

MALDI MSI of Lipids in Experimental Model of Traumatic Brain Injury Detects Acylcarnitines as Injury Related Markers

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Figure S1: A) Spatially segmented cluster images after processing lipid MALDI MSI data of lesion segments for all three replicates of sham brain and 1 day, 3 day, 7 day, and 10 day injured brains. In addition, the cluster tree corresponding to the imaged sections based on Manhattan distance calculation method is also shown. B) Transparent image of the spatial segmentation shown in figure S1A, with the highlighted selected regions that were further processed in principle component analysis. C) 3-Dimensional Principle component analysis of the regions selected in S1B. This part of the figure shows three different visualization panels for the same 3-Dimensional distribution result.

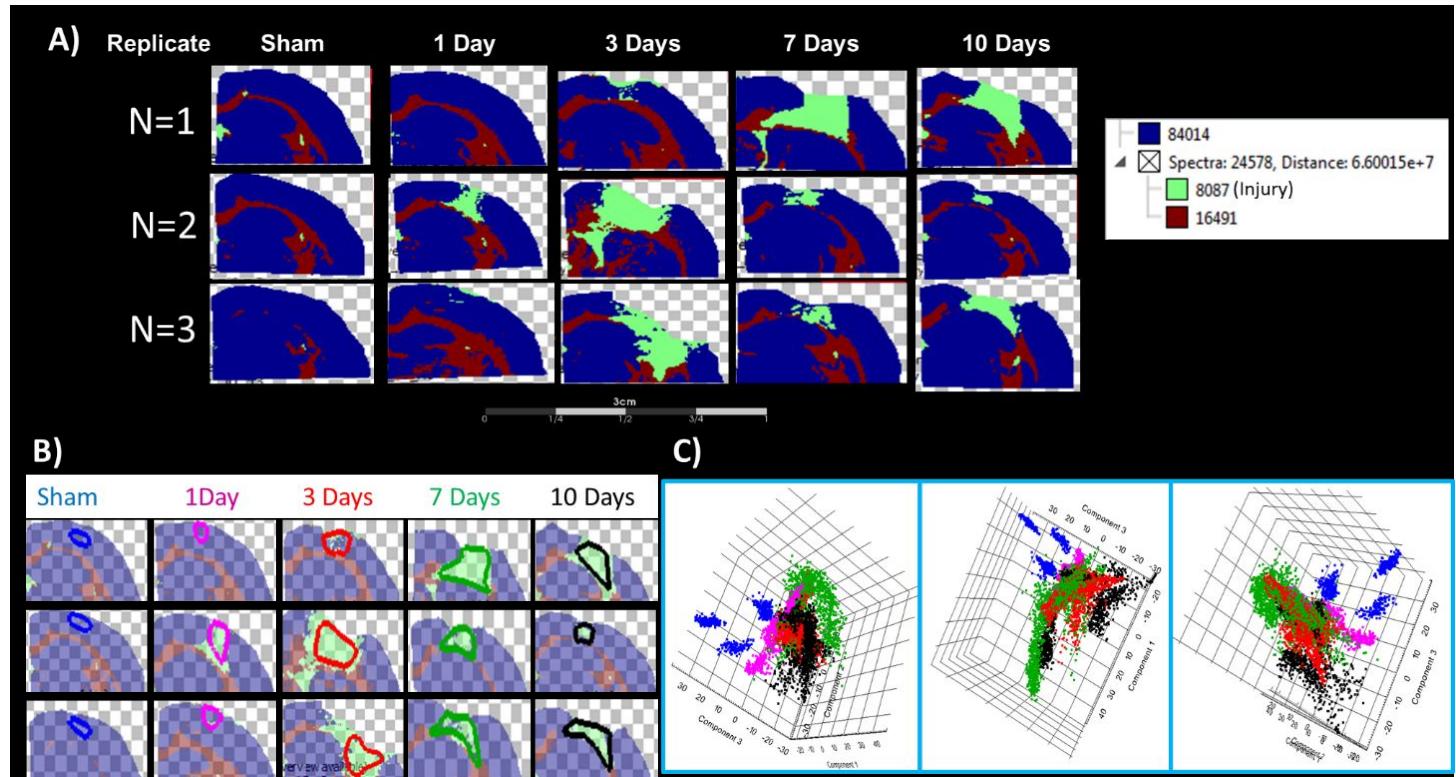


Figure S2: Plotted Ion images of m/z 769.57 and m/z 798.53 along with their corresponding intensity box plot expression for all three replicates in all conditions: sham, 1 day, 3 days, 7 days, and 10 days.

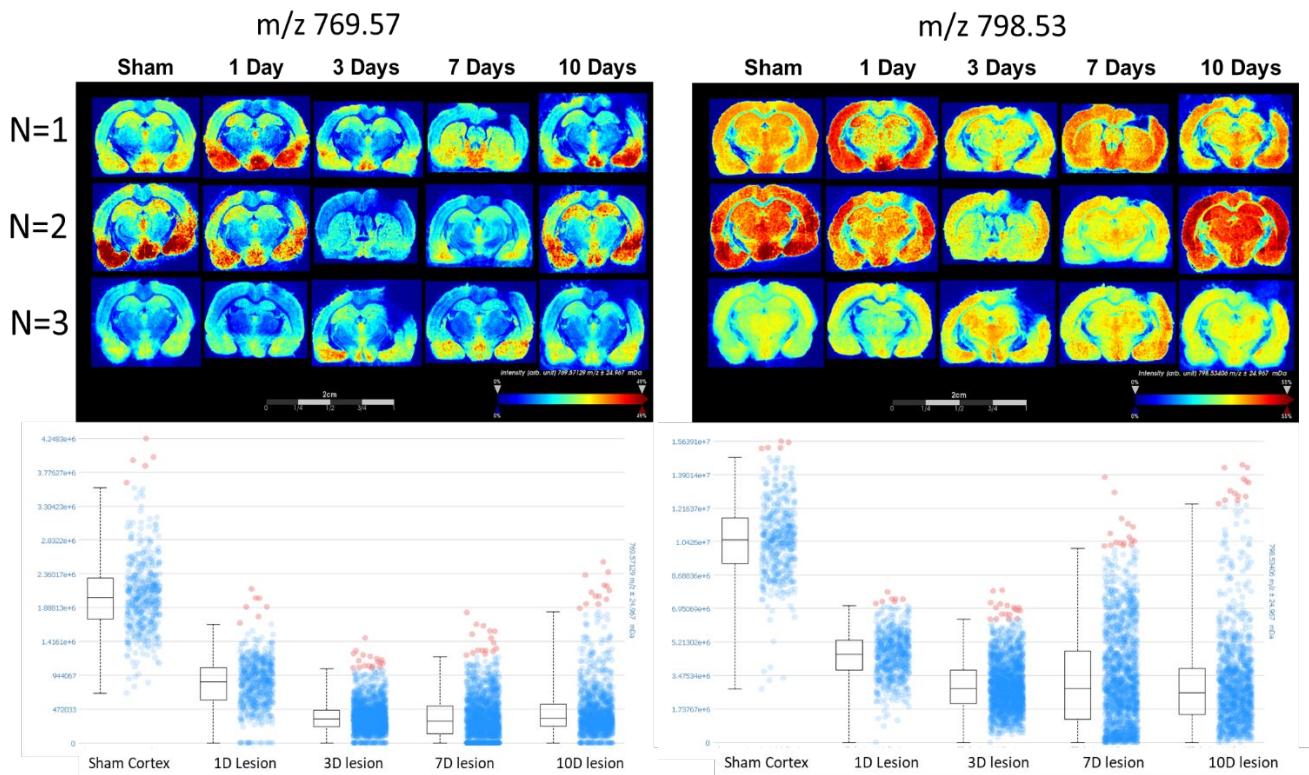
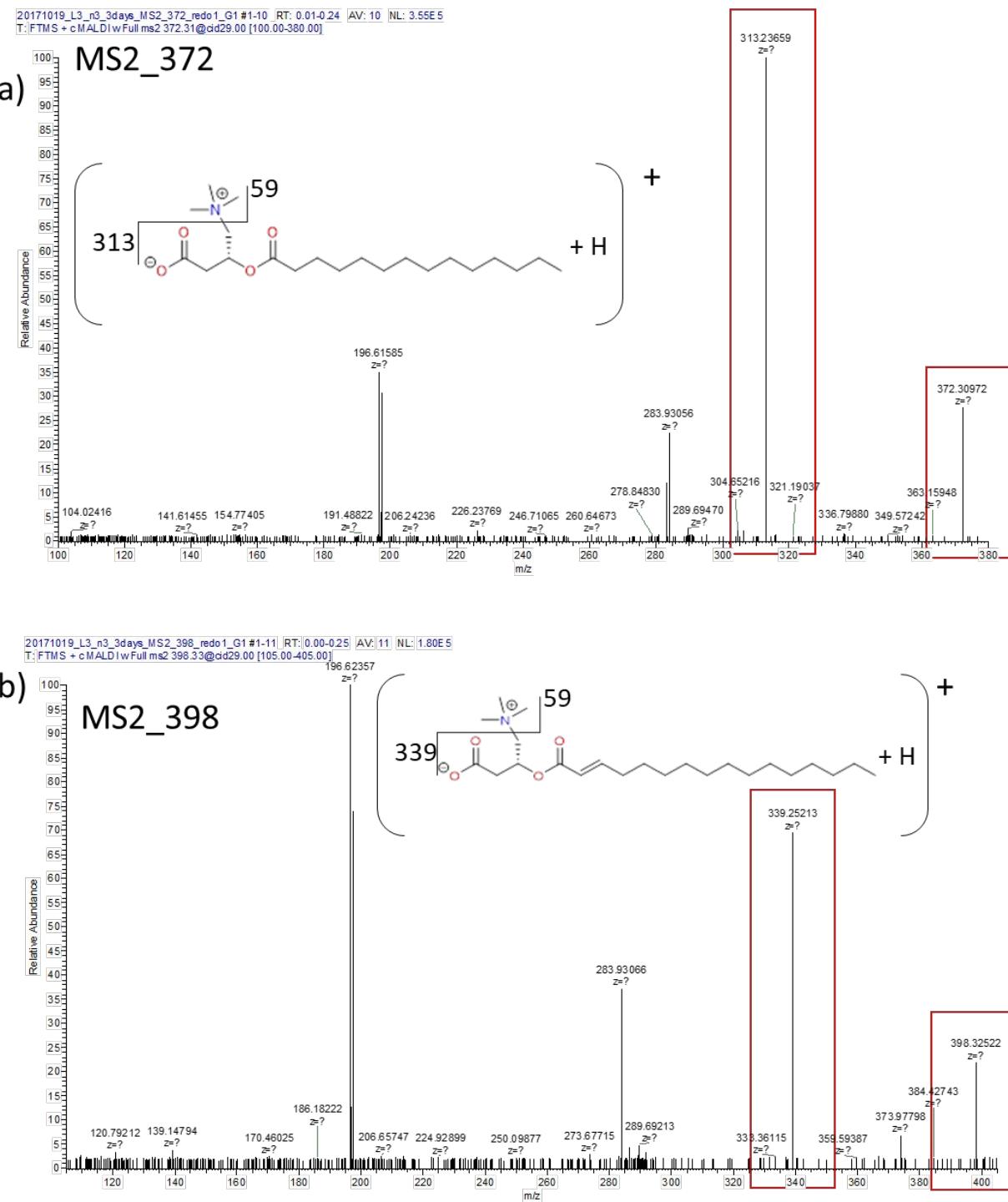


Figure S3: MS/MS spectra showing the fragmentation pattern of *m/z* a) 372.31, b) 398.32, and c) 426.36 from lipid extract at 3 days post injury.



20171018_L3_n3_3Days_MS2_426_B1 #1-7 | RT: 0.00-0.48 | AV: 7 | NL: 4.55E5
T: FTMS + cMALDIw Full ms 2 426.36@cid30.00 [115.00-440.00]

c) MS2_426

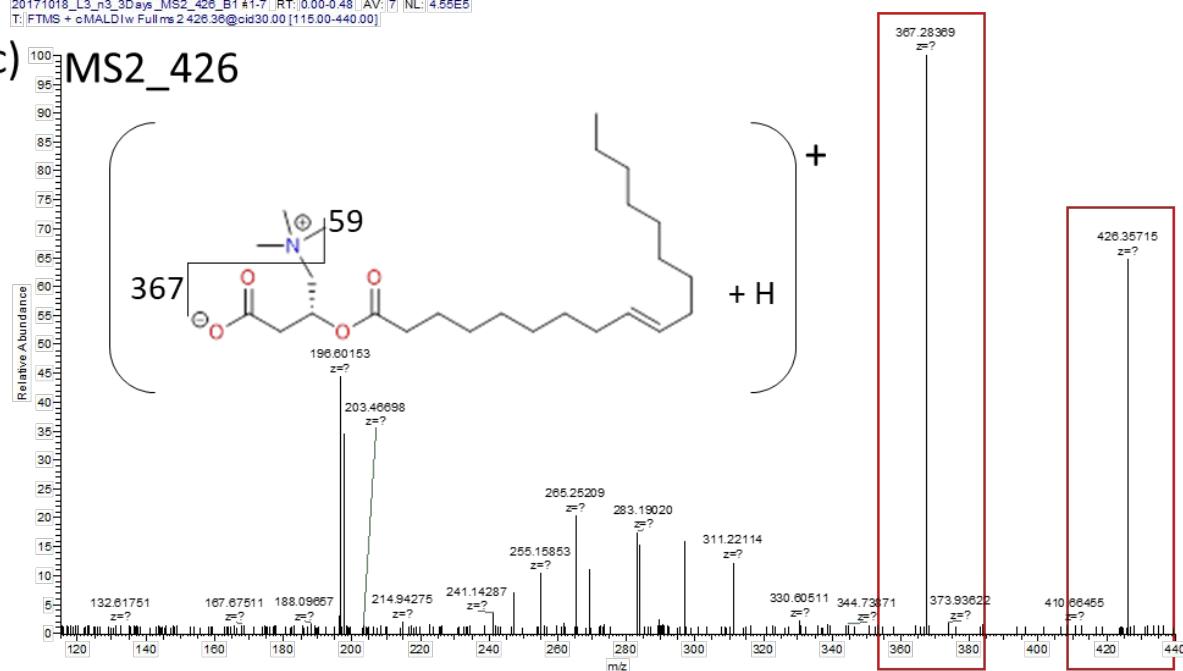
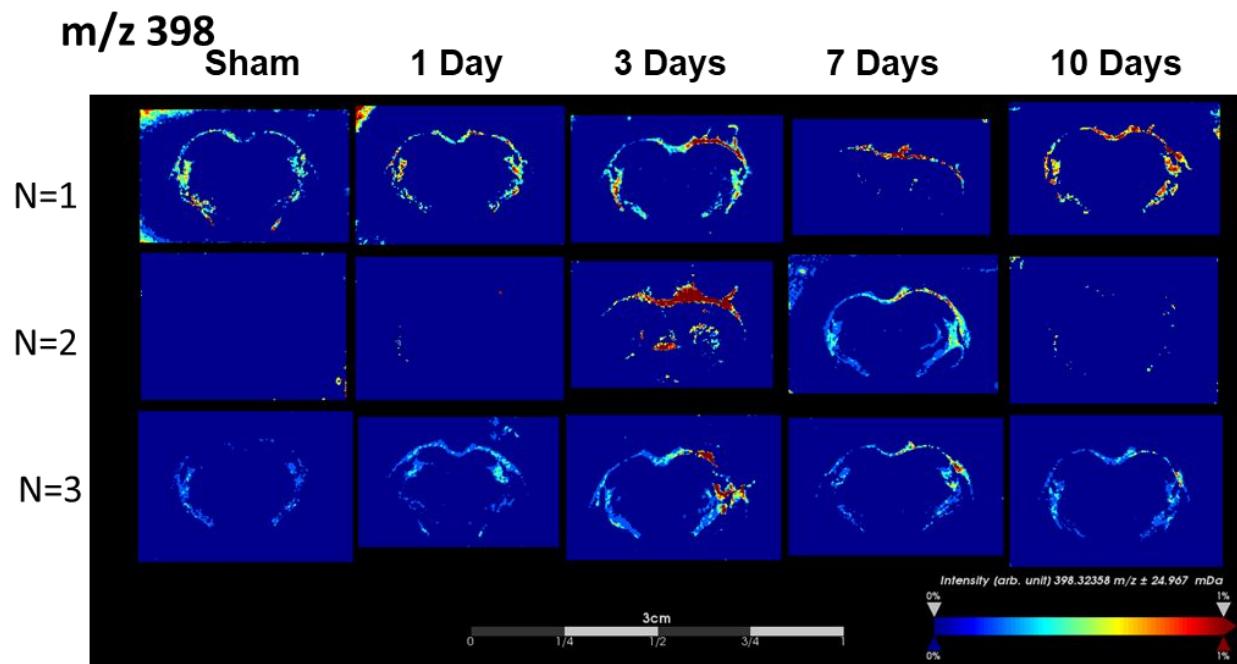
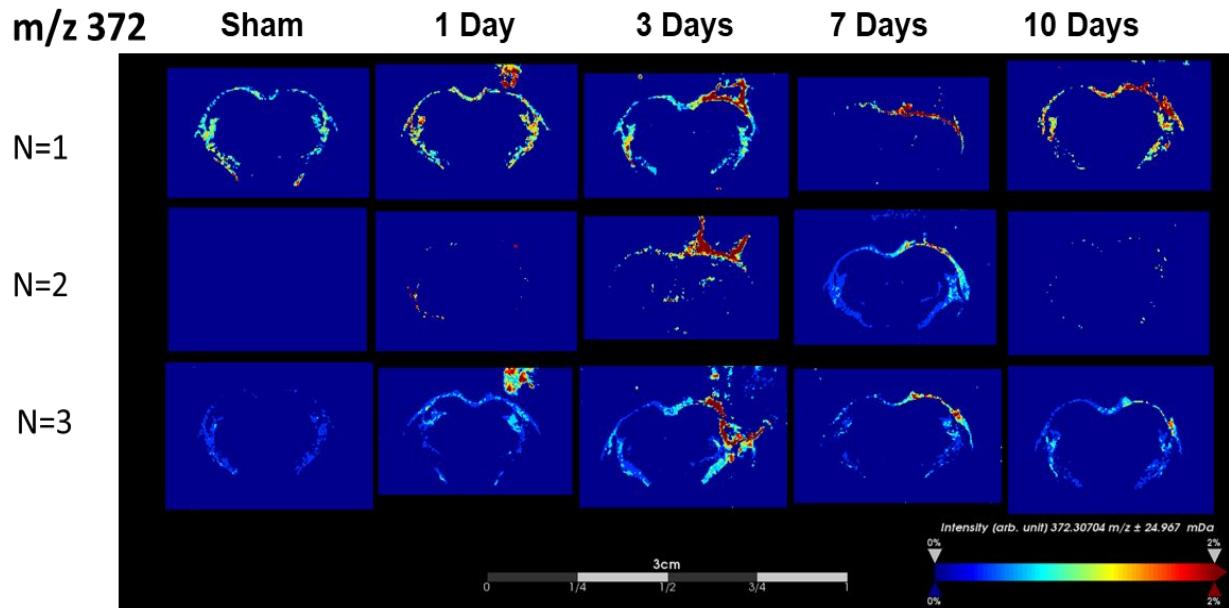
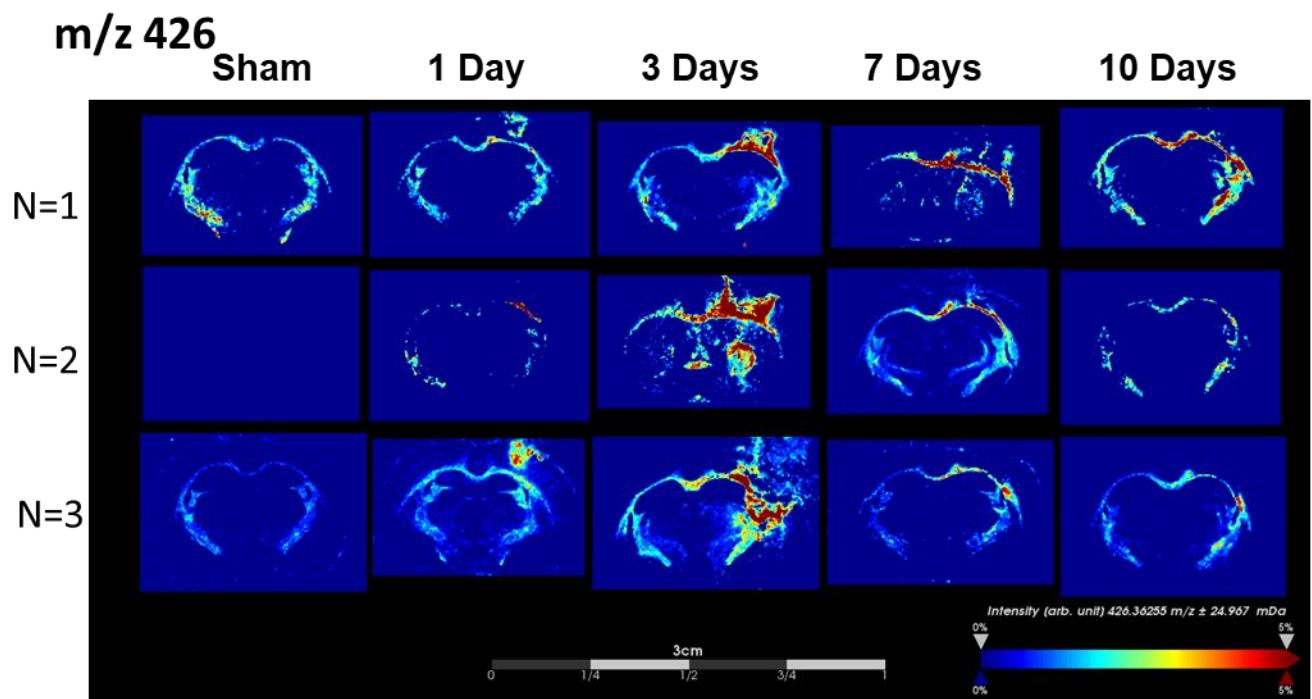


Figure S4: Plotted Ion images of m/z 372.31, 398.32, and 426.36 for all three replicates in all conditions: sham, 1 day, 3 days, 7 days, and 10 days.





Supplementary Tables:

Table S1: ROC analysis of Sham versus of all injured area in lesion segments. List of all 67 *m/z* values that discriminate the sham region from the injury region after applying threshold=0.75.

Centroid [<i>m/z</i>] ± 24.967 [mDa]		
393.93	773.54	844.52
423.99	774.54	845.47
614.92	775.54	845.52
615.97	785.45	846.55
617.99	786.47	848.57
710.50	797.59	849.57
711.50	798.53	852.49
713.44	800.56	853.46
714.47	801.53	868.47
738.51	802.48	869.47
739.46	814.51	870.47
740.48	820.53	870.54
741.48	821.53	871.54
753.59	824.45	872.56
754.59	825.42	873.56
767.50	826.57	874.51
767.55	827.57	875.51
769.57	830.52	896.48
770.52	831.52	912.46
770.57	840.43	913.46
771.57	841.45	914.46
772.52	844.47	934.43
		963.47

Table S2: ROC analysis of all injured area in lesion segments versus sham. List of all 82 *m/z* values that discriminate the sham region from the injury region after applying threshold=0.75.

Centroid [<i>m/z</i>] ± 24.967 [mDa]		
313.03	535.30	744.00
331.04	544.34	752.97
350.98	546.36	757.96
353.03	547.37	758.98
374.00	551.03	759.98
375.00	560.32	760.98
389.98	562.34	768.60
390.98	563.34	780.56
391.98	564.98	780.96
400.35	565.98	781.56
412.95	566.98	792.19
427.39	568.01	808.17
428.38	581.96	808.60
449.36	582.96	809.17
450.36	583.96	809.59
459.25	584.96	835.66
475.22	641.34	851.64
487.28	666.48	919.00
496.35	682.46	928.97
497.35	703.58	933.98
518.32	725.55	934.98
519.32	726.55	935.98
522.36	736.99	949.94
524.39	741.53	950.96
525.39	741.98	951.96
527.01	742.53	952.96
534.30	743.01	956.96
		972.93

Table S3: List of m/z ion colocalized with m/z 400. List of 15 m/z ions that were found to be colocalized with m/z 400 at a threshold=0.3.

Centroid [m/z] \pm 24.967 [Da]
339.30
344.29
370.28
372.31
398.32
400.35
401.34
426.36
428.38
429.38
438.30
518.27
522.36
524.39
525.39