

Effects of Thymoquinone on Small-Molecule Metabolites in a Rat Model of Cerebral Ischemia Reperfusion Injury Assessed using MALDI-MSI

Fang Tian ^{1,2}, Runzhe Liu ^{1,2}, Chaoxin Fan ^{1,2}, Yi Sun ^{1,2}, Xi Huang ^{3,4}, Zongxiu Nie ^{3,4}, Xin Zhao ^{1,2}, and Xiaoping Pu ^{1,2*}

1 National Key Research Laboratory of Natural and Biomimetic Drugs, Peking University, Beijing 100191, China

2 Department of Molecular and Cellular Pharmacology, School of Pharmaceutical Sciences, Peking University, Beijing 100191, China

3 Key Laboratory of Analytical Chemistry for Living Biosystems, Institute of Chemistry Chinese Academy of Sciences, Beijing 100190, China

4 Beijing National Laboratory for Molecular Sciences, Beijing 100190, China

* Correspondence: pxp123@bjmu.edu.cn; Tel: +86-10-82802431

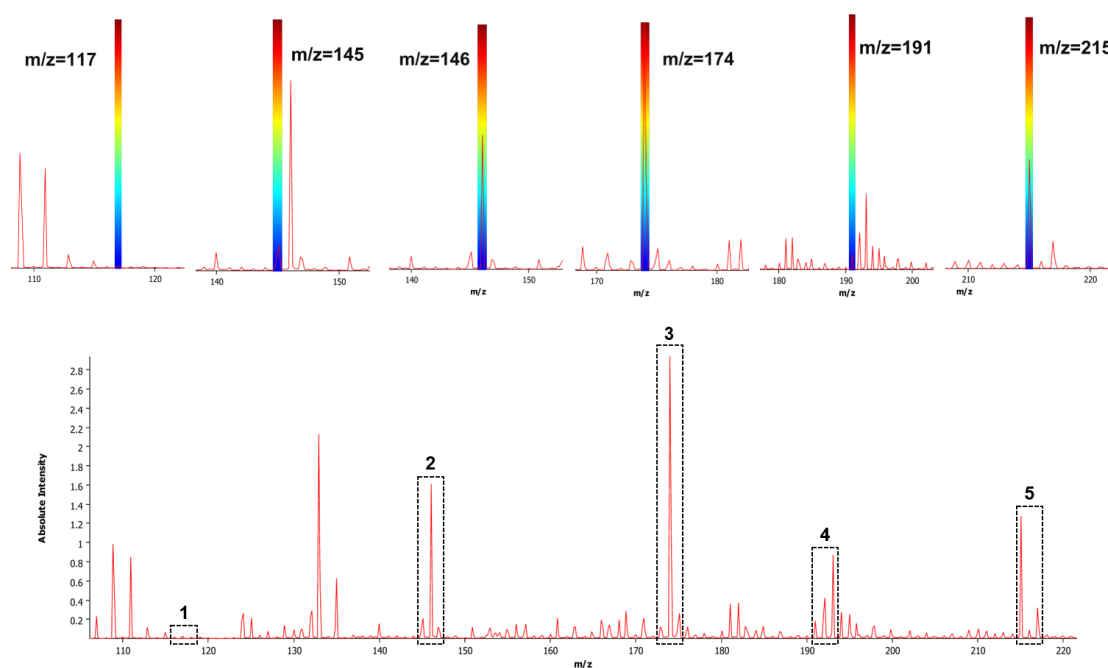


Figure S1. Negative ion mode mass spectrum of aerobic oxidation-related molecules and amino acids using a 1, 5-DAN hydrochloride matrix. Whole mass spectrometry ion peak map with m/z ranging from 110 to 220. Black rectangular areas in the whole mass spectrometry were amplified and displayed. 1: Succinate $m/z=117$, 2: Glutamine $m/z=145$ and Glutamate $m/z=146$, 3: N-acetyl-L-aspartate $m/z=174$, 4: Citric acid $m/z=191$, 5: Glucose $m/z=215$.

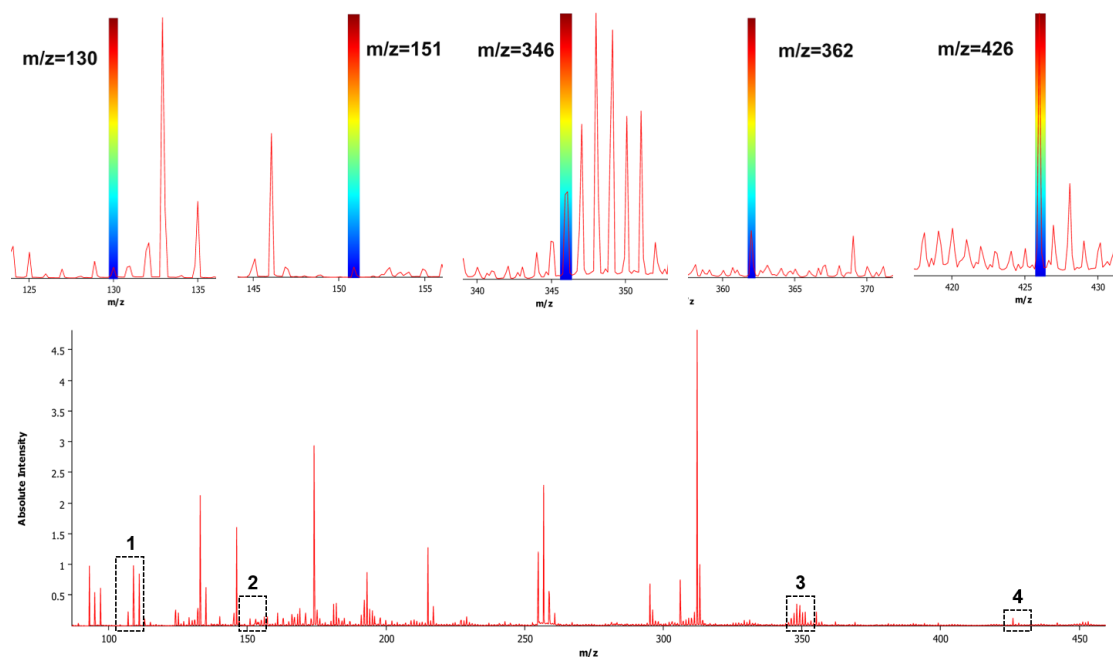


Figure S2. Negative ion mode mass spectrum of energy metabolism-related molecules using a 1, 5-DAN hydrochloride matrix. Whole mass spectrometry ion peak map with m/z ranging from 100 to 450. Black rectangular areas in the whole mass spectrometry were amplified and displayed. 1: Creatine $m/z=130$, 2: Xanthine $m/z=151$, 3: AMP $m/z=346$ and GMP $m/z=362$, 4: ADP $m/z=426$.

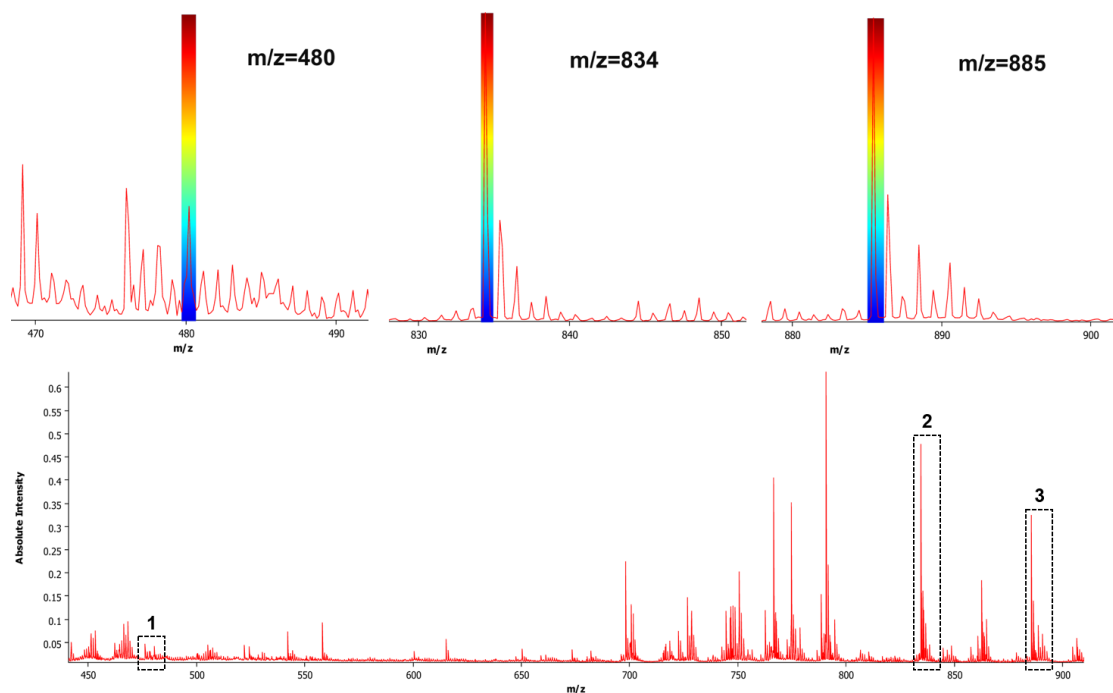


Figure S3. Negative ion mode mass spectrum of phospholipid molecules using a 1, 5-DAN hydrochloride matrix. Whole mass spectrometry ion peak map with m/z ranging from 450 to 900. Black rectangular areas in the whole mass spectrometry were amplified and displayed. 1: PE (18:0) $m/z=480$, 2: PS (18:0/22:6) $m/z=834$, 3: PI (18:0/20:4) $m/z=885$.

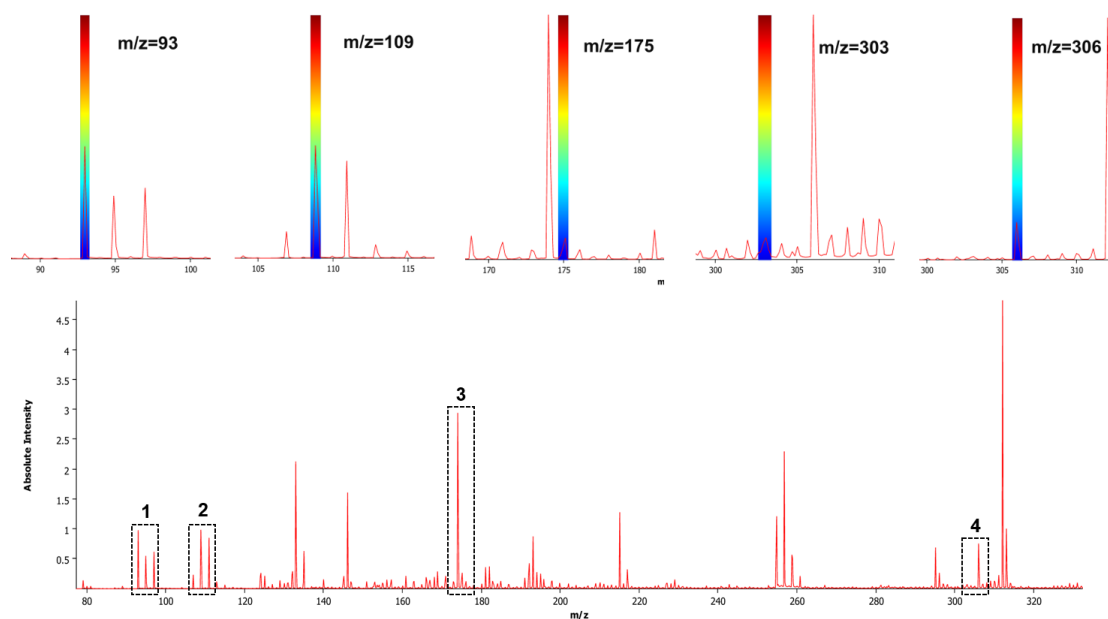


Figure S4. Negative ion mode mass spectrum of other metabolic molecules using a 1, 5-DAN hydrochloride matrix. Whole mass spectrometry ion peak map with m/z ranging from 80 to 320. Black rectangular areas in the whole mass spectrometry were amplified and displayed. 1: Na^+ $m/z=93$, 2: K^+ $m/z=109$, 3: Ascorbic acid $m/z=175$, 4: Arachidonic acid $m/z=303$ and Glutathione $m/z=306$.