

## Supplementary information

### Spatially resolved multi-omics highlights cell-specific metabolic remodeling and interactions in gastric cancer

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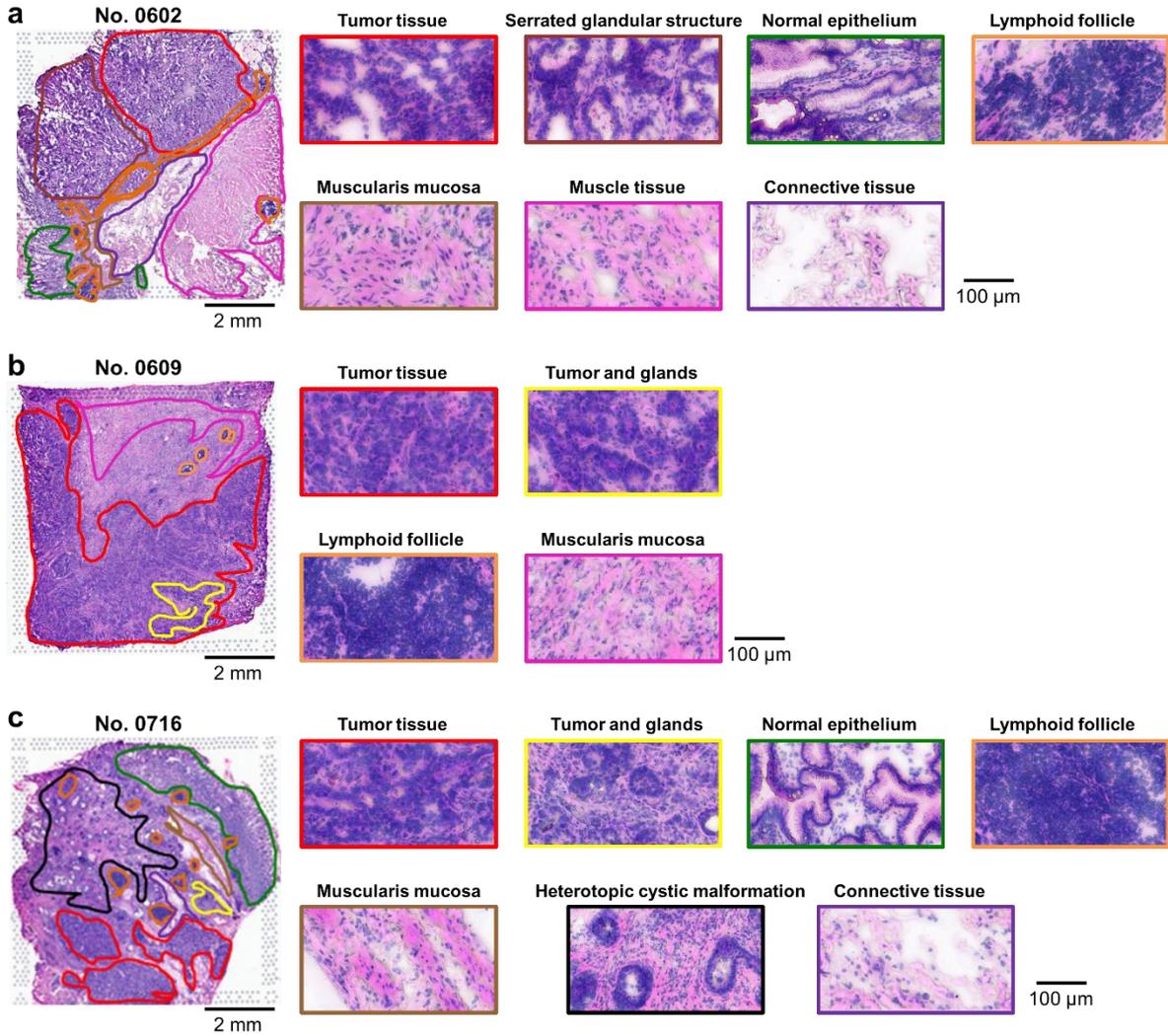
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<sup>7</sup> Shanghai Key Laboratory of Gastric Neoplasms, Department of General Surgery, Shanghai Institute of Digestive Surgery, Ruijin Hospital, Shanghai Jiao Tong University School of Medicine, Shanghai 200025, China.

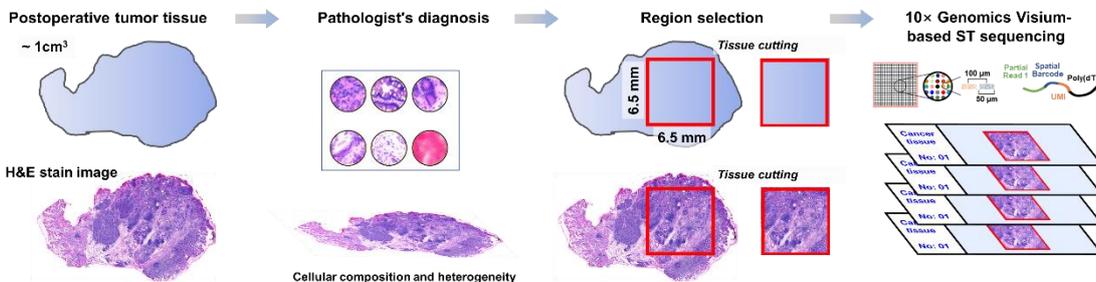
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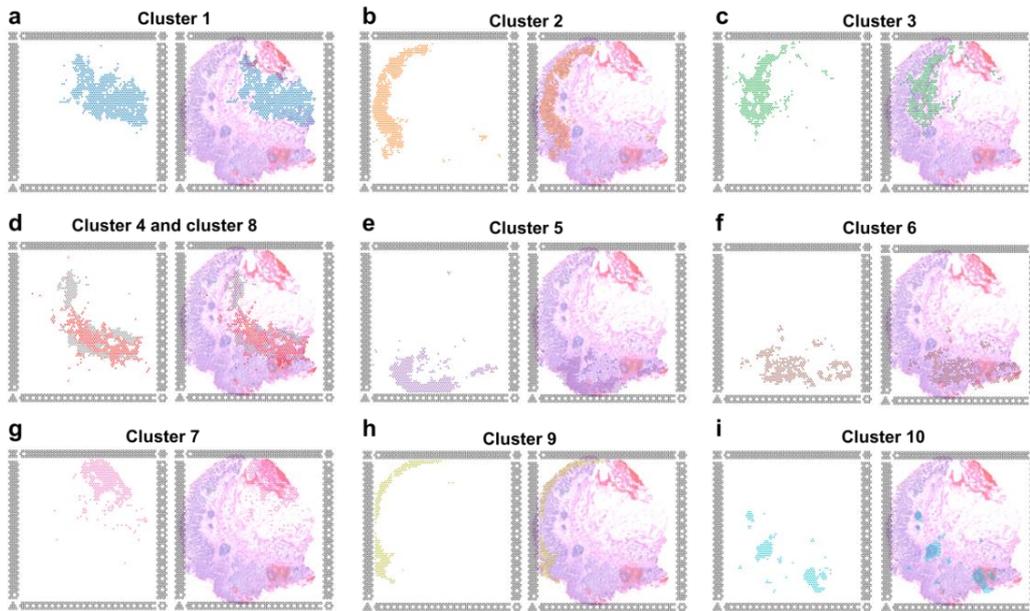
\* These authors jointly supervised this work: Wentao Dai, [dwent\\_job@163.com](mailto:dwent_job@163.com); Zhaode Bu, [buzhaode@cjcrcn.org](mailto:buzhaode@cjcrcn.org); Jiafu Ji, [jijiafu@hsc.pku.edu.cn](mailto:jijiafu@hsc.pku.edu.cn); Jiuming He, [hejiuming@imm.ac.cn](mailto:hejiuming@imm.ac.cn)



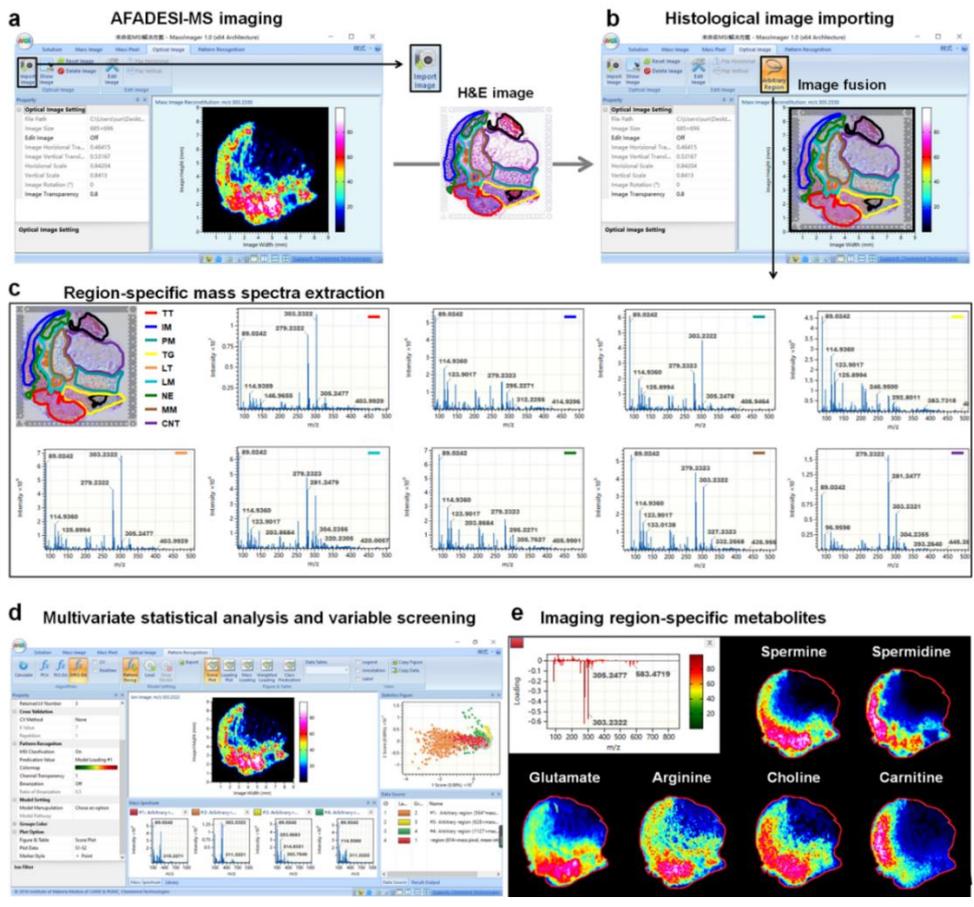
**Supplementary Figure 1 | H&E stain image of gastric cancer tissue section from different patients. a,** Typical H&E staining image of gastric cancer tissue for patients “No.0602”. **b,** Typical H&E staining image of gastric cancer tissue for patients “No.0609”. **c,** Typical H&E staining image of gastric cancer tissue for patients “No.0716”. scale bar = 2 mm for whole tissue sections, scale bar = 100 μm for magnified image. The experiment was repeated three times.



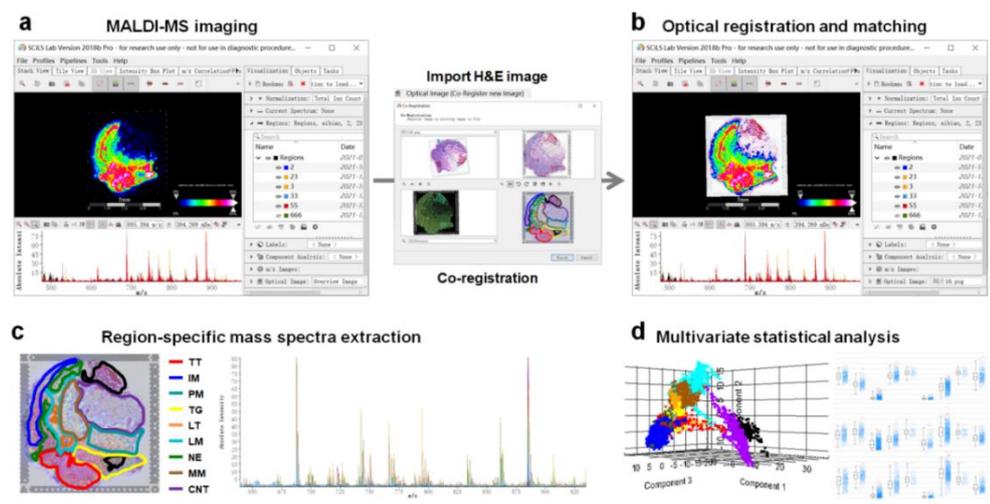
**Supplementary Figure 2 | The process of selecting scan area for 10x Genomics sequencing.**



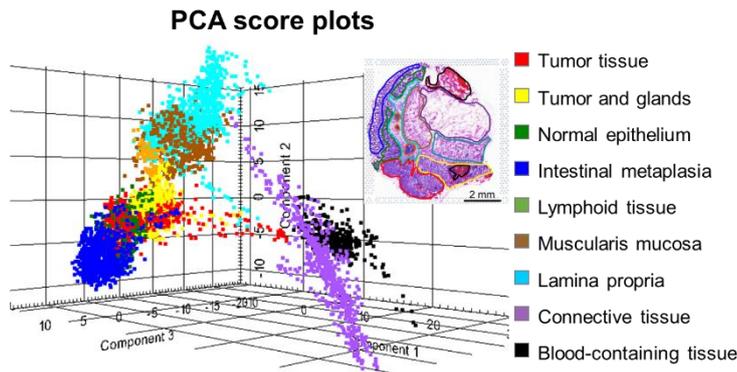
**Supplementary Figure 3 | Visium array spots colored by graph-based clustering algorithm for gastric cancer tissue section.** **a**, Graph-based Visium array spots of cluster 1. **b**, Graph-based Visium array spots of cluster 2. **c**, Graph-based Visium array spots of cluster 3. **d**, Graph-based Visium array spots of cluster 4 and cluster 8. **e**, Graph-based Visium array spots of cluster 5. **f**, Graph-based Visium array spots of cluster 6. **g**, Graph-based Visium array spots of cluster 7. **h**, Graph-based Visium array spots of cluster 9. **i**, Graph-based Visium array spots of cluster 10.



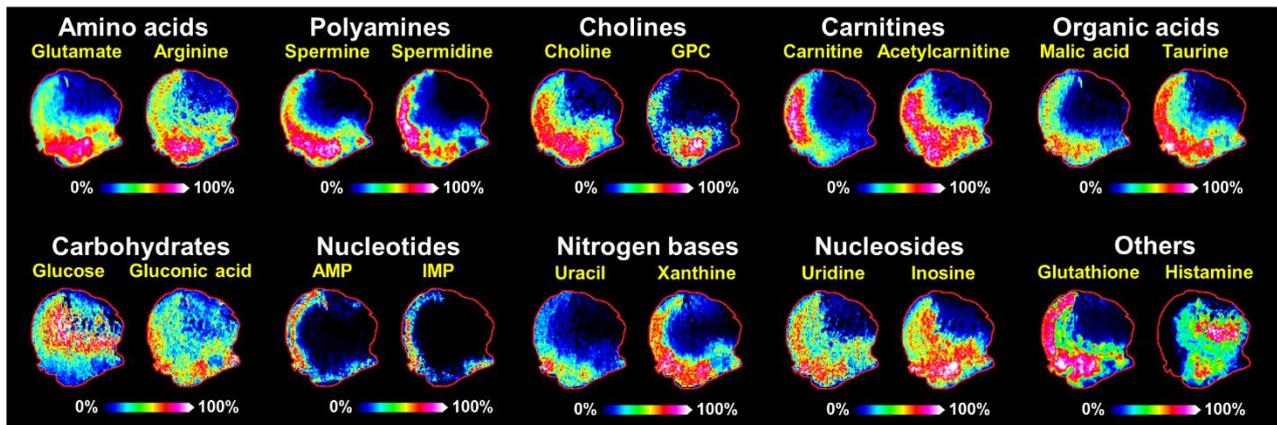
**Supplementary Figure 4 | Spots-labeled H&E image was imported into AFADESI-MSI software MassImager for image fusion and feature metabolites screening.** a, The operation interface of MassImager software. b, Import histological staining images into MassImager software. c, Extraction of AFADESI MS data from different tissue regions. d, *In situ* multivariate statistical analysis. e, MS images of screened region-specific metabolites.



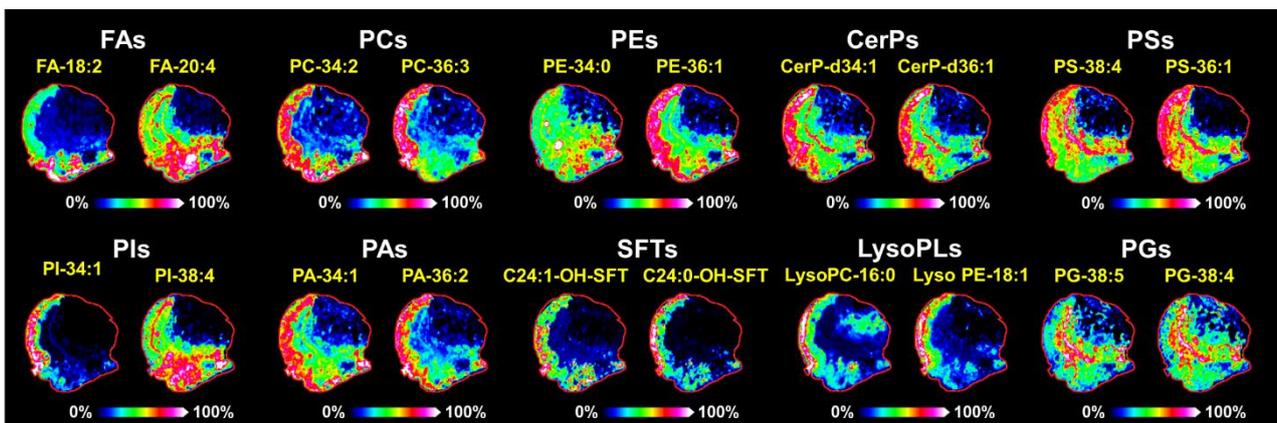
**Supplementary Figure 5 | Spots-labeled H&E image was imported into MALDI-MSI software SCiLS Lab for image fusion and feature lipids screening.** a, The operation interface of SCiLS Lab software. b, Import histological staining images into SCiLS Lab software. c, Extraction of MALDI MS data from different tissue regions. d, *In situ* multivariate statistical analysis.



**Supplementary Figure 6 | PCA score plots for different gastric cancer tissue regions based on the metabolite and lipid profiles.**

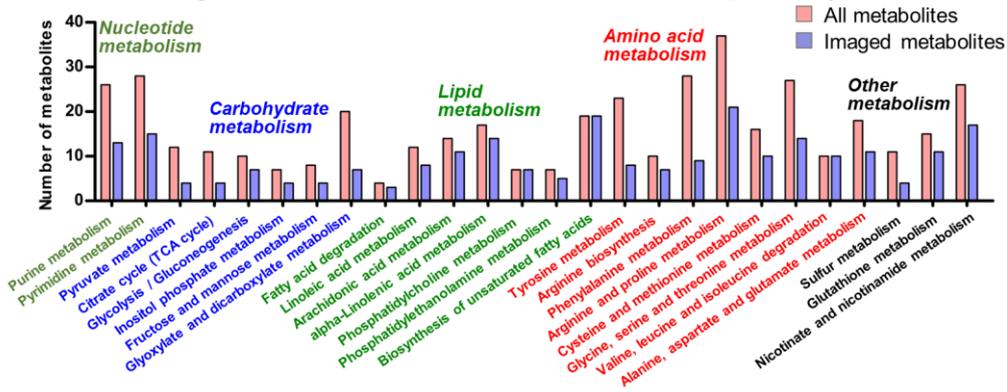


**Supplementary Figure 7 | Representative metabolites that imaged by AFADESI-MSI based platform. GPC: glycerophosphorylcholine, AMP: adenosine monophosphate, IMP: inosine monophosphate, intensity in colour scale is relative value.**



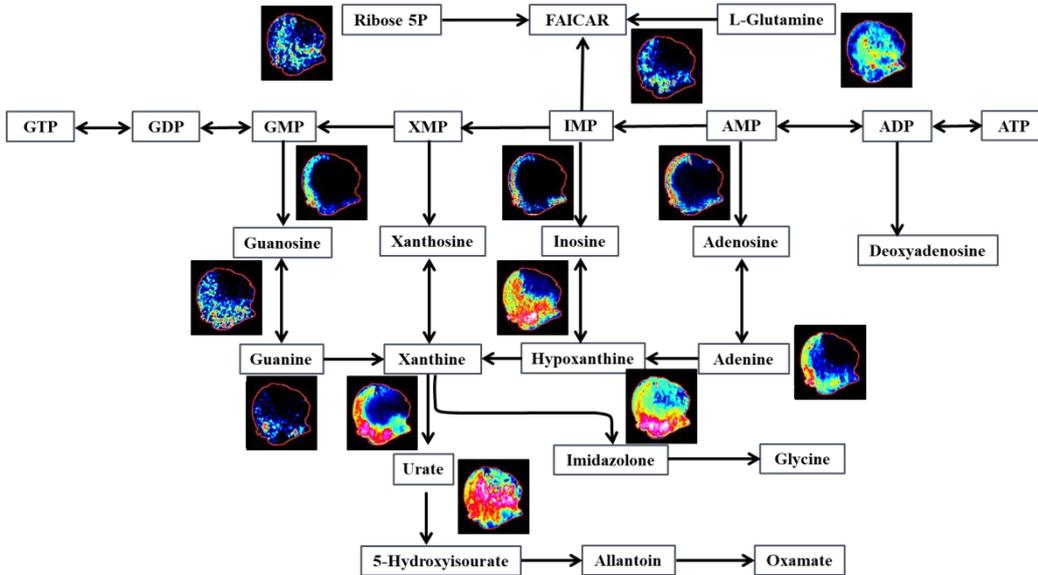
**Supplementary Figure 8 | Representative lipids that imaged by MALDI-MSI based platform. PC: Phosphatidylcholine, LysoPL: Lysophosphatide, PC: phosphatidylcholine, PE: phosphatidylethanolamine, CerP: ceramide-phosphate, PS: phosphatidylserine, PG: phosphatidylglycerol, PI: phosphatidylinositol, PA: phosphatidic acid, SFT: sulfatide, intensity in colour scale is relative value.**

### Imaged metabolites in different metabolic pathways



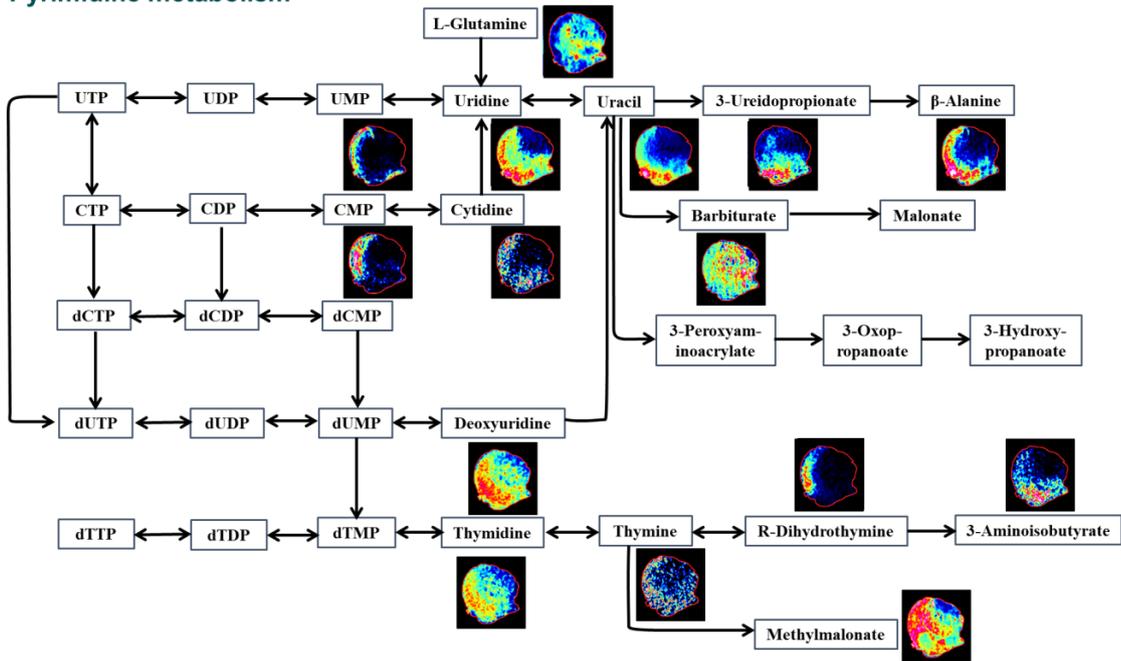
Supplementary Figure 9 | Imaged metabolites and lipids in different metabolic pathways.

### Purine metabolism



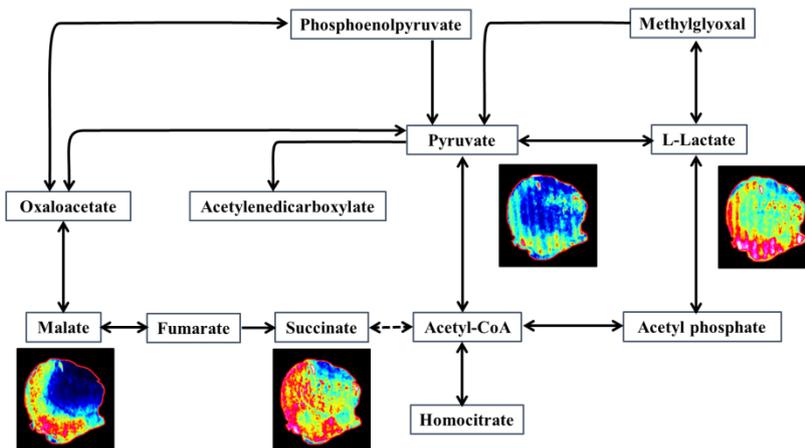
Supplementary Figure 10 | MS images of detected metabolites in purine metabolism pathway (intensity in colour scale is relative value).

### Pyrimidine metabolism



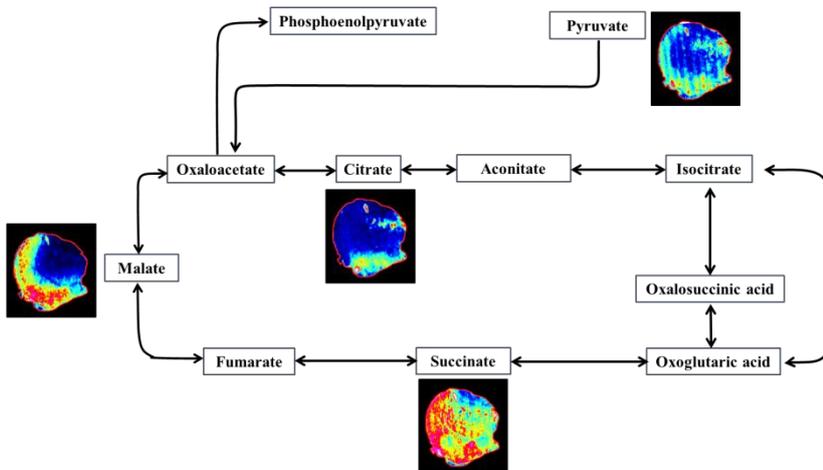
Supplementary Figure 11 | MS images of detected metabolites in pyrimidine metabolism pathway (intensity in colour scale is relative value).

### Pyruvate metabolism



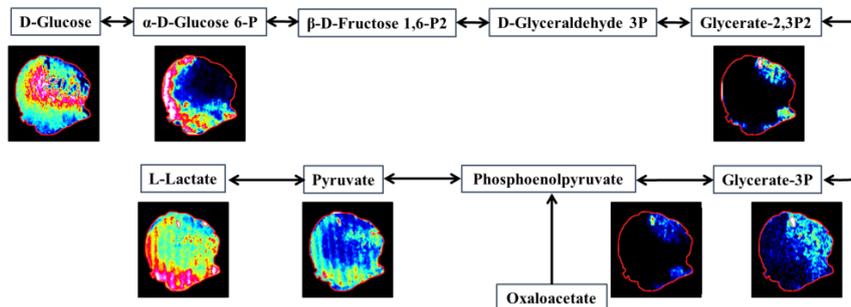
Supplementary Figure 12 | MS images of detected metabolites in pyruvate metabolism pathway (intensity in colour scale is relative value).

### Citrate cycle (TCA cycle)



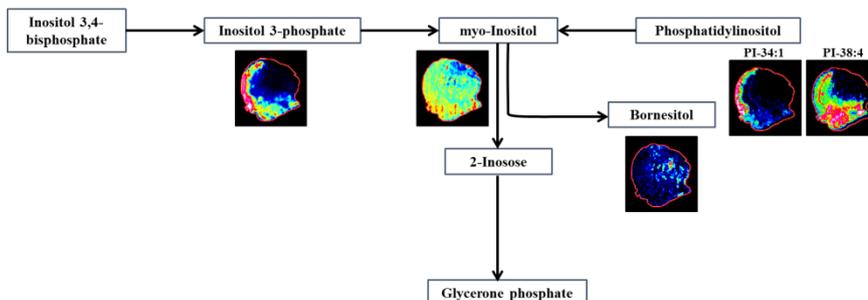
Supplementary Figure 13 | MS images of detected metabolites in citrate cycle pathway (intensity in colour scale is relative value).

### Glycolysis / Gluconeogenesis



Supplementary Figure 14 | MS images of detected metabolites in glycolysis and gluconeogenesis pathways (intensity in colour scale is relative value).

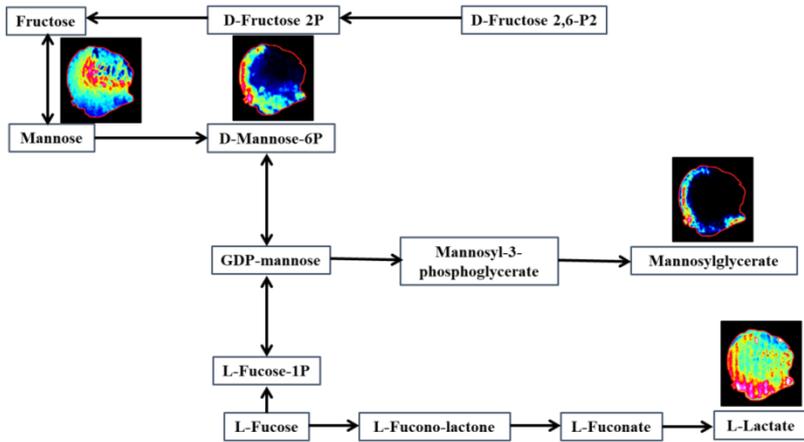
### Inositol phosphate metabolism



Supplementary Figure 15 | MS images of detected metabolites in inositol phosphate pathway (intensity in colour

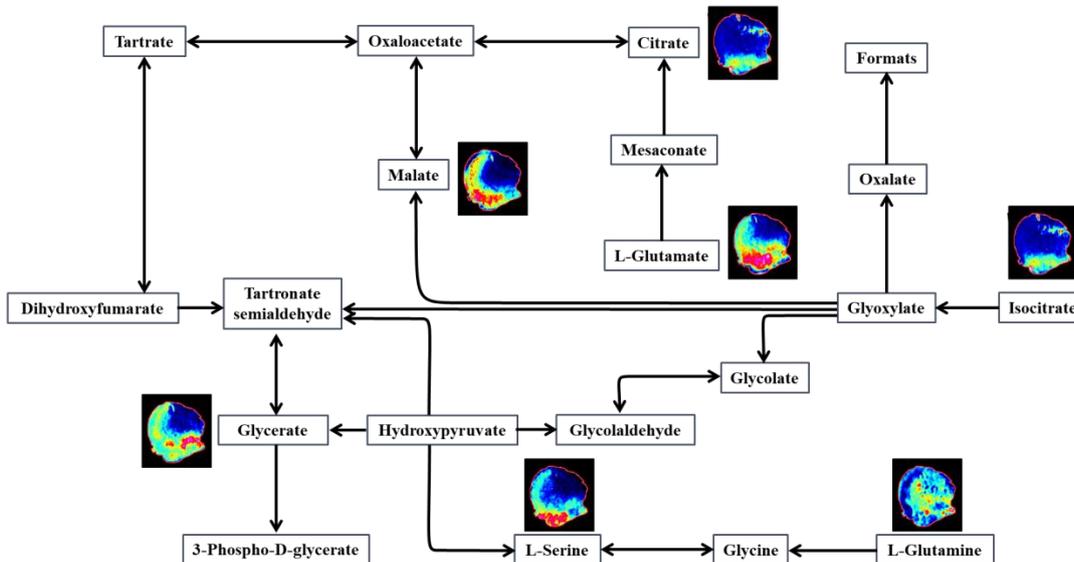
scale is relative value).

### Fructose and mannose metabolism



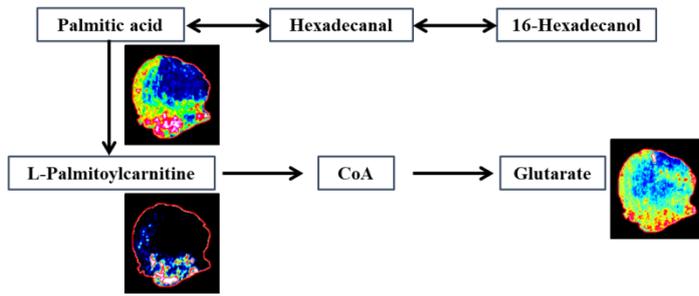
Supplementary Figure 16 | MS images of detected metabolites in fructose and mannose metabolism pathway (intensity in colour scale is relative value).

### Glyoxylate and dicarboxylate metabolism



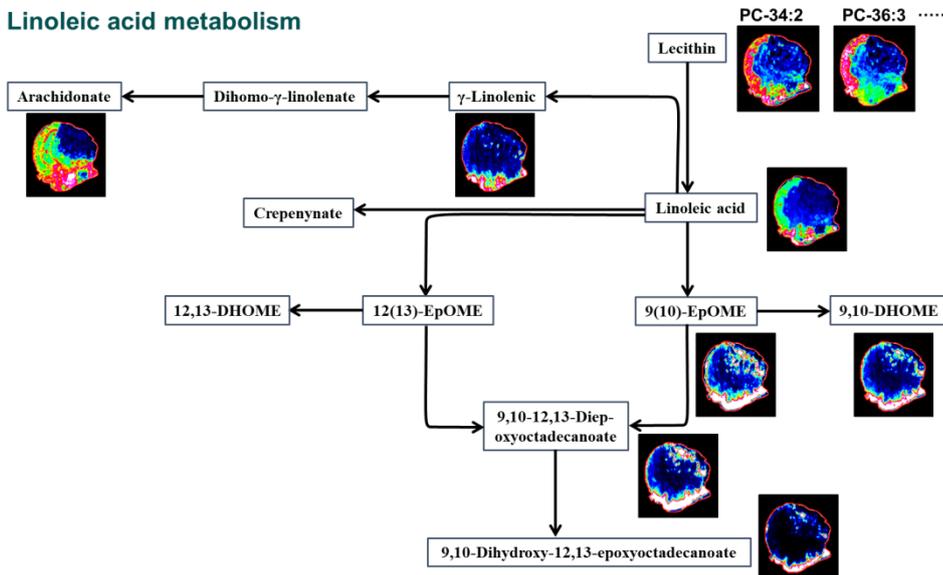
Supplementary Figure 17 | MS images of detected metabolites in glyoxylate and dicarboxylate pathway (intensity in colour scale is relative value).

### Fatty acid degradation



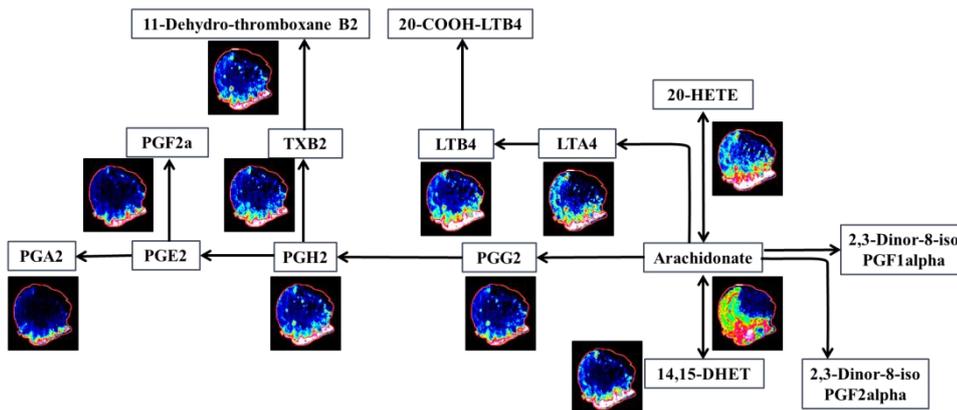
Supplementary Figure 18 | MS images of detected metabolites in fatty acid degradation pathway (intensity in colour scale is relative value).

### Linoleic acid metabolism



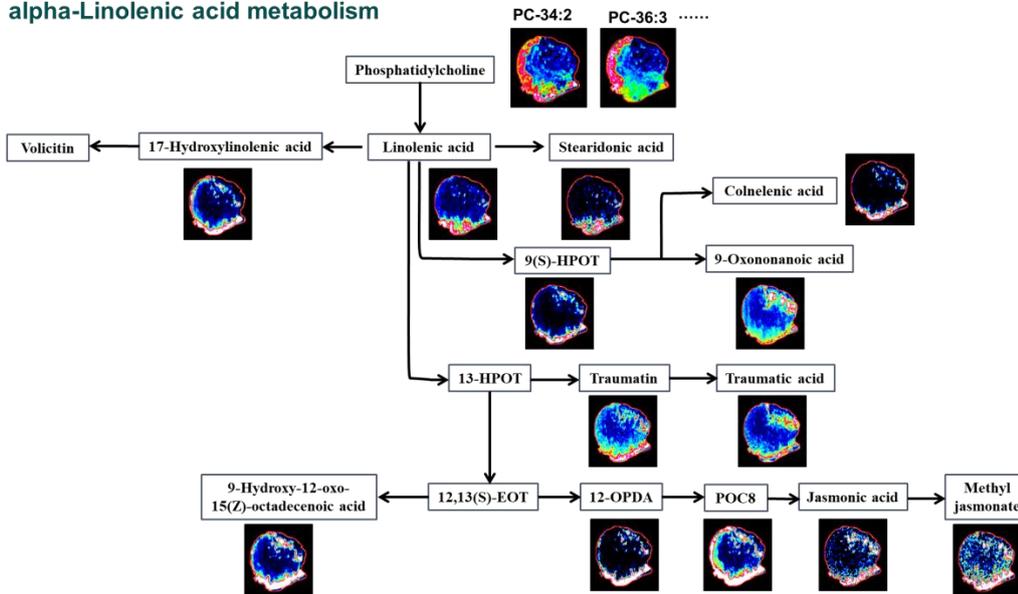
Supplementary Figure 19 | MS images of detected metabolites in linoleic acid metabolism pathway (intensity in colour scale is relative value).

### Arachidonic acid metabolism



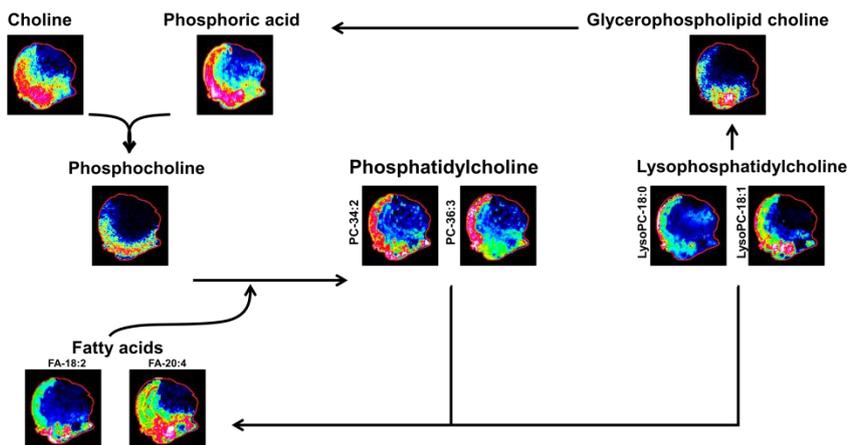
Supplementary Figure 20 | MS images of detected metabolites in arachidonic acid metabolism pathway (intensity in colour scale is relative value).

**alpha-Linolenic acid metabolism**



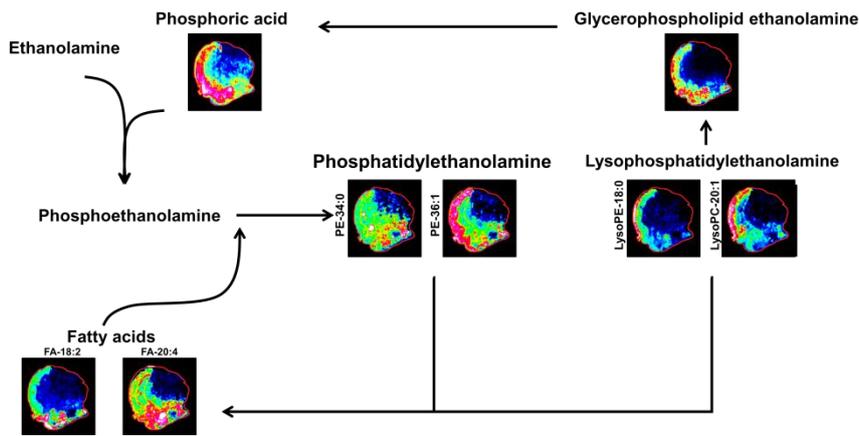
Supplementary Figure 21 | MS images of detected metabolites in alpha-linolenic acid metabolism pathway (intensity in colour scale is relative value).

**Phosphatidylcholine metabolism**



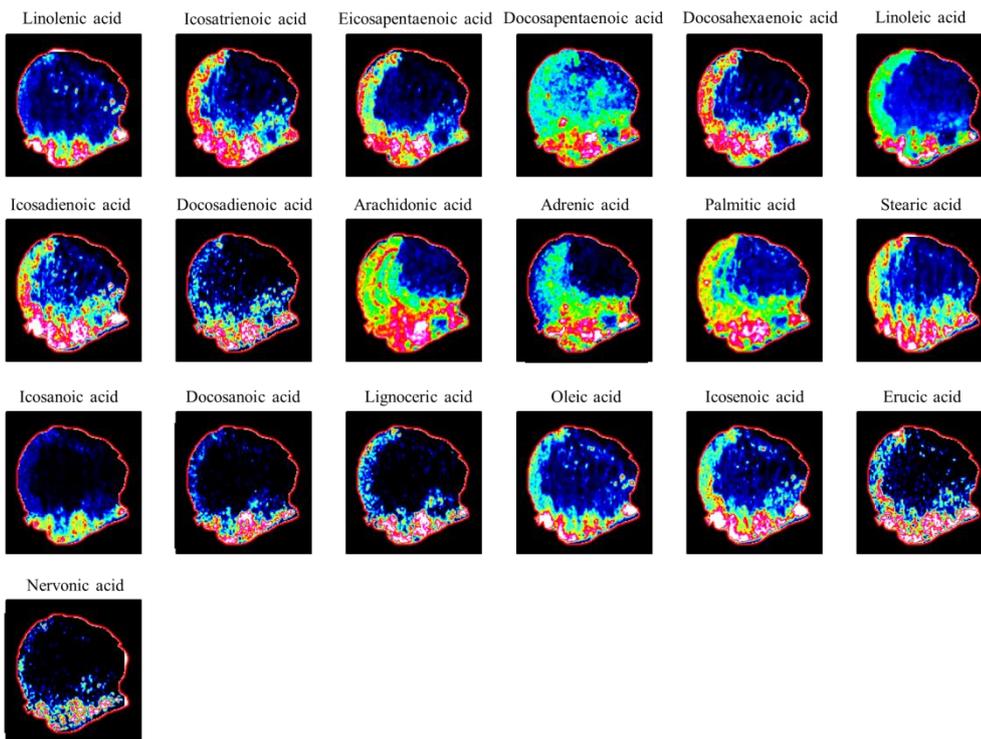
Supplementary Figure 22 | MS images of detected metabolites in phosphatidylcholine metabolism pathway (intensity in colour scale is relative value).

### Phosphatidylethanolamine metabolism



Supplementary Figure 23 | MS images of detected metabolites in phosphatidylethanolamine metabolism pathway (intensity in colour scale is relative value).

### Biosynthesis of unsaturated fatty acids

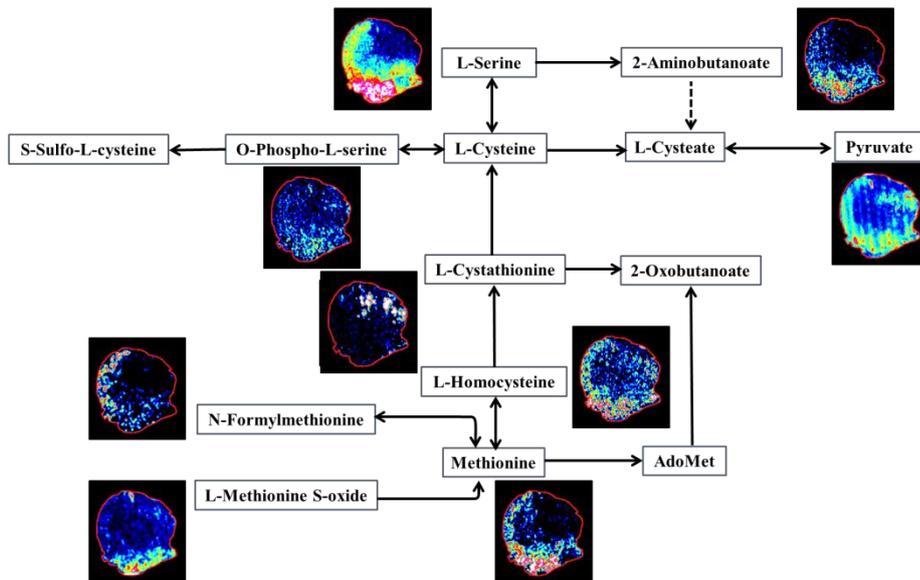


Supplementary Figure 24 | MS images of detected metabolites in biosynthesis of unsaturated fatty acids pathway (intensity in colour scale is relative value).



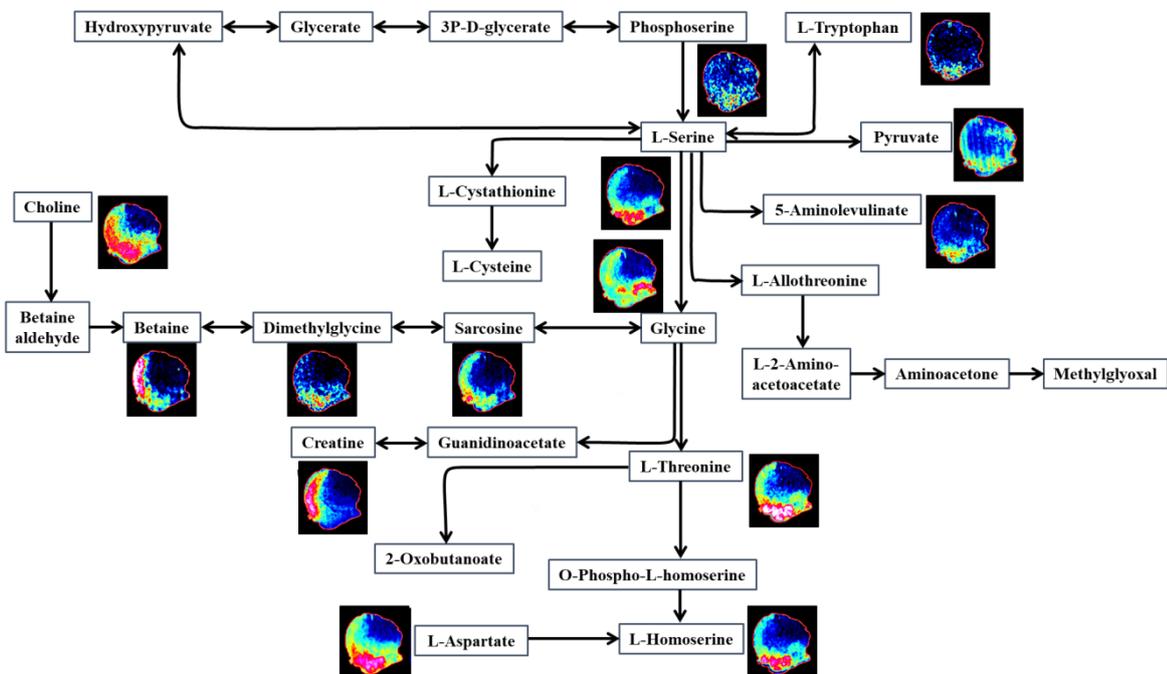


### Cysteine and methionine metabolism



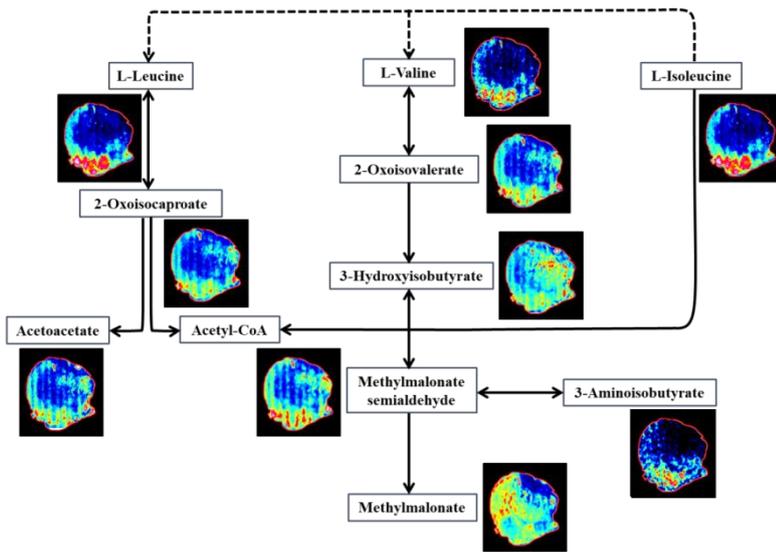
Supplementary Figure 29 | MS images of detected metabolites in cysteine and methionine metabolism pathway (intensity in colour scale is relative value).

### Glycine, serine and threonine metabolism



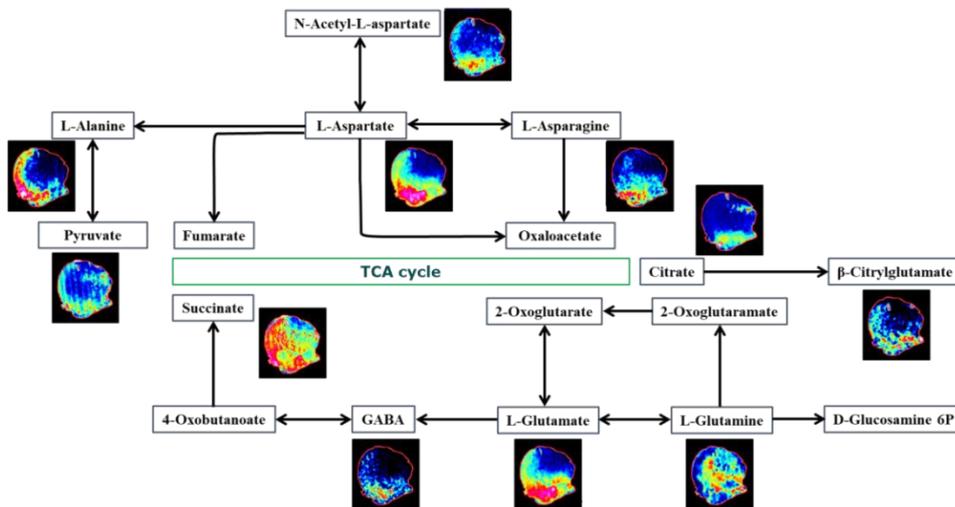
Supplementary Figure 30 | MS images of detected metabolites in glycine, serine and threonine metabolism pathway (intensity in colour scale is relative value).

### Valine, leucine and isoleucine degradation



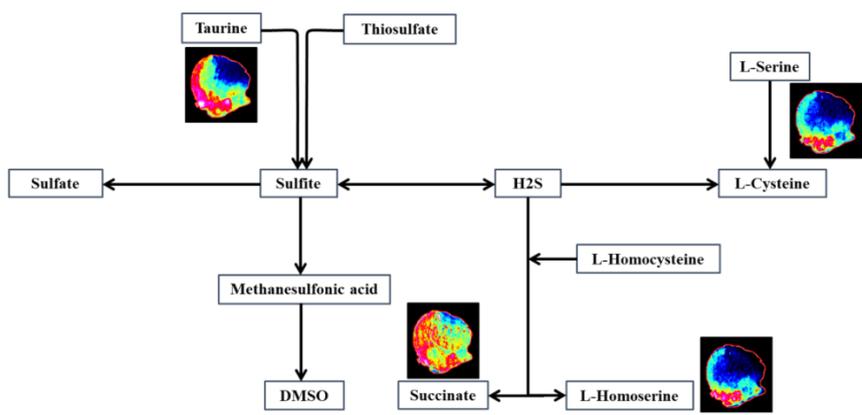
Supplementary Figure 31 | MS images of detected metabolites in valine, leucine and isoleucine degradation pathway (intensity in colour scale is relative value).

### Alanine, aspartate and glutamate metabolism



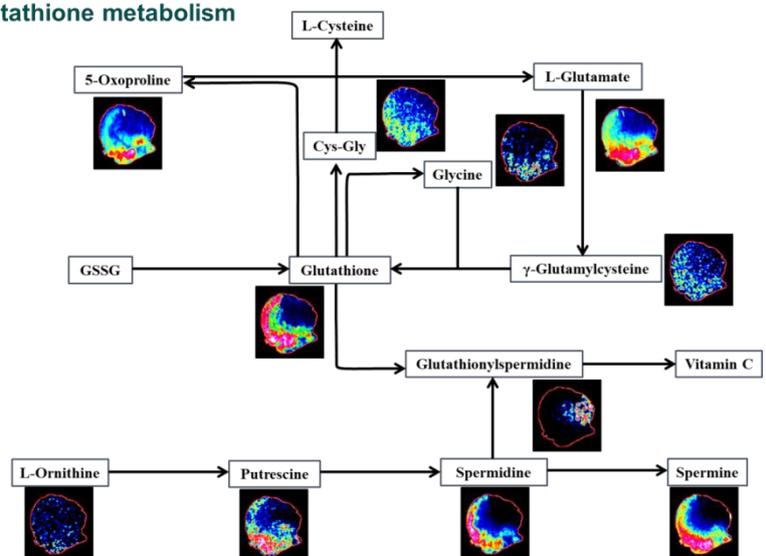
Supplementary Figure 32 | MS images of detected metabolites in alanine, aspartate and glutamate metabolism pathway (intensity in colour scale is relative value).

### Sulfur metabolism



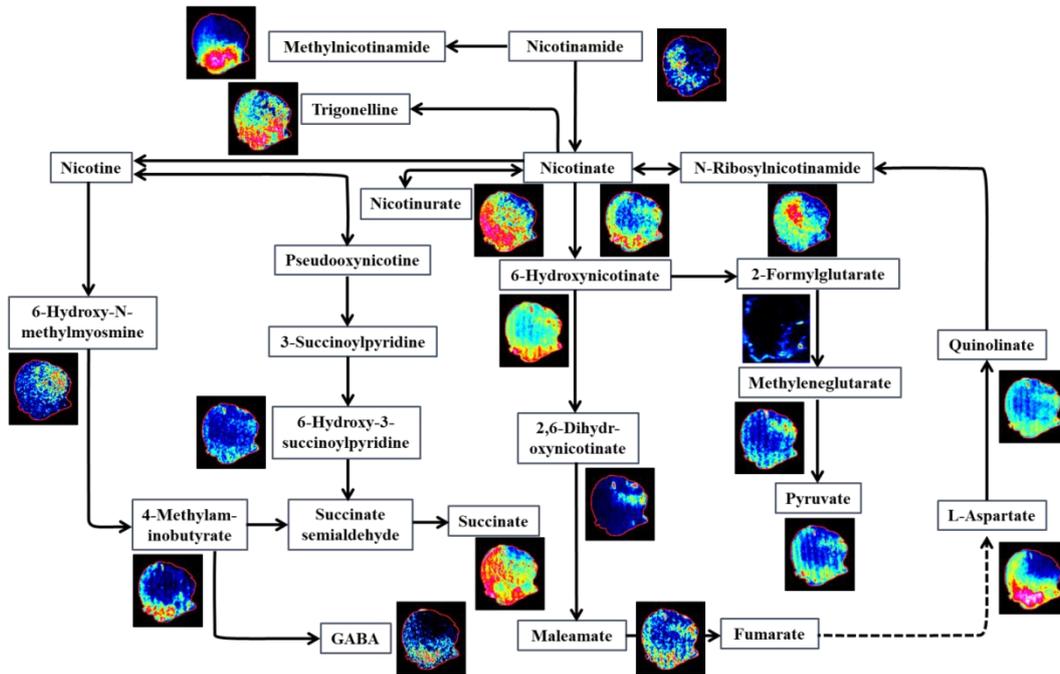
Supplementary Figure 33 | MS images of detected metabolites in sulfur metabolism pathway (intensity in colour scale is relative value).

### Glutathione metabolism

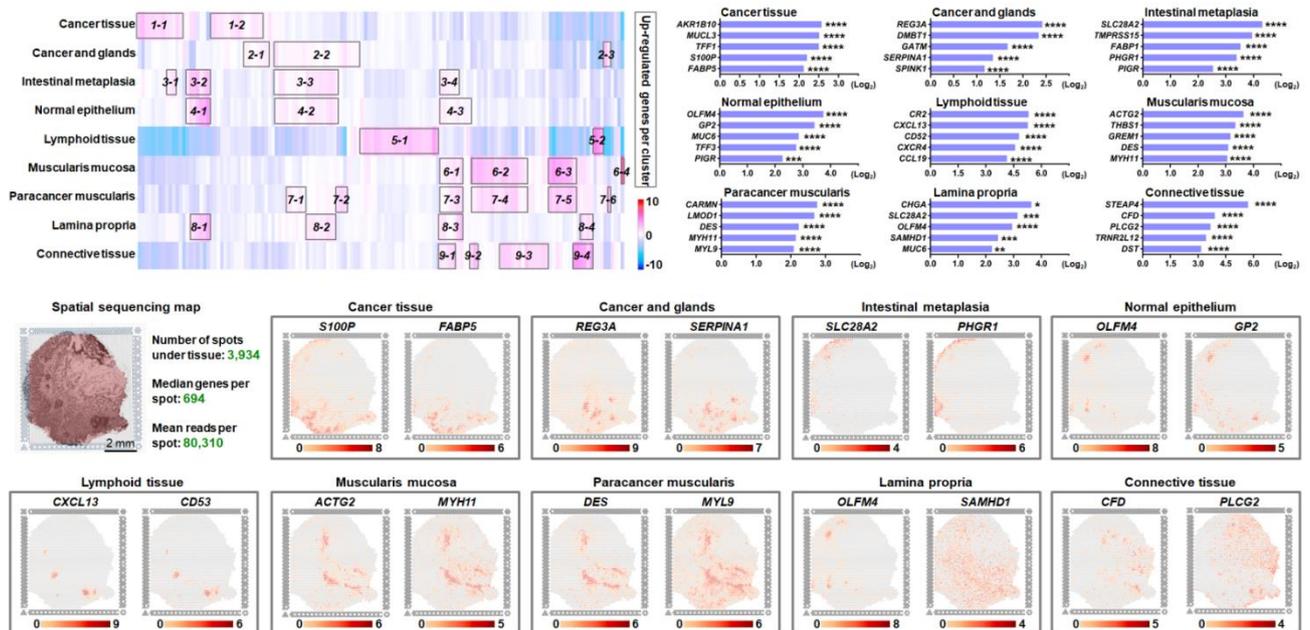


Supplementary Figure 34 | MS images of detected metabolites in glutathione metabolism pathway (intensity in colour scale is relative value).

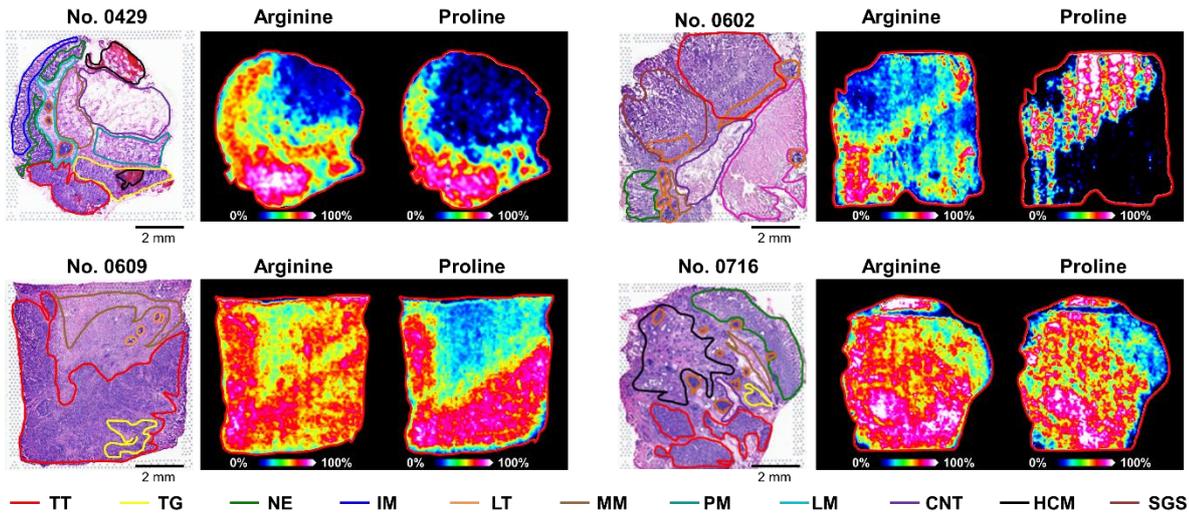
### Nicotinate and nicotinamide metabolism



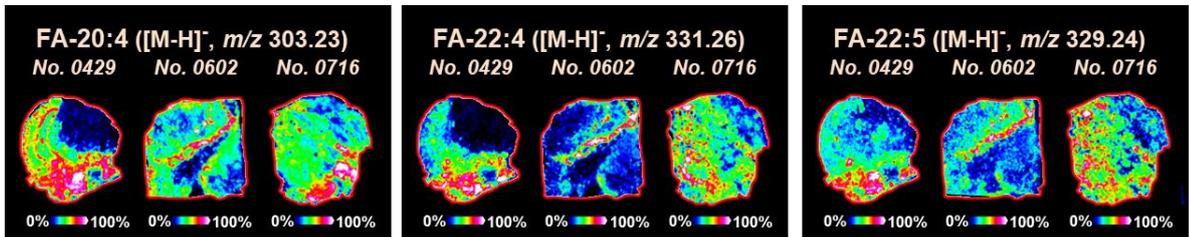
Supplementary Figure 35 | MS images of detected metabolites in nicotinate and nicotinamide metabolism pathway (intensity in colour scale is relative value).



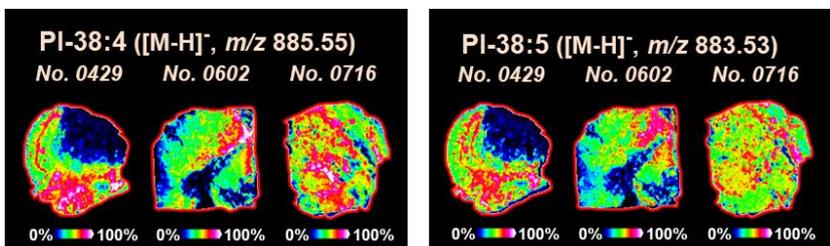
Supplementary Figure 36 | Visualization of region-specific genes in gastric cancer tissue. All scanning spots ( $n = 3934$ , the  $n$  number means the total number of spatial transcriptomics sequencing spots from patient "No.0429") were used for statistical analysis, \*\*\*\* $p < 0.001$ , \*\*\* $p < 0.01$ , \*\* $p < 0.05$ , \* $p < 0.1$ ,  $p$ -values are adjusted using the Benjamini-Hochberg correction for multiple tests, intensity in colour scale is log2 transformed.



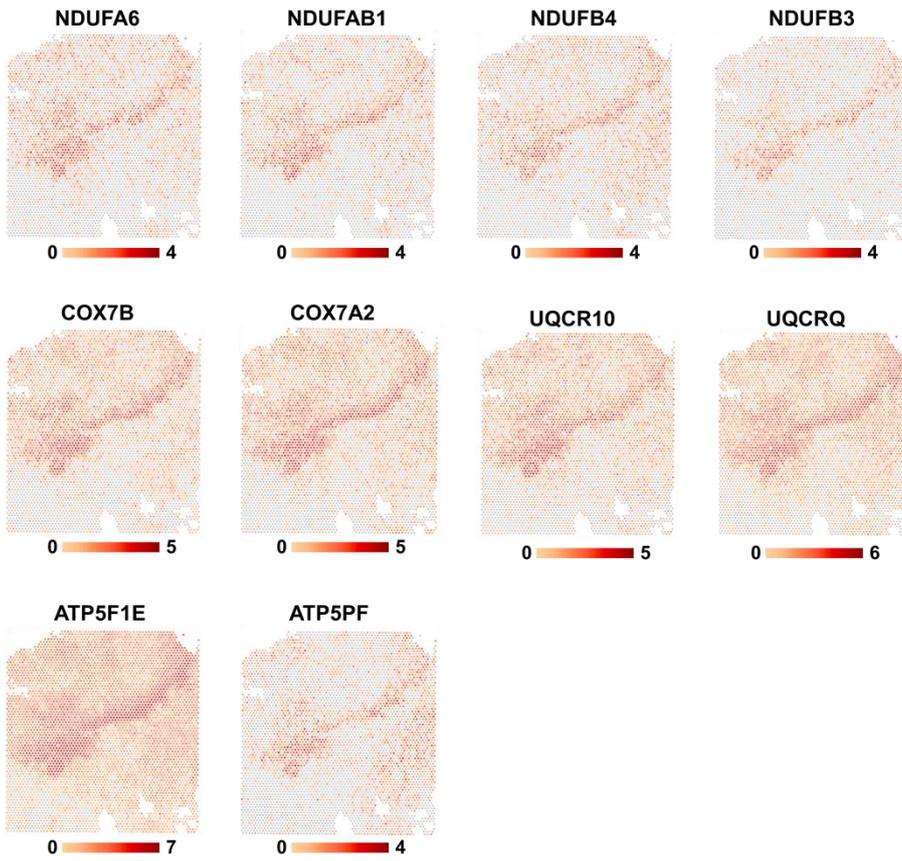
**Supplementary Figure 37 | MS images of arginine and proline in gastric cancer tissue sections.** TT: tumor tissue, TG: tumor and gland tissue, NE: normal epithelium, IM: intestinal metaplasia, LT: lymphoid tissue, MM: muscularis mucosa, PM: peritumoral muscularis, LM: lamina propria, CNT: connective tissue, SGS: serrated glandular structure, HCM: heterotopic cystic malformation, intensity in colour scale is relative value. Scale bar = 2 mm



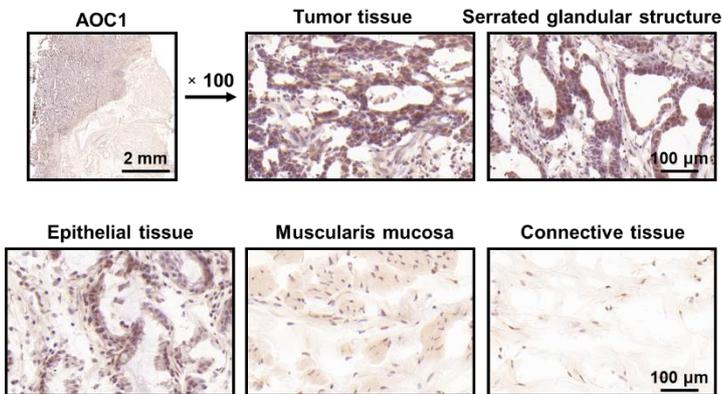
**Supplementary Figure 38 | MS images of representative polyunsaturated long-chain fatty acids in gastric cancer tissue sections, intensity in colour scale is relative value.**



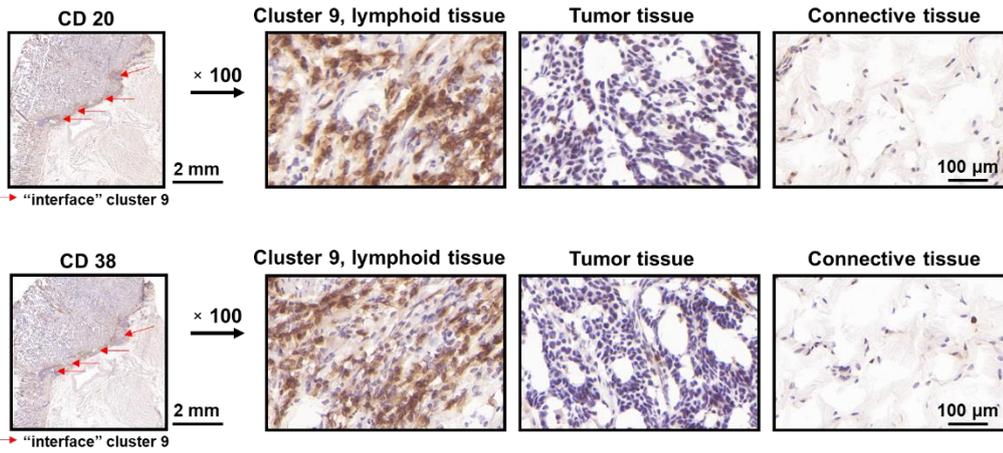
**Supplementary Figure 39 | MS images of representative polyunsaturated PIs in gastric cancer tissue sections, intensity in colour scale is relative value.**



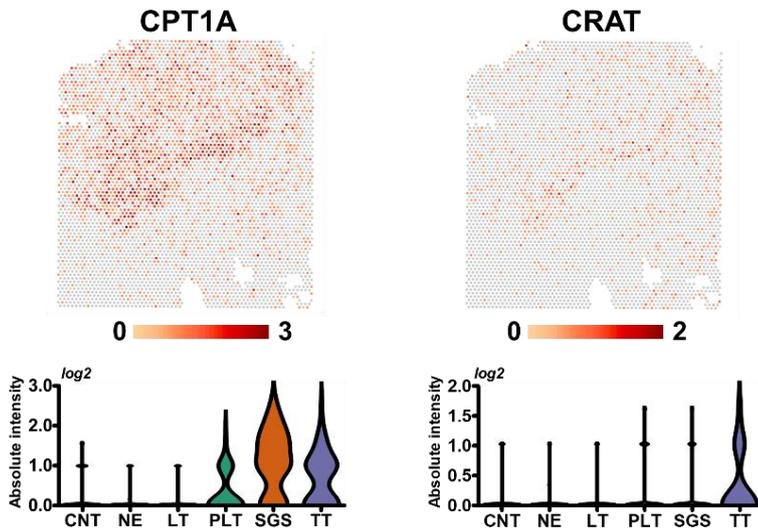
**Supplementary Figure 40 | Other altered genes in oxidative phosphorylation pathway, intensity in colour scale is  $\log_2$  transformed.**



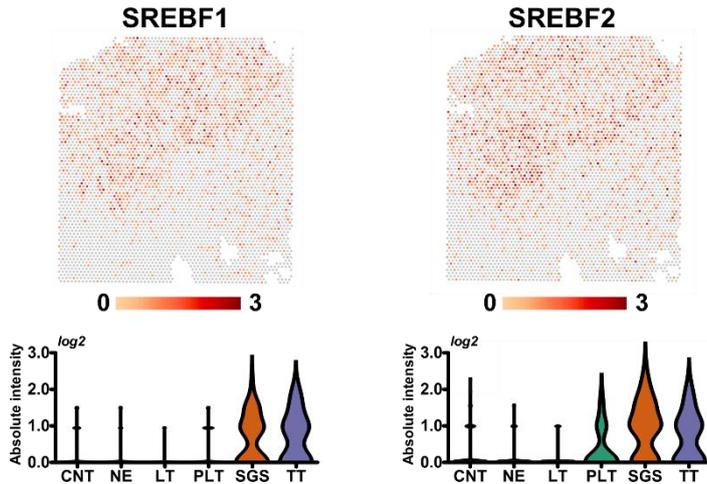
**Supplementary Figure 41 | Expression of AOC1 in different tissue regions of the gastric cancer tissue section.** Scale bar = 2 mm for whole tissue sections, scale bar = 100  $\mu\text{m}$  for magnified image. The IHC images are representative of one patient "No.0602", and the experiment was repeated three times.



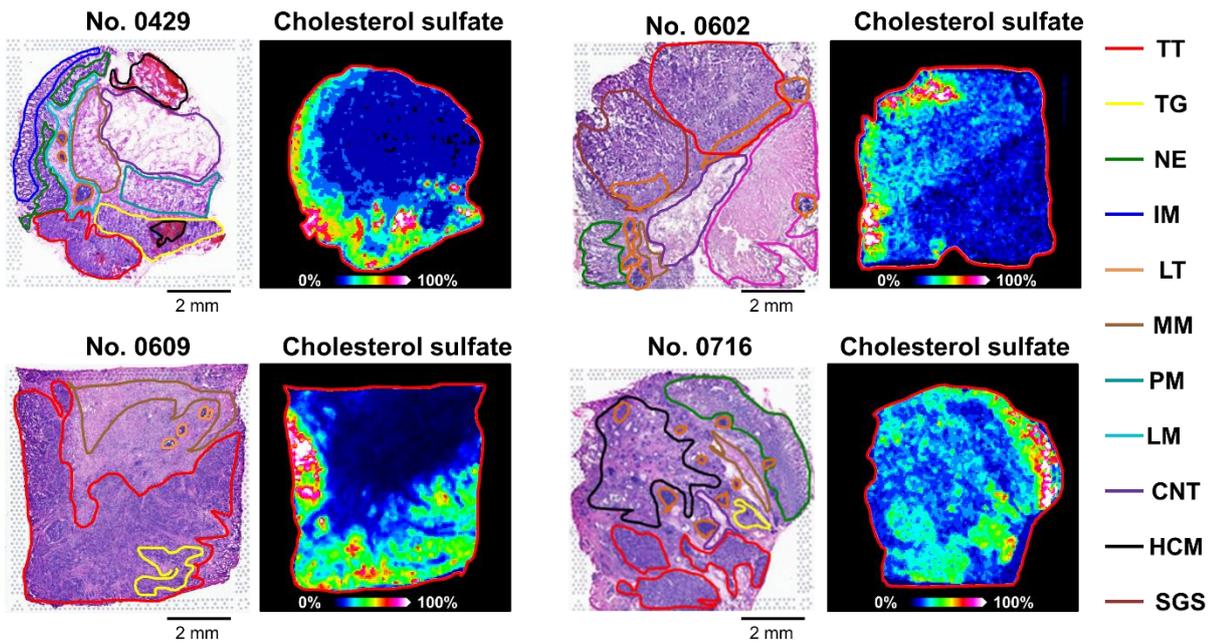
**Supplementary Figure 42 | IHC stain image of CD20 and CD 38 in adjacent gastric cancer tissue sections from patient “No.0602”.** Scale bar = 2 mm for whole tissue sections, scale bar = 100 μm for magnified image. The IHC images are representative of one patient “No.0602”, and the experiment was repeated three times.



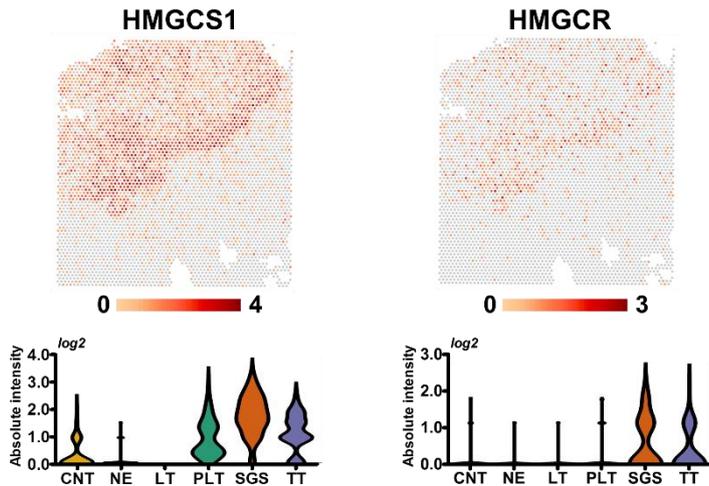
**Supplementary Figure 43 | Expressions of CPT1A and CRAT genes, intensity in colour scale is log2 transformed.**



**Supplementary Figure 44 | Expressions of SREBF1 and SREBF2 genes, intensity in colour scale is log<sub>2</sub> transformed.**



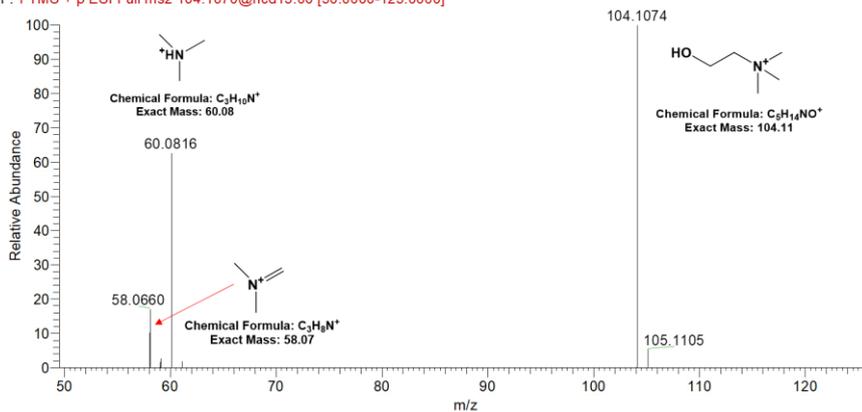
**Supplementary Figure 45 | MS images of cholesterol sulfate in different gastric cancer tissue sections. TT: tumor tissue, TG: tumor and gland tissue, NE: normal epithelium, IM: intestinal metaplasia, LT: lymphoid tissue, MM: muscularis mucosa, PM: peritumoral muscularis, LM: lamina propria, CNT: connective tissue, SGS: serrated glandular structure, HCM: heterotopic cystic malformation, intensity in colour scale is relative value. Scale bar = 2 mm.**



Supplementary Figure 46 | Expressions of HMGCS1 and HMGR genes, intensity in colour scale is log2 transformed.

#### Choline

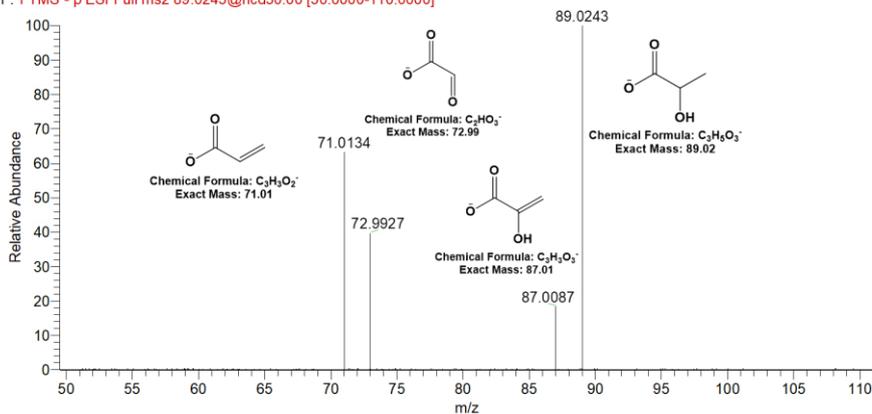
TUMOR-PRM-POS1 #289-358 RT: 1.00-1.14 AV: 2 SB: 7 0.26-0.68, 2.66-3.26 NL: 3.90E7  
 F: FTMS + p ESI Full ms2 104.1070@hcd15.00 [50.0000-125.0000]



Supplementary Figure 47 | The MS/MS spectrum and the fragmentation pathway of choline.

#### Lactic acid

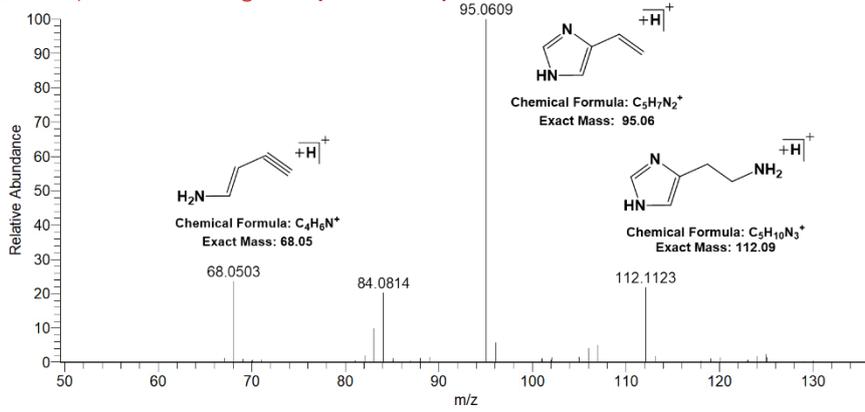
TUMOR-PRM-NEG89 #450-496 RT: 1.54-1.68 AV: 23 SB: 601 0.00-0.90, 10.03-13.32 NL: 2.50E5  
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Supplementary Figure 48 | The MS/MS spectrum and the fragmentation pathway of lactic acid.

### Histamine

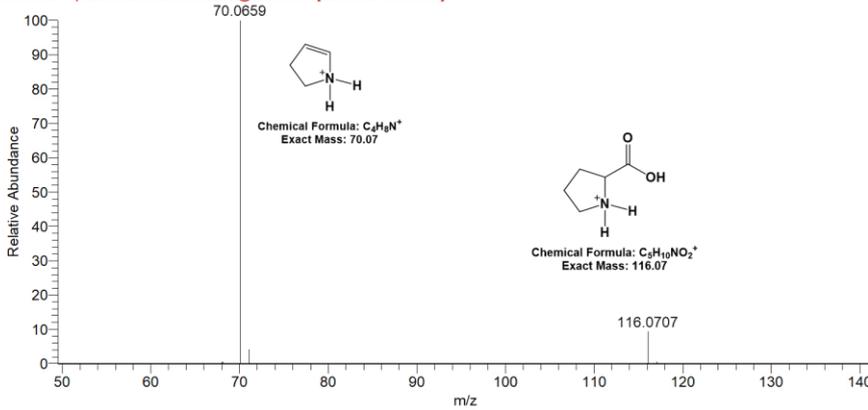
TUMOR-PRM-POS1 #232 RT: 0.87 AV: 1 SB: 9 0.11-0.52, 4.92-5.74 NL: 1.94E6  
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Supplementary Figure 49 | The MS/MS spectrum and the fragmentation pathway of histamine.

### Proline

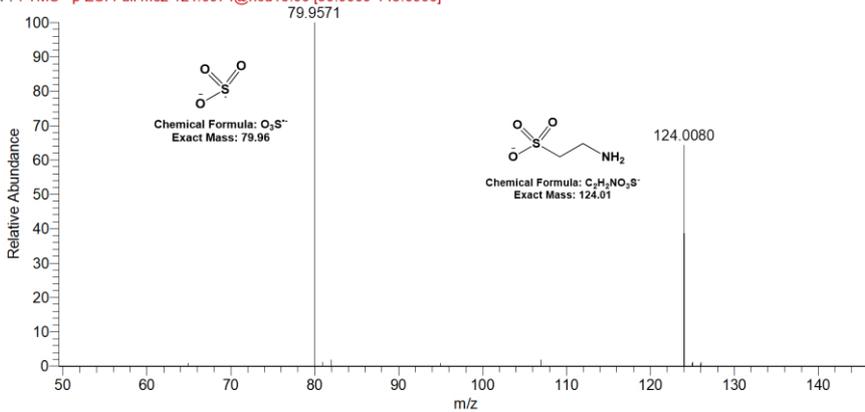
TUMOR-PRM-POS1 #323 RT: 1.16 AV: 1 SB: 8 0.30-0.79, 1.80-2.36 NL: 3.34E8  
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Supplementary Figure 50 | The MS/MS spectrum and the fragmentation pathway of proline.

### Taurine

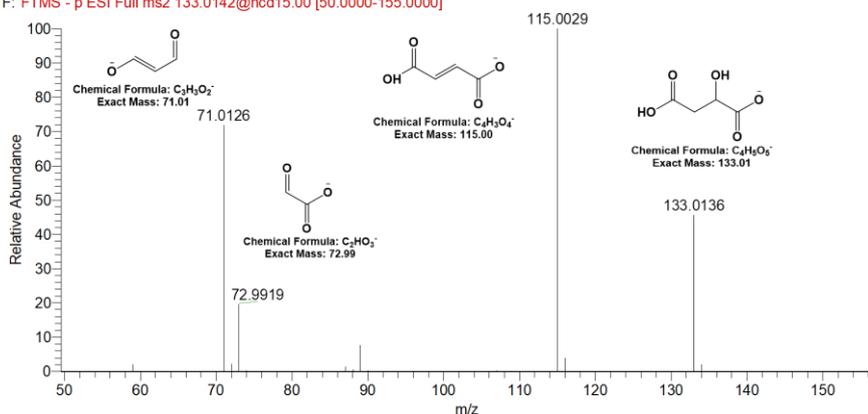
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Supplementary Figure 51 | The MS/MS spectrum and the fragmentation pathway of taurine.

### Malic acid

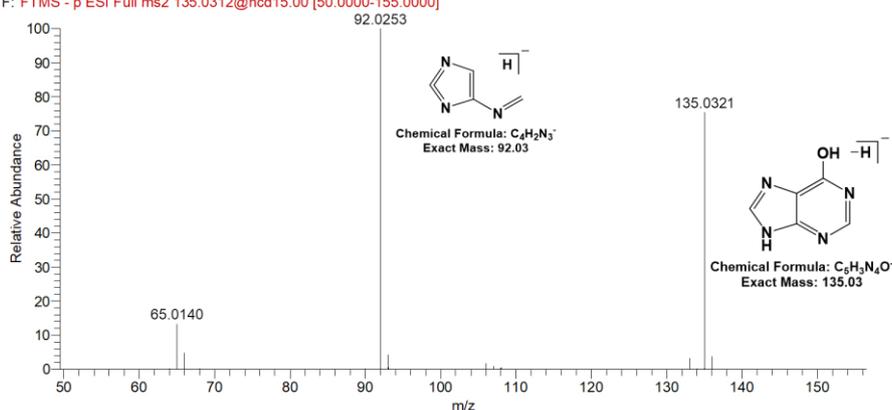
TUMOR-PRM-NEG1-15V-3 #349-430 RT: 1.32-1.44 AV: 2 SB: 12 0.11-0.72, 2.46-3.30 NL: 1.34E7  
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Supplementary Figure 52 | The MS/MS spectrum and the fragmentation pathway of malic acid.

### Hypoxanthine

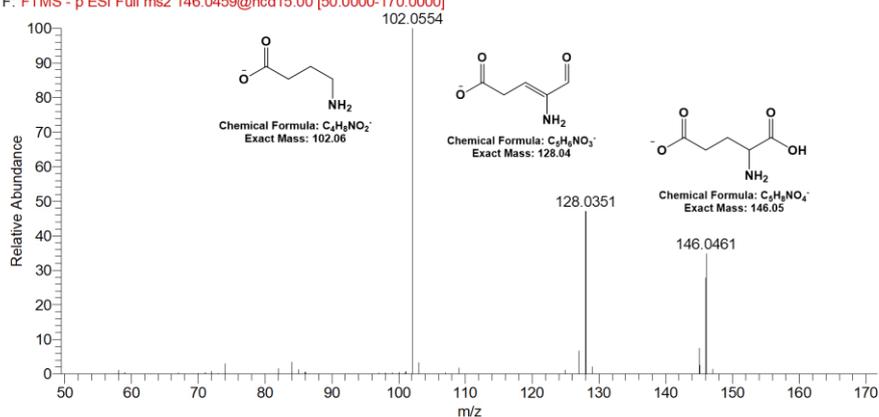
TUMOR-PRM-NEG1-15V #608 RT: 2.12 AV: 1 SB: 4 1.74-1.89, 2.48-2.78 NL: 1.20E7  
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Supplementary Figure 53 | The MS/MS spectrum and the fragmentation pathway of hypoxanthine.

### Glutamate

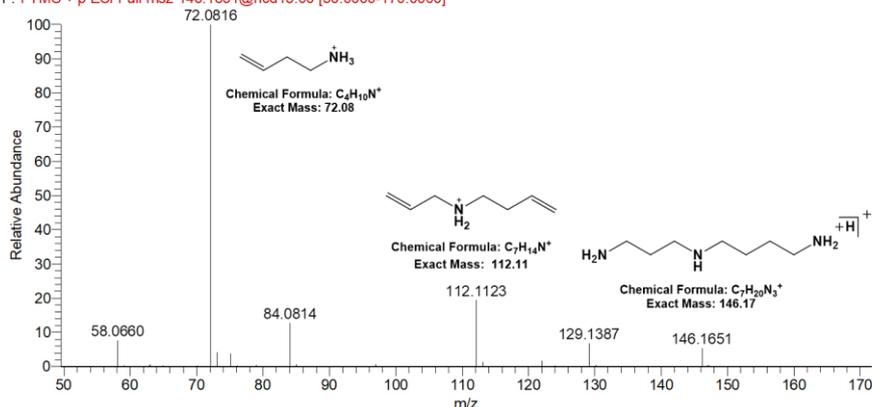
TUMOR-PRM-NEG1-15V-2 221116233731 #278 RT: 1.05 AV: 1 SB: 2 0.71-0.82, 1.49-1.64 NL: 1.79E7  
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Supplementary Figure 54 | The MS/MS spectrum and the fragmentation pathway of glutamate.

### Spermidine

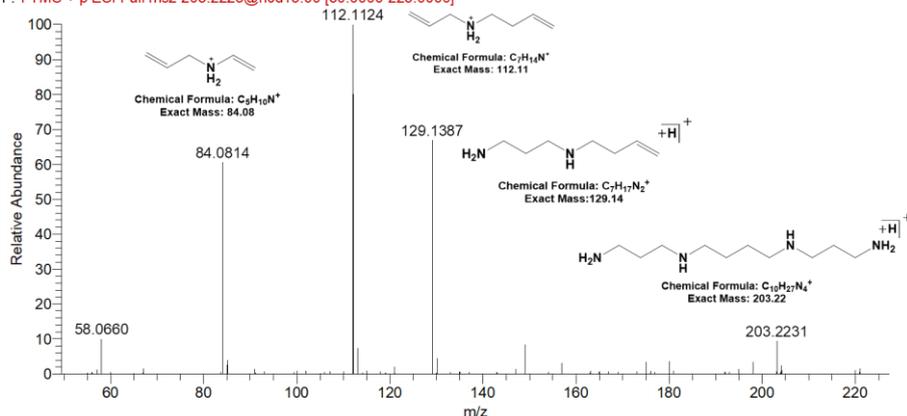
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Supplementary Figure 55 | The MS/MS spectrum and the fragmentation pathway of spermidine.

### Spermine

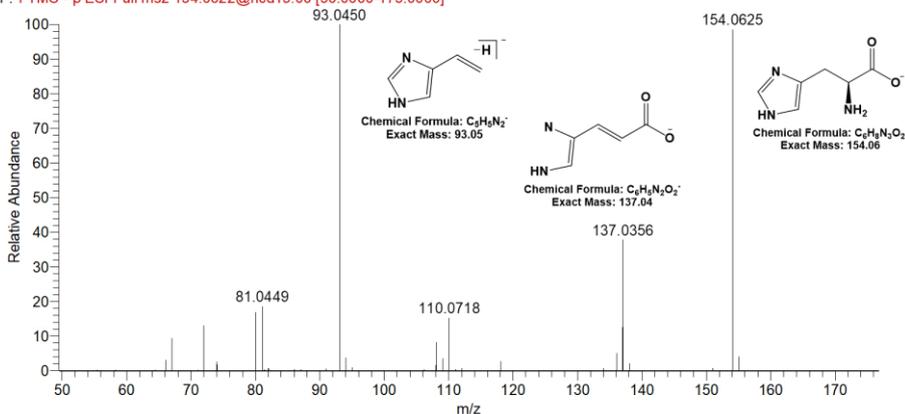
TUMOR-PRM-POS1 #220 RT: 0.80 AV: 1 SB: 4 0.33-0.51, 1.16-1.52 NL: 2.69E5  
 F: FTMS + p ESI Full ms2 203.2228@hcd15.00 [50.0000-225.0000]



Supplementary Figure 56 | The MS/MS spectrum and the fragmentation pathway of spermine.

### Histidine

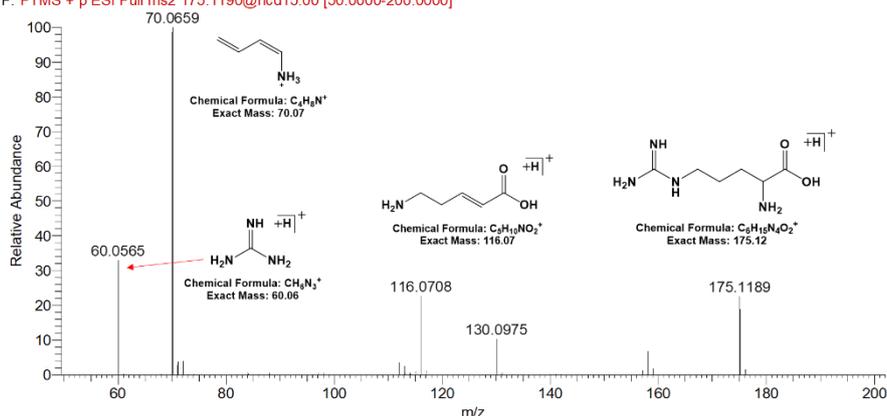
TUMOR-PRM-NEG1-15V-2 221116233731 #239 RT: 0.93 AV: 1 SB: 11 0.11-0.62, 2.09-3.09 NL: 3.05E5  
 F: FTMS - p ESI Full ms2 154.0622@hcd15.00 [50.0000-175.0000]



Supplementary Figure 57 | The MS/MS spectrum and the fragmentation pathway of histidine.

### Arginine

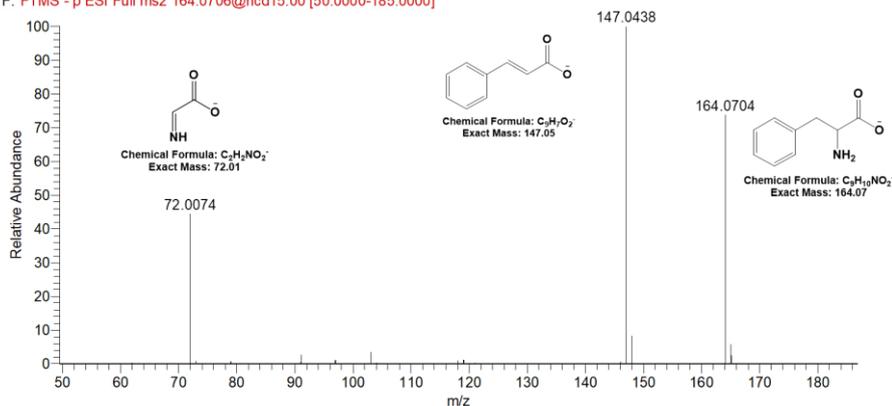
TUMOR-PRM-POS1 #298 RT: 1.07 AV: 1 SB: 7 0.41-0.72, 1.94-2.66 NL: 2.01E7  
 F: FTMS + p ESI Full ms2 175.1190@hcd15.00 [50.0000-200.0000]



Supplementary Figure 58 | The MS/MS spectrum and the fragmentation pathway of arginine.

### Phenylalanine

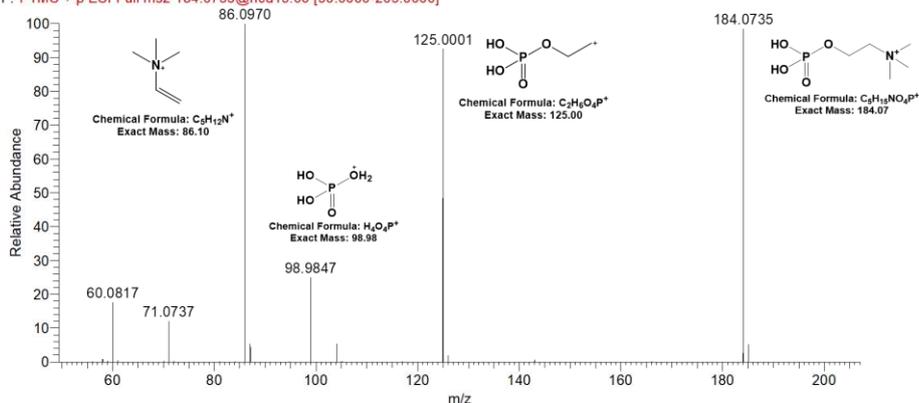
TUMOR-PRM-NEG1-15V-2 #814-870 RT: 2.83-2.96 AV: 2 SB: 12 1.59-2.20, 4.66-5.53 NL: 1.90E6  
 F: FTMS - p ESI Full ms2 164.0706@hcd15.00 [50.0000-185.0000]



Supplementary Figure 59 | The MS/MS spectrum and the fragmentation pathway of phenylalanine.

### Phosphocholine

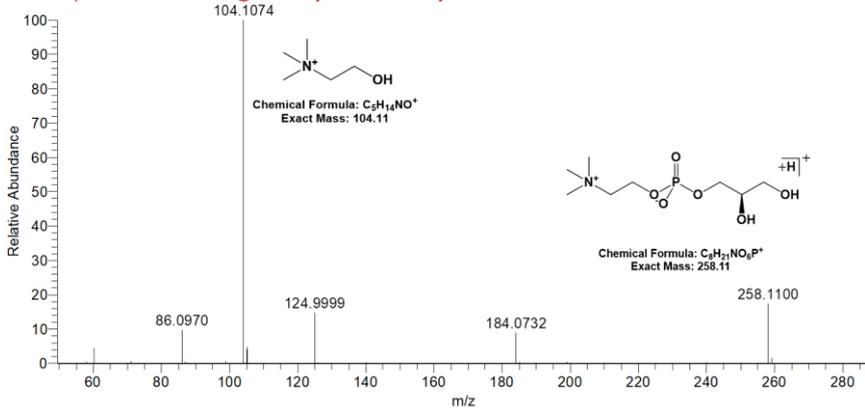
TUMOR-PRM-POS1 #302 RT: 1.07 AV: 1 SB: 5 0.42-0.71, 1.83-2.26 NL: 2.59E7  
 F: FTMS + p ESI Full ms2 184.0733@hcd15.00 [50.0000-205.0000]



Supplementary Figure 60 | The MS/MS spectrum and the fragmentation pathway of phosphocholine.

Glycerophosphocholine

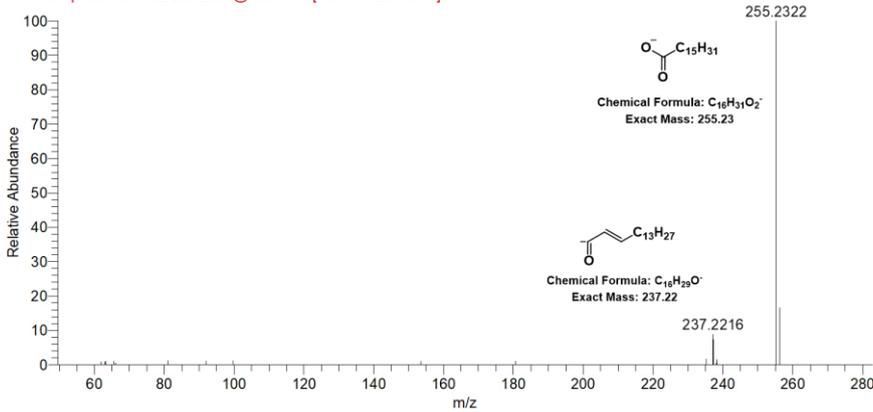
TUMOR-PRM-POS1 #309 RT: 1.09 AV: 1 SB: 4 0.60-0.81, 1.77-2.13 NL: 3.93E7  
 F: FTMS + p ESI Full ms2 258.1101@hcd15.00 [50.0000-285.0000]



Supplementary Figure 61 | The MS/MS spectrum and the fragmentation pathway of glycerophosphocholine.

FA-16:0

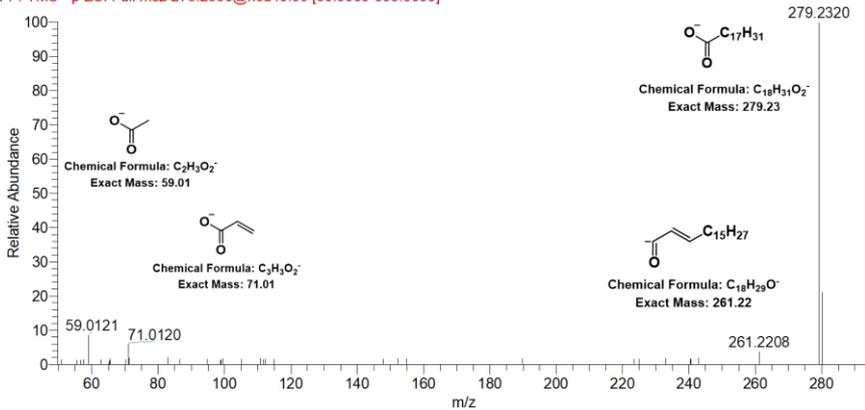
TUMOR-PRM-NEG2-40V #6355 RT: 22.47 AV: 1 SB: 11 21.17-21.74, 23.93-24.61 NL: 1.11E5  
 F: FTMS - p ESI Full ms2 255.2330@hcd40.00 [50.0000-280.0000]



Supplementary Figure 62 | The MS/MS spectrum and the fragmentation pathway of FA-16:0.

FA-18:2

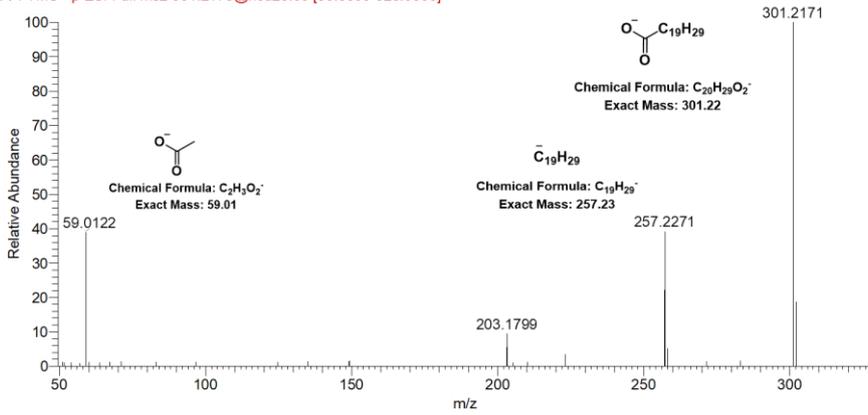
TUMOR-PRM-NEG2-40V #6181-6260 RT: 21.79-22.01 AV: 3 SB: 20 20.12-21.21, 22.80-23.93 NL: 2.21E4  
 F: FTMS - p ESI Full ms2 279.2330@hcd40.00 [50.0000-305.0000]



Supplementary Figure 63 | The MS/MS spectrum and the fragmentation pathway of FA-18:2.

FA-20:5

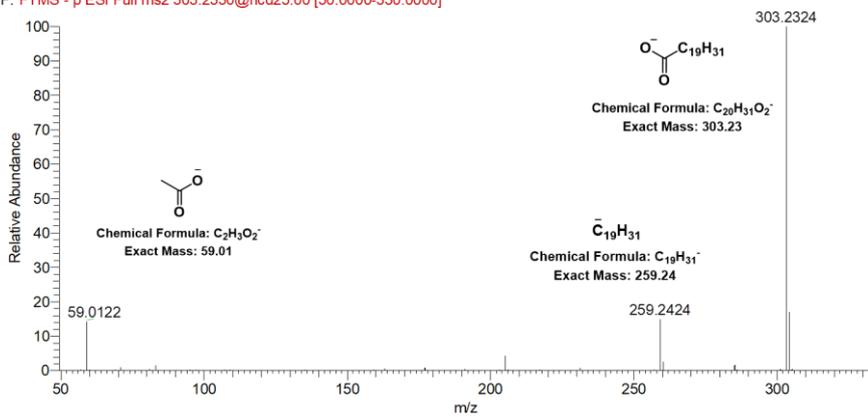
TUMOR-PRM-NEG2-25V #5901-5958 RT: 21.09-21.22 AV: 2 SB: 20 18.91-19.85 , 23.14-24.50 NL: 4.64E4  
 F: FTMS - p ESI Full ms2 301.2173@hcd25.00 [50.0000-325.0000]



Supplementary Figure 64 | The MS/MS spectrum and the fragmentation pathway of FA-20:5.

FA-20:4

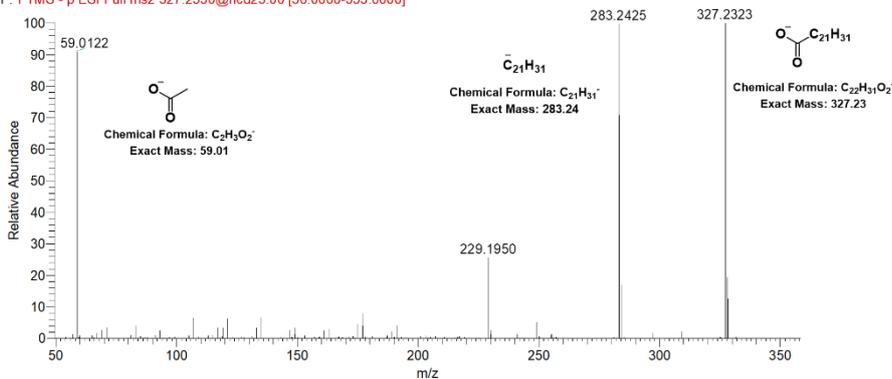
TUMOR-PRM-NEG2-25V #6055 RT: 21.73 AV: 1 SB: 14 19.78-20.69 , 22.72-23.70 NL: 2.30E6  
 F: FTMS - p ESI Full ms2 303.2330@hcd25.00 [50.0000-330.0000]



Supplementary Figure 65 | The MS/MS spectrum and the fragmentation pathway of FA-20:4.

FA-22:6

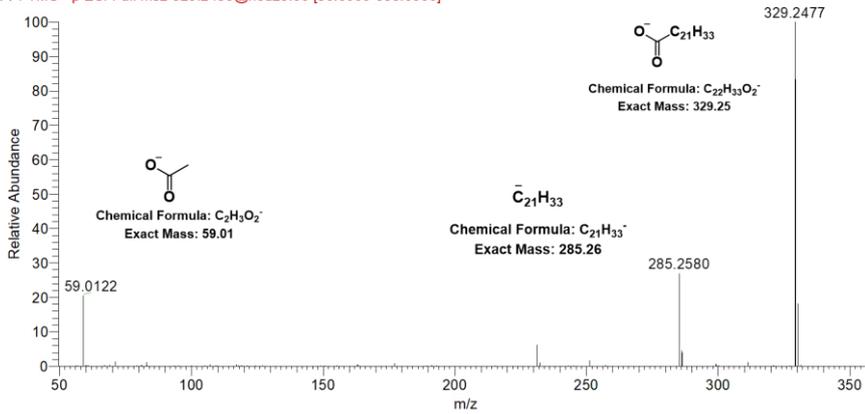
TUMOR-PRM-NEG2-25V #5986-6045 RT: 21.50-21.62 AV: 2 SB: 17 19.29-20.49 , 23.02-23.89 NL: 2.26E5  
 F: FTMS - p ESI Full ms2 327.2330@hcd25.00 [50.0000-355.0000]



Supplementary Figure 66 | The MS/MS spectrum and the fragmentation pathway of FA-22:6.

FA-22:5

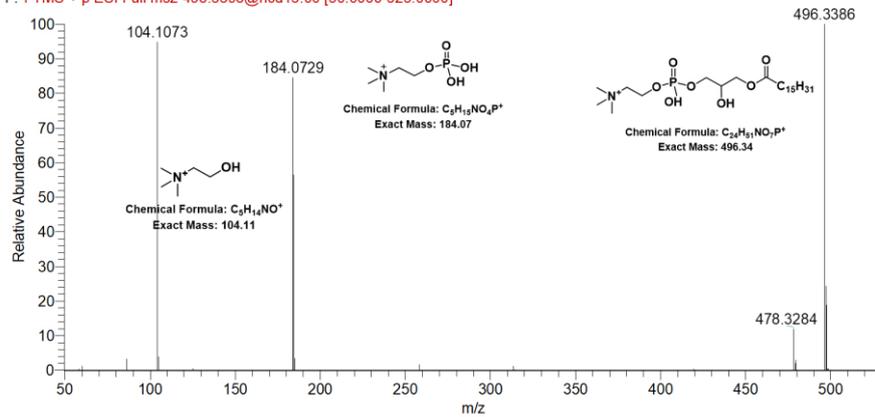
TUMOR-PRM-NEG2-25V #6105-6143 RT: 21.87-22.00 AV: 2 SB: 15 20.04-20.76 , 23.51-24.68 NL: 3.32E5  
F: FTMS - p ESI Full ms2 329.2486@hcd25.00 [50.0000-355.0000]



Supplementary Figure 67 | The MS/MS spectrum and the fragmentation pathway of FA-22:5.

Lyso PC-16:0

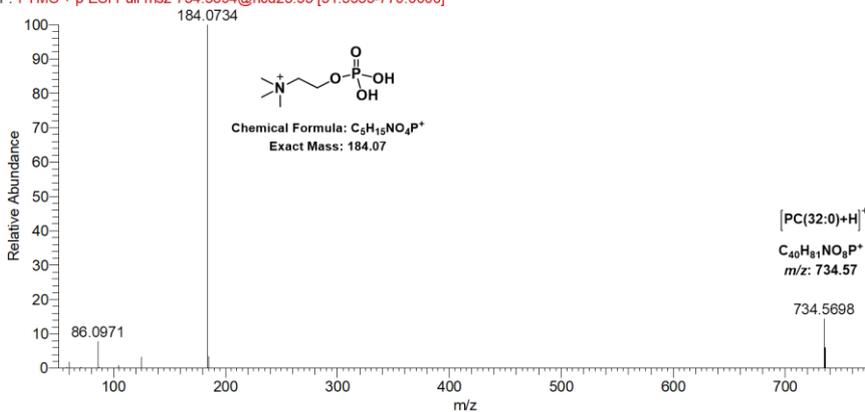
TUMOR-PRM-POS1 #3914 RT: 13.17 AV: 1 SB: 20 10.99-12.08 , 14.89-16.62 NL: 6.56E7  
F: FTMS + p ESI Full ms2 496.3398@hcd15.00 [50.0000-525.0000]



Supplementary Figure 68 | The MS/MS spectrum and the fragmentation pathway of lysoPC-16:0.

PC-32:0

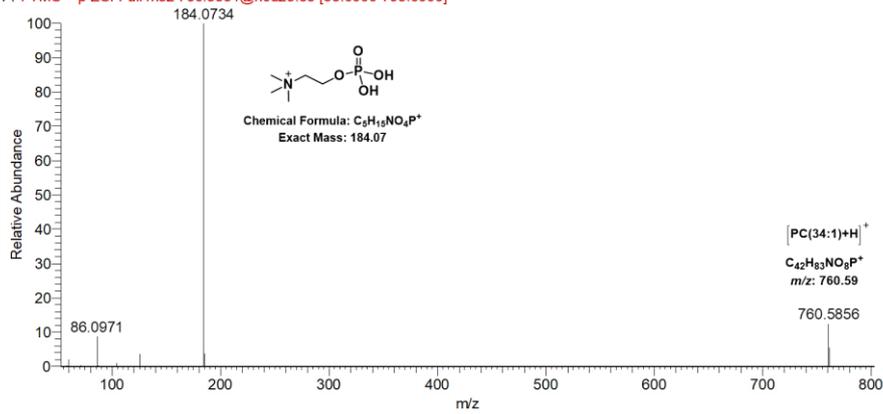
TUMOR-L-POS1 #4330-4422 RT: 14.24-14.50 AV: 11 SB: 62 12.72-13.43 , 16.31-17.21 NL: 1.09E8  
F: FTMS + p ESI Full ms2 734.5694@hcd23.33 [51.3333-770.0000]



Supplementary Figure 69 | The MS/MS spectrum and the fragmentation pathway of PC-32:0.

PC-34:1

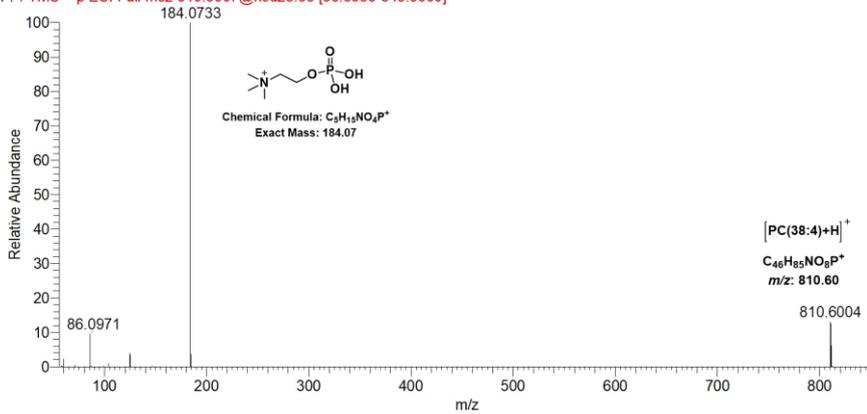
TUMOR-L-POS1 #4342-4411 RT: 14.27-14.48 AV: 9 SB: 87 12.12-13.21, 15.79-16.99 NL: 3.20E8  
F: FTMS + p ESI Full ms2 760.5851@hcd23.33 [53.0000-795.0000]



Supplementary Figure 70 | The MS/MS spectrum and the fragmentation pathway of PC-34:1.

PC-38:4

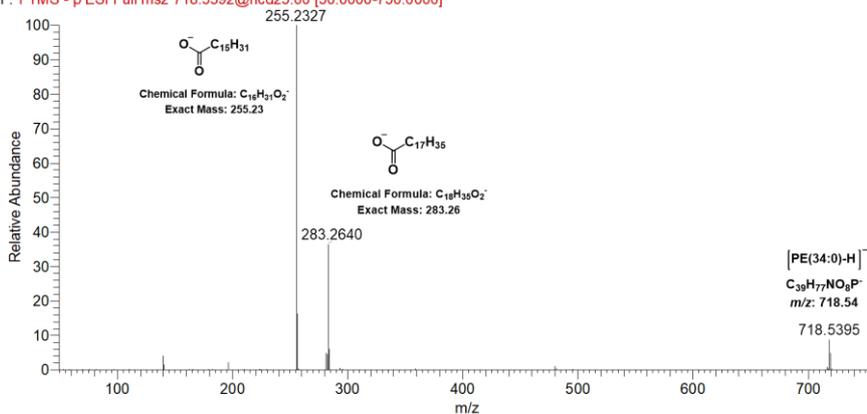
TUMOR-L-POS1 #4319-4365 RT: 14.18-14.31 AV: 6 SB: 77 12.16-12.87, 17.40-18.71 NL: 8.89E7  
F: FTMS + p ESI Full ms2 810.6007@hcd23.33 [56.3333-845.0000]



Supplementary Figure 71 | The MS/MS spectrum and the fragmentation pathway of PC-38:4.

PE-34:0

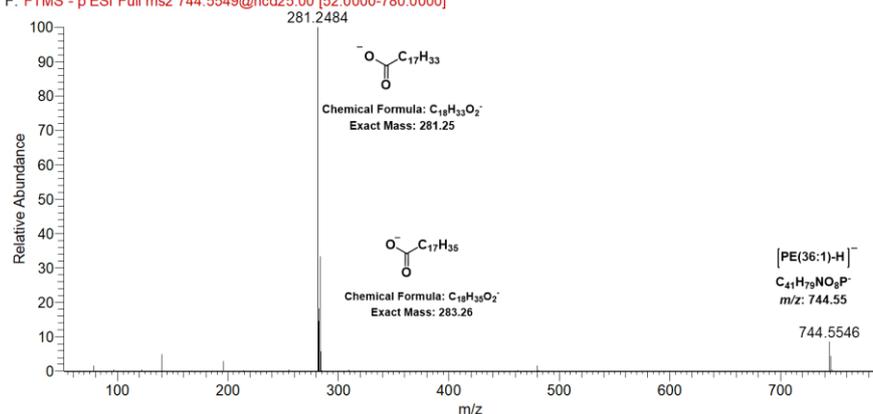
TUMOR-L-NEG1 #4302-4357 RT: 15.56-15.66 AV: 2 SB: 21 11.93-12.91, 16.61-17.96 NL: 3.12E5  
F: FTMS - p ESI Full ms2 718.5392@hcd25.00 [50.0000-750.0000]



Supplementary Figure 72 | The MS/MS spectrum and the fragmentation pathway of PE-34:0.

## PE-36:1

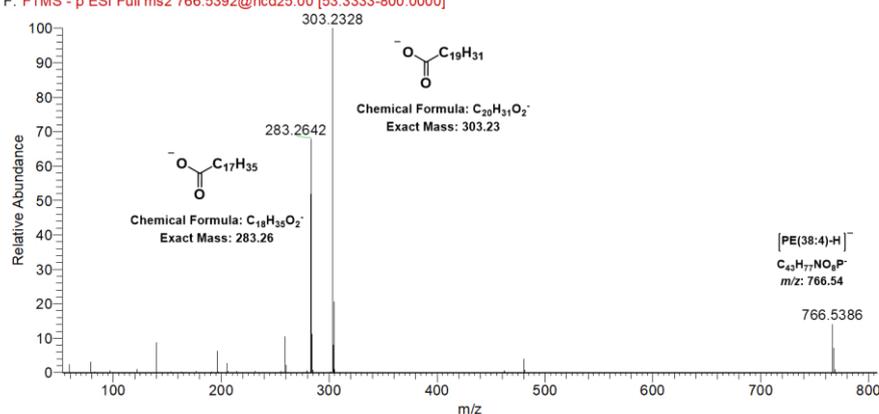
TUMOR-L-NEG1 #4302-4357 RT: 15.56-15.67 AV: 2 SB: 17 13.28-14.18 , 16.57-17.51 NL: 1.83E7  
 F: FTMS - p ESI Full ms2 744.5549@hcd25.00 [52.0000-780.0000]



Supplementary Figure 73 | The MS/MS spectrum and the fragmentation pathway of PE-36:1.

## PE-38:4

TUMOR-L-NEG1 #3980 RT: 14.49 AV: 1 SB: 19 11.49-12.72 , 16.05-16.99 NL: 1.09E7  
 F: FTMS - p ESI Full ms2 766.5392@hcd25.00 [53.3333-800.0000]



Supplementary Figure 74 | The MS/MS spectrum and the fragmentation pathway of PE-38:4.

Supplementary Table 1 | Annotated metabolites among the metabolic pathways analyzed in this study.

Name	Formula	Ion type	Theoretical m/z	Measured m/z	Relative error (ppm)
Choline	$C_5H_{13}NO$	$[M+H]^+$	104.107	104.1066	-3.85
Histamine	$C_5H_9N_3$	$[M+H]^+$	112.0869	112.0865	-3.57
Proline	$C_5H_9NO_2$	$[M+H]^+$	116.0706	116.0702	-3.45
Spermine	$C_{10}H_{26}N_4$	$[M+H]^+$	203.2228	203.2225	-1.48
Spermidine	$C_7H_{19}N_3$	$[M+H]^+$	146.1651	146.1648	-2.05
Arginine	$C_6H_{14}N_4O_2$	$[M+H]^+$	175.119	175.1185	-2.86
L-Carnitine*	$C_7H_{15}NO_3$	$[M+H]^+$	162.1122	162.112	-1.23
Betaine*	$C_5H_{11}NO_2$	$[M+H]^+$	118.0863	118.0860	-2.54

Phosphocholine	C <sub>5</sub> H <sub>14</sub> NO <sub>4</sub> P	[M+H] <sup>+</sup>	184.0733	184.0729	-2.17
Glycerophosphocholine	C <sub>8</sub> H <sub>20</sub> NO <sub>6</sub> P	[M+H] <sup>+</sup>	258.1101	258.1092	-3.49
Lyso PC-16:0	C <sub>24</sub> H <sub>50</sub> NO <sub>7</sub> P	[M+H] <sup>+</sup>	496.3398	496.3386	-2.42
Lyso PC-18:0	C <sub>26</sub> H <sub>54</sub> NO <sub>7</sub> P	[M+H] <sup>+</sup>	524.3711	524.3694	-3.24
Lyso PC-18:1	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P	[M+H] <sup>+</sup>	522.3554	522.3538	-3.06
PC-32:0	C <sub>40</sub> H <sub>80</sub> NO <sub>8</sub> P	[M+H] <sup>+</sup>	734.5694	734.5664	-4.09
PC-34:1	C <sub>42</sub> H <sub>82</sub> NO <sub>8</sub> P	[M+H] <sup>+</sup>	760.5851	760.5815	-4.74
PC-34:2	C <sub>42</sub> H <sub>80</sub> NO <sub>8</sub> P	[M+H] <sup>+</sup>	758.5694	758.5662	-4.22
PC-36:2	C <sub>44</sub> H <sub>84</sub> NO <sub>8</sub> P	[M+H] <sup>+</sup>	786.6007	786.5981	-3.31
PC-38:4	C <sub>46</sub> H <sub>84</sub> NO <sub>8</sub> P	[M+H] <sup>+</sup>	810.6007	810.5972	-4.32
Lactic acid	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	[M-H] <sup>-</sup>	89.0244	89.0240	-4.49
Taurine	C <sub>2</sub> H <sub>7</sub> NO <sub>3</sub> S	[M-H] <sup>-</sup>	124.0074	124.0068	-4.84
Malic acid	C <sub>4</sub> H <sub>5</sub> O <sub>5</sub>	[M-H] <sup>-</sup>	133.0142	133.0136	-4.51
Hypoxanthine	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O	[M-H] <sup>-</sup>	135.0312	135.0306	-4.44
Glutamate	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	[M-H] <sup>-</sup>	146.0459	146.0452	-4.79
Histidine	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	154.0622	154.0615	-4.55
Phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	[M-H] <sup>-</sup>	164.0706	164.0709	1.83
Glucose-phosphate	C <sub>6</sub> H <sub>13</sub> O <sub>9</sub> P	[M-H] <sup>-</sup>	259.0224	259.0217	-2.70
FA-16:1	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	253.2173	253.2163	-3.95
FA-18:1	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	281.2486	281.2473	-4.63
FA-20:1	C <sub>20</sub> H <sub>38</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	309.2799	309.2785	-4.53
FA-22:1	C <sub>22</sub> H <sub>42</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	337.3112	337.3096	-4.75
FA-24:1	C <sub>14</sub> H <sub>26</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	365.3425	365.3408	-4.66
FA-16:0	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	255.2330	255.2319	-4.31
FA-18:0	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	283.2643	283.2630	-4.59
FA-20:0	C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	311.2956	311.2942	-4.50
FA-22:5	C <sub>22</sub> H <sub>34</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	329.2486	329.2471	-4.56
FA-22:6	C <sub>22</sub> H <sub>32</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	327.2330	323.2317	-3.96
FA-20:5	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	301.2173	301.2161	-3.99
FA-18:2	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	279.2330	279.2317	-4.66
FA-20:4	C <sub>20</sub> H <sub>32</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	303.2330	303.2320	-3.30
PE-36:2	C <sub>41</sub> H <sub>78</sub> NO <sub>8</sub> P	[M-H] <sup>-</sup>	742.5392	742.5377	-2.02
PE-36:1	C <sub>41</sub> H <sub>80</sub> NO <sub>8</sub> P	[M-H] <sup>-</sup>	744.5549	744.5518	-4.17

PE-34:1	C <sub>39</sub> H <sub>76</sub> NO <sub>8</sub> P	[M-H] <sup>-</sup>	716.5235	716.5215	-2.79
PE-34:0	C <sub>39</sub> H <sub>78</sub> NO <sub>8</sub> P	[M-H] <sup>-</sup>	718.5392	718.5360	-4.46
PE-38:6	C <sub>43</sub> H <sub>74</sub> NO <sub>8</sub> P	[M-H] <sup>-</sup>	762.5079	762.5066	-1.71
PE-38:4	C <sub>43</sub> H <sub>78</sub> NO <sub>8</sub> P	[M-H] <sup>-</sup>	766.5392	766.5375	-2.22
PI-36:4	C <sub>45</sub> H <sub>79</sub> O <sub>13</sub> P	[M-H] <sup>-</sup>	857.5186	857.5160	-3.03
PI-38:5	C <sub>47</sub> H <sub>81</sub> O <sub>13</sub> P	[M-H] <sup>-</sup>	883.5342	883.5314	-3.17
PI-38:4	C <sub>47</sub> H <sub>83</sub> O <sub>13</sub> P	[M-H] <sup>-</sup>	885.5499	885.5479	-2.26
PI-36:1	C <sub>45</sub> H <sub>85</sub> O <sub>13</sub> P	[M-H] <sup>-</sup>	863.5655	863.5651	-0.46
PI-34:1	C <sub>43</sub> H <sub>81</sub> O <sub>13</sub> P	[M-H] <sup>-</sup>	835.5342	835.5316	-3.11
PS-36:2	C <sub>42</sub> H <sub>78</sub> NO <sub>10</sub> P	[M-H] <sup>-</sup>	786.5291	786.5277	-1.78
PS-36:1	C <sub>42</sub> H <sub>80</sub> NO <sub>10</sub> P	[M-H] <sup>-</sup>	788.5447	788.5430	-2.16
PS-38:4	C <sub>44</sub> H <sub>78</sub> NO <sub>10</sub> P	[M-H] <sup>-</sup>	810.5291	810.5263	-3.46
PS-38:6	C <sub>44</sub> H <sub>74</sub> NO <sub>10</sub> P	[M-H] <sup>-</sup>	806.4978	806.4951	-3.35
PG-38:4	C <sub>44</sub> H <sub>79</sub> O <sub>10</sub> P	[M-H] <sup>-</sup>	797.5338	797.5301	-4.64
PG-38:5	C <sub>44</sub> H <sub>77</sub> O <sub>10</sub> P	[M-H] <sup>-</sup>	795.5182	795.5156	-3.27
PG-38:3	C <sub>44</sub> H <sub>81</sub> O <sub>10</sub> P	[M-H] <sup>-</sup>	799.5495	799.5482	-1.63
PG-36:4	C <sub>42</sub> H <sub>75</sub> O <sub>10</sub> P	[M-H] <sup>-</sup>	769.5025	769.5010	-1.95
C24:1-OH-ST	C <sub>48</sub> H <sub>91</sub> NO <sub>12</sub> S	[M-H] <sup>-</sup>	904.6189	904.6180	-0.99
C24:0-OH-ST	C <sub>48</sub> H <sub>93</sub> NO <sub>12</sub> S	[M-H] <sup>-</sup>	906.6346	906.6324	-2.42