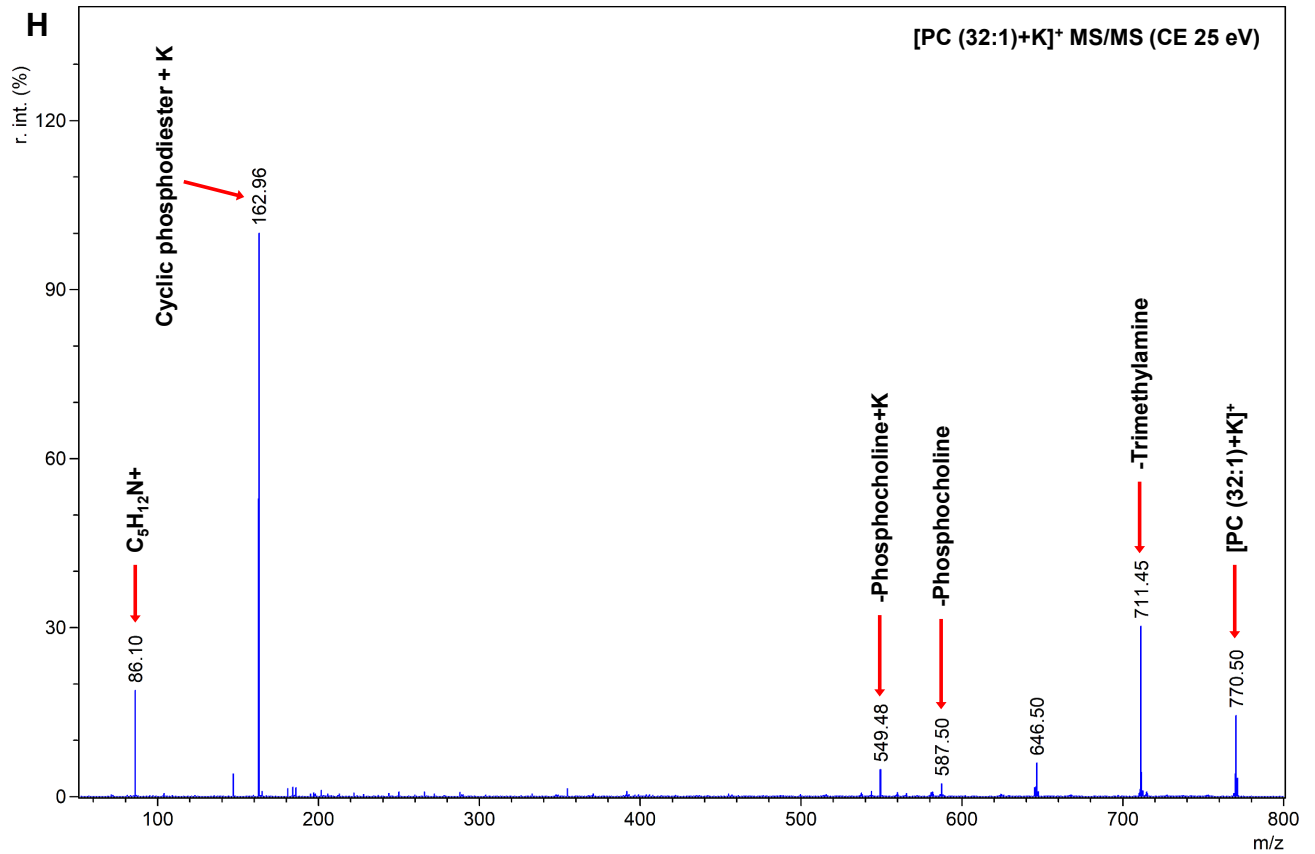
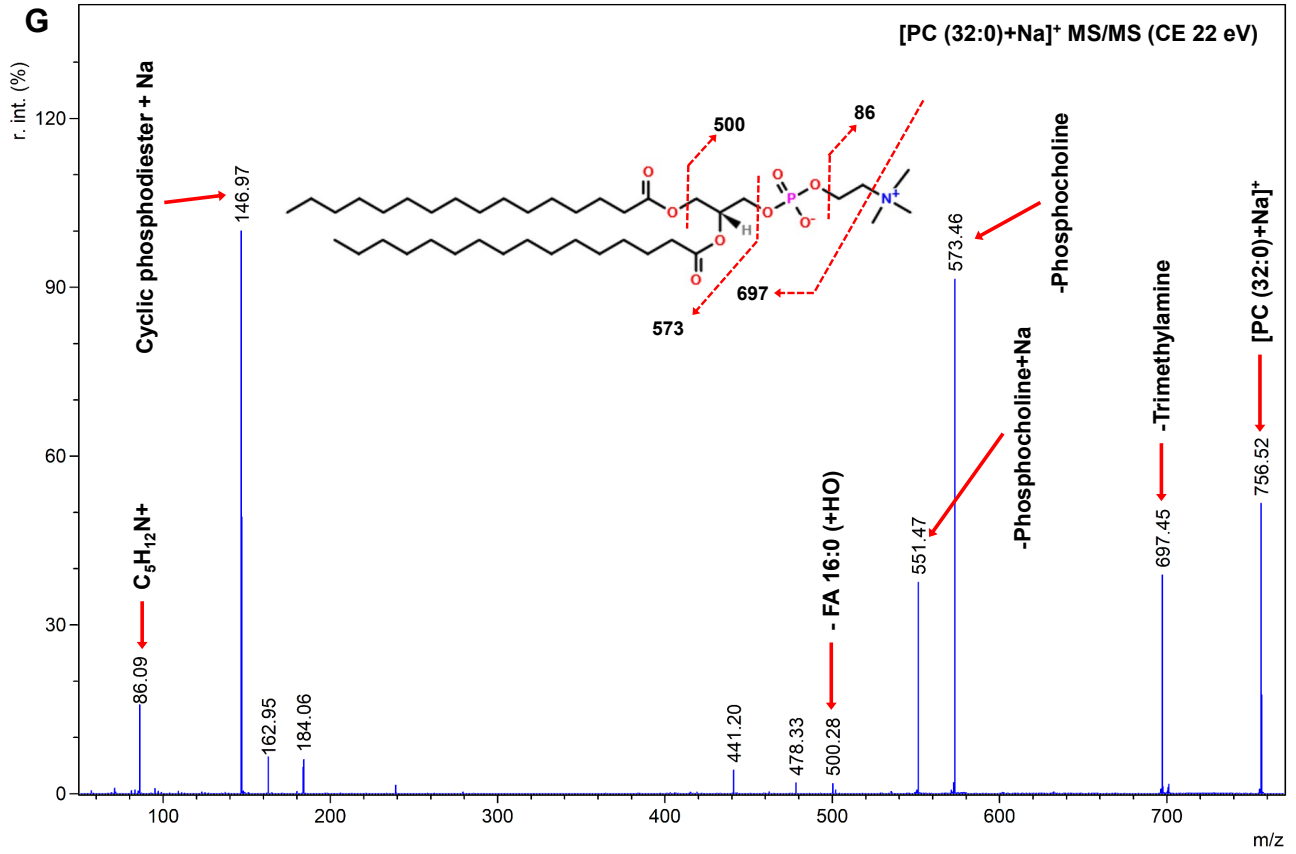


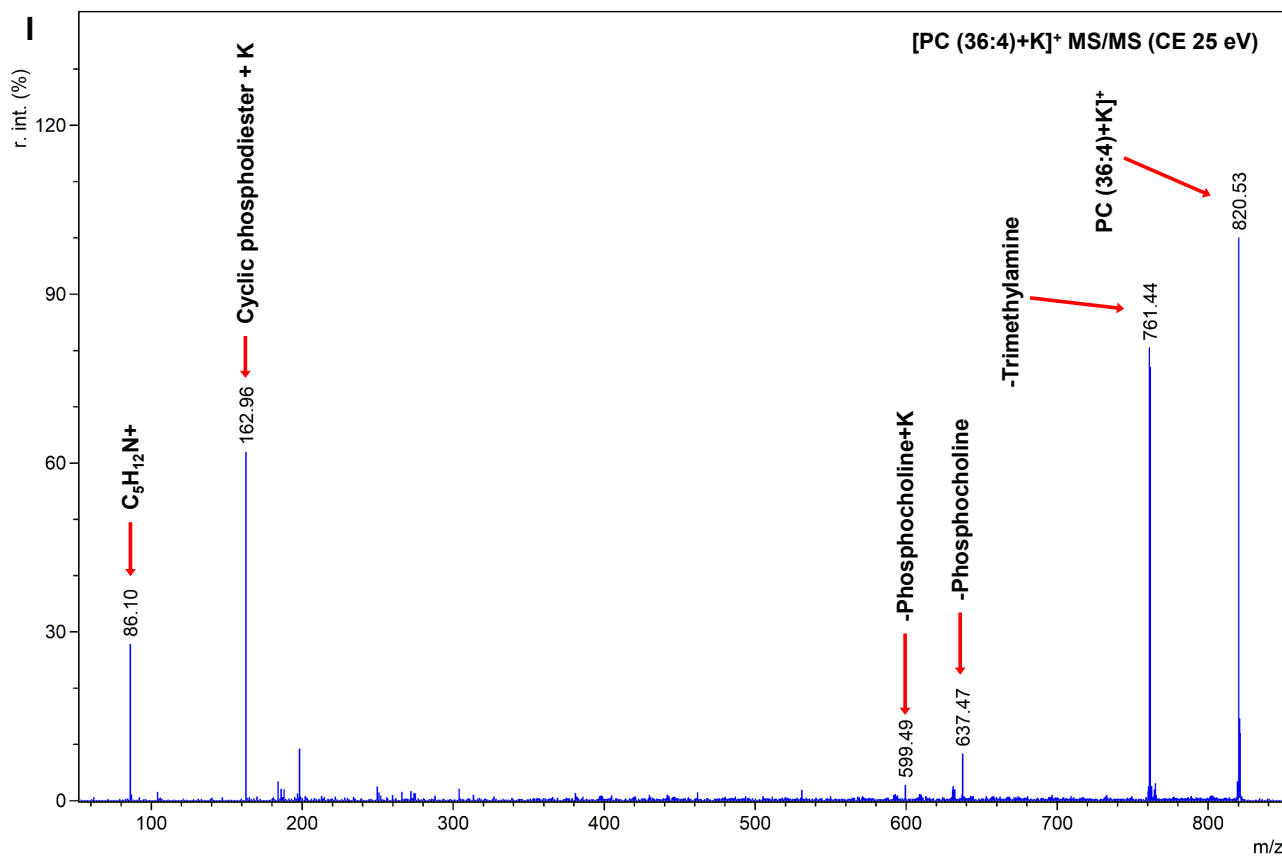
**Figure S1:** Workflow of sample preparation. A) Frozen rat lung tissue, B) rat lung tissue in liquid gelatin, C) frozen gelatin block with homogenate fiducial markers and D) block face showing the rat lung tissue embedded in frozen gelatin with fiducial markers.





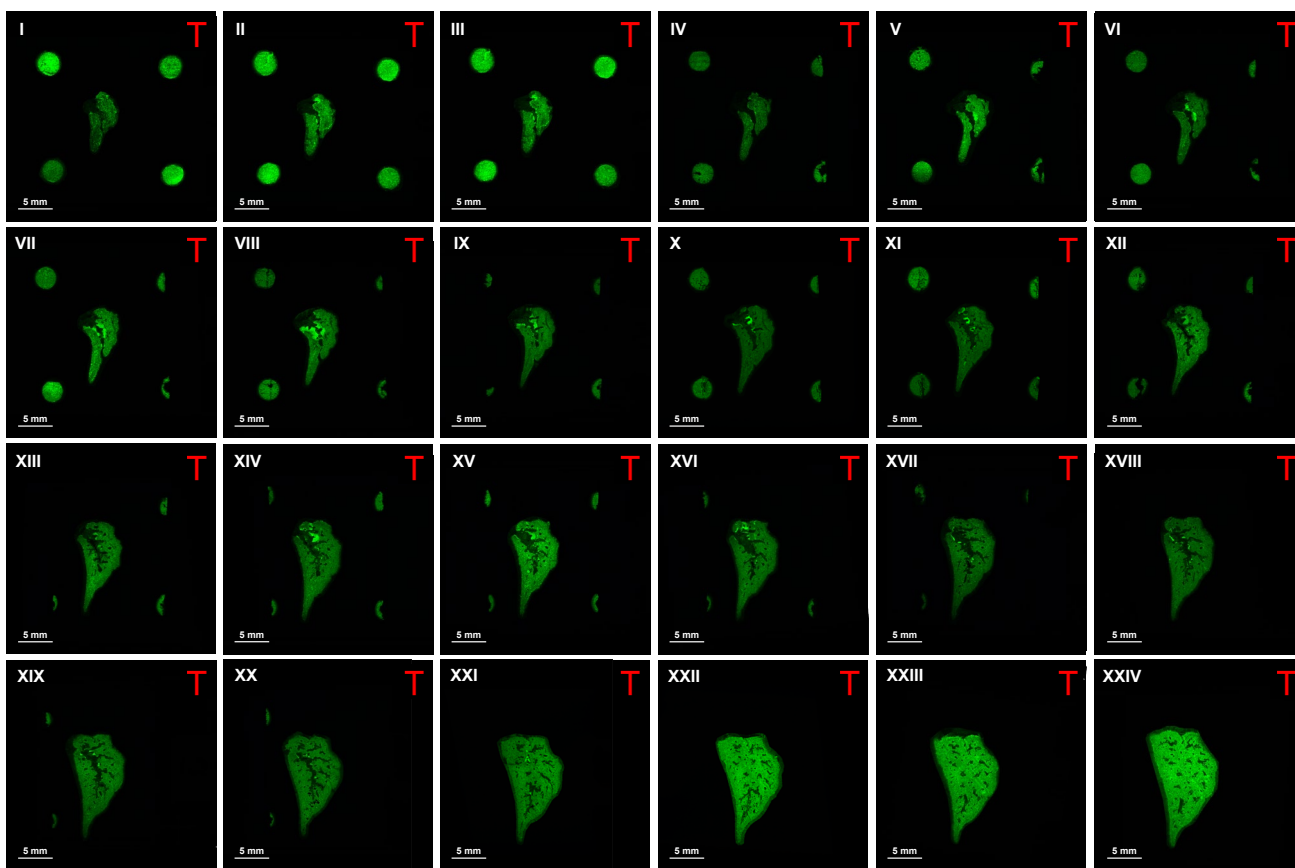




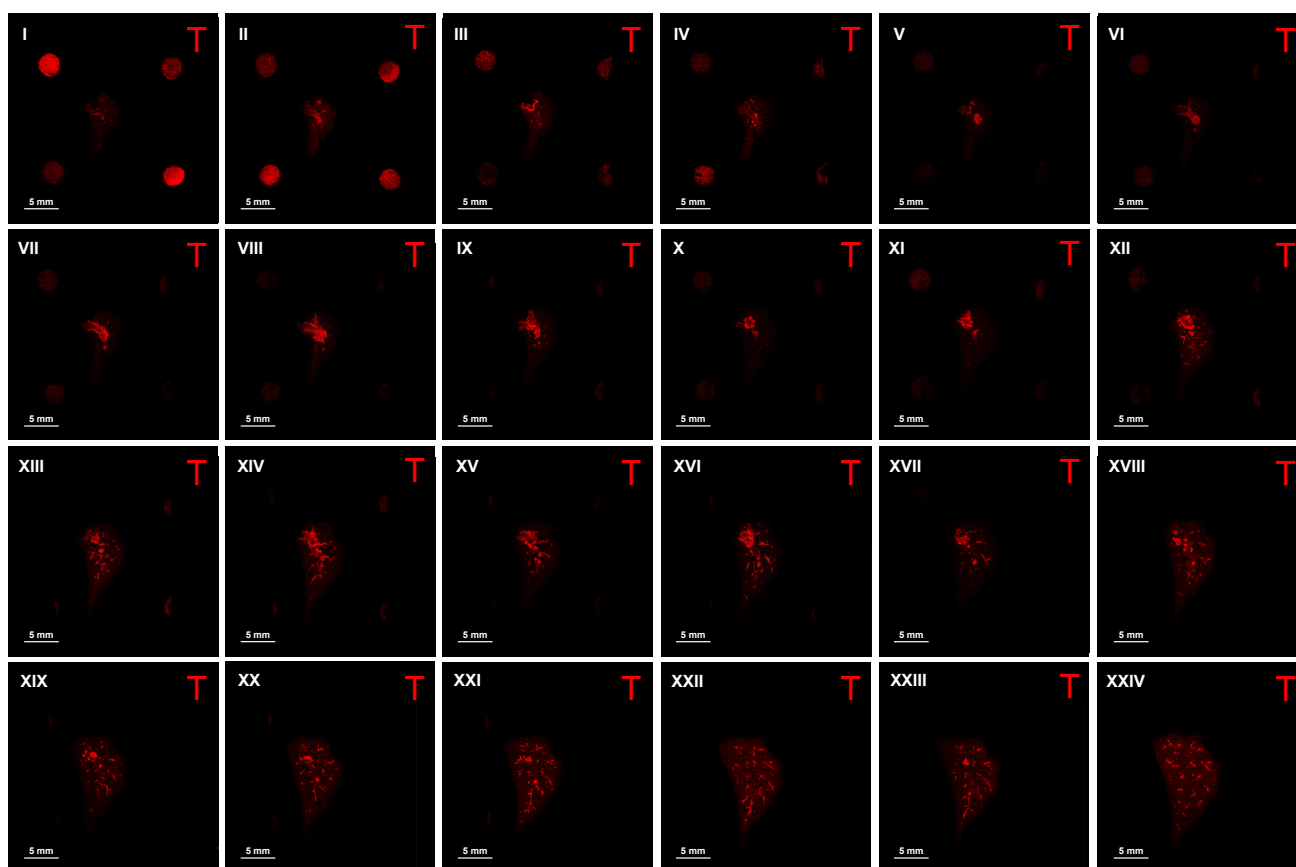


**Figure S2:** MALDI-MS/MS spectra of selected molecular species. A) Phosphocholine at  $m/z$  184.08, B) [LPC (16:0)+H]<sup>+</sup> at  $m/z$  496.32, C) [LPC (16:0)+Na]<sup>+</sup> at  $m/z$  518.29, D) [LPC (18:0)+H]<sup>+</sup> at  $m/z$  524.32, E) [LPC (16:0)+K]<sup>+</sup> at  $m/z$  534.24, F) [PC (16:0/16:0)+H]<sup>+</sup> at  $m/z$  734.55, G) [PC (32:0)+Na]<sup>+</sup> at  $m/z$  756.52, H) [PC (32:1)+K]<sup>+</sup> at  $m/z$  770.49 and I) [PC (36:4)+K]<sup>+</sup> at  $m/z$  820.52 (Collision energy quoted on spectra).





**Figure S3:** MALDI-MS images showing the distribution of  $[\text{PC (32:1)+K}]^+$  at  $m/z$  770.51 that highlights the parenchyma throughout the 24 tissue sections. Spatial resolution  $50 \times 50 \mu\text{m}$ , normalized with TIC as indicated by the red “T” in the top right corner based on reporting nomenclature.



**Figure S4:** MALDI-MS images showing the distribution of  $[\text{PC (36:4)+K}]^+$  at  $m/z$  820.52 that highlights the airways throughout the 24 tissue sections. Spatial resolution  $50 \times 50 \mu\text{m}$ , normalized with TIC as indicated by the red “T” in the top right corner based on reporting nomenclature.

<i>Identification</i>	<i>Observed mass</i>	<i>Theoretical mass</i>	<i>Formula</i>	<i>Error (ppm)</i>	<i>MS/MS</i>
Choline	104.1071	104.1070	C5H14NO	0.960	N
Phosphocholine	184.0734	184.0733	C5H15NO4P	0.543	Y
[LPA (18:1)+Na] <sup>+</sup>	459.2487	459.2482	C21H41O7PNa	1.089	N
[LPC 16:0+H-H <sub>2</sub> O] <sup>+</sup>	478.3296	478.3292	C24H49NO6P	0.836	N
[LPC 16:0+H] <sup>+</sup>	496.3400	496.3398	C24H51NO7P	0.403	Y
[LPC 16:0+Na] <sup>+</sup>	518.3223	518.3217	C24H50NO7PNa	1.158	Y
[LPC 18:0+H] <sup>+</sup>	524.3716	524.3711	C26H55NO7P	0.934	Y
[LPC 16:0+K] <sup>+</sup>	534.2964	534.2956	C24H50NO7PK	1.497	Y
[PC 16:0/16:0+H] <sup>+</sup>	734.5699	734.5694	C40H81NO8P	0.681	Y
[PC 32:0+Na] <sup>+</sup>	756.5520	756.5514	C40H80NO8PNa	0.793	Y
[PC (32:1)+K] <sup>+</sup>	770.5105	770.5097	C40H78NO8PK	1.038	Y
[PC (36:4)+K] <sup>+</sup>	820.5261	820.5253	C44H80NO8PK	0.975	Y

**Table S1: List of masses observed in lung tissue.**