

Figure S 1. Multivariate statistical analysis results from the LC/MS-only analysis. A) PCA model; B) OSC PLS-DA score plot; C) OSC PLS-DA loading plot, top 100 ions on the VIP list were marked with red square; D) S-Plot, top 100 ions on the VIP list were marked with red square; E) Jack-knifing confidence of selected differential variables.

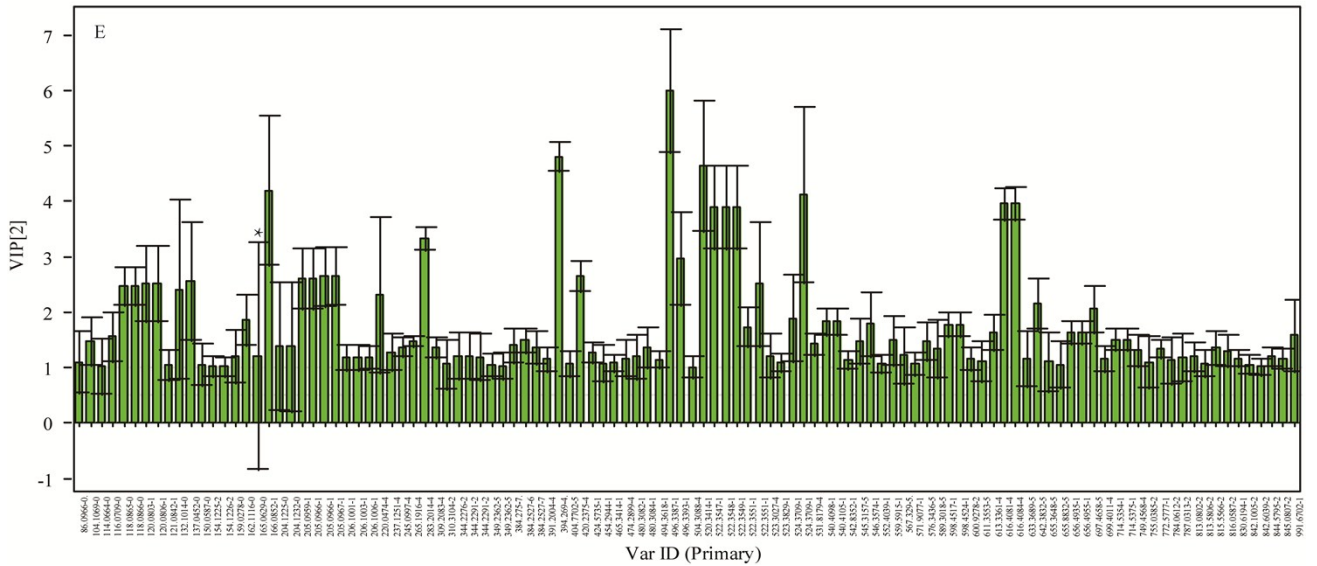
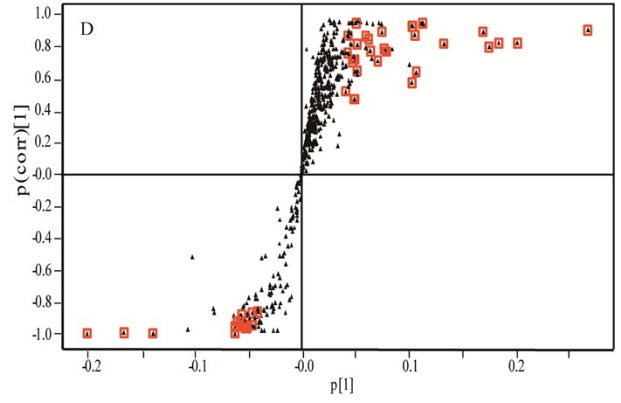
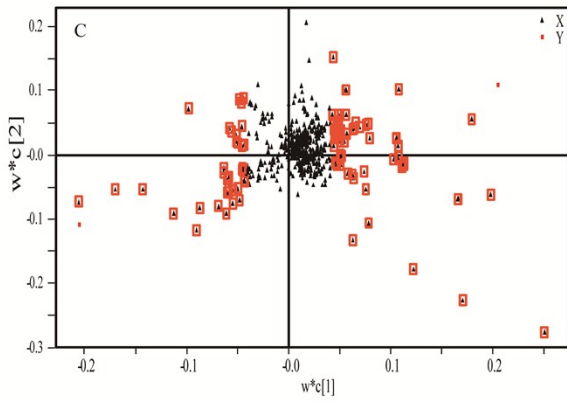
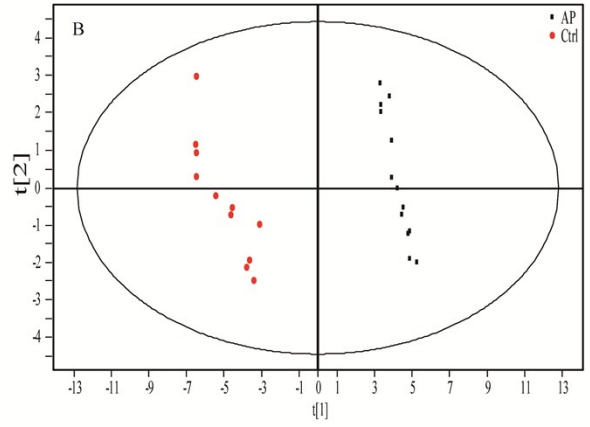
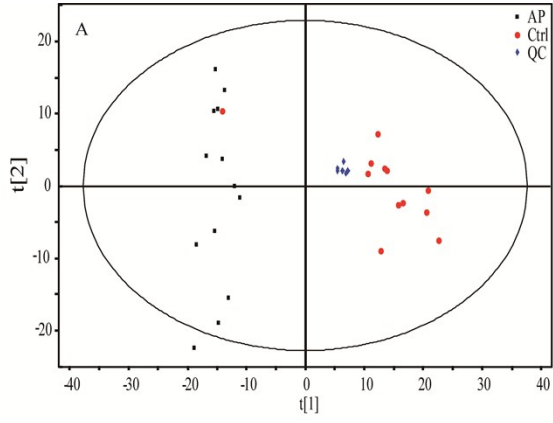


Table S 1. Identified candidate metabolite ions of acute pancreatitis from LC/MS-only analysis

\*: metabolites validated by authentic standard compounds, UN: unknow, metabolites that unable to assign an unambiguous structure.

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| <b>No.</b> | <b>VIP[1]</b> | <b>t<sub>R</sub></b> | <b>m/z</b> | <b>MS/MS spectrum</b>                  | <b>Identification</b>         |
|------------|---------------|----------------------|------------|--|-------------------------------|
| <b>1</b>   | 1.488         | 0.67                 | 104.107    | 104.11, 60.08                          | choline*                      |
| <b>2</b>   | 1.572         | 0.68                 | 116.071    | 116.07, 70.06                          | proline*                      |
| <b>3</b>   | 1.892         | 0.69                 | 162.112    | 161.11, 103.04, 102.08, 85.03, 60.08   | carnitine*                    |
| <b>4</b>   | 1.337         | 0.69                 | 204.122    | 204.12, 145.05, 85.03, 60.8            | acetylcarnitine*              |
| <b>5</b>   | 2.516         | 0.72                 | 118.087    | 118, 72                                | valine*                       |
| <b>6</b>   | 2.449         | 0.72                 | 132.101    | 132.10, 86.10, 69.07                   | isoleucine*                   |
| <b>7</b>   | 1.335         | 0.72                 | 204.123    |  | UN1                           |
| <b>8</b>   | 1.116         | 0.74                 | 86.0966    | 86.10, 69.07                           | ion of isoleucine             |
| <b>9</b>   | 1.220         | 0.78                 | 159.028    | 118.09, 72.08                          | Zymonic acid                  |
| <b>10</b>  | 2.508         | 0.80                 | 118.087    | 118.09, 72.08                          | Ion of 159.028                |
| <b>11</b>  | 1.070         | 0.83                 | 150.059    | 150.06, 133.03, 104.05, 102.06, 61.02  | methionine*                   |
| <b>12</b>  | 4.267         | 1.10                 | 166.085    | 120.08, 103.05, 93.07                  | phenylalanine*                |
| <b>13</b>  | 2.552         | 1.12                 | 120.080    | 120.08, 103.05, 93.07                  | ion of phenylalanine          |
| <b>14</b>  | 1.059         | 1.12                 | 121.084    |  | Isotope 120.080               |
| <b>15</b>  | 2.689         | 1.88                 | 205.097    | 118.07, 146.06, 188.07                 | tryptophan*                   |
| <b>16</b>  | 1.207         | 1.88                 | 206.100    | 119.07, 147.06, 189.07                 | Isotope of tryptophan         |
| <b>17</b>  | 1.027         | 2.73                 | 154.122    | 154.12, 98.06, 70.07                   | 2-isobutyl-4,5-dimethyloxaole |
| <b>18</b>  | 1.235         | 2.85                 | 344.228    | 327.20, 177.11, 133.09, 89.06          | UN2                           |
| <b>19</b>  | 3.387         | 4.22                 | 283.201    | 283.20, 265.19, 180.14, 124.08         | UN3                           |
| <b>20</b>  | 1.504         | 4.22                 | 265.192    |  | Ion of 283.201                |
| <b>21</b>  | 4.879         | 4.60                 | 394.269    | 394, 376.26, 291.21, 235.14, 206.15    | UN4                           |
| <b>22</b>  | 1.377         | 4.60                 | 245.100    | 243.04, 224.61, 215.59, 173.07, 157.99 | UN5                           |
| <b>23</b>  | 4.021         | 4.76                 | 616.408    |  | UN6                           |

|           |       |       |         |                                |                    |
|-----------|-------|-------|---------|--------------------------------|--------------------|
| <b>24</b> | 1.382 | 4.78  | 309.208 |                                | Ion of 616.408     |
| <b>25</b> | 1.166 | 4.79  | 474.290 |                                | Ion of 616.408     |
| <b>26</b> | 4.022 | 4.83  | 616.408 |                                | UN7                |
| <b>27</b> | 1.514 | 6.91  | 384.253 |                                | UN8                |
| <b>28</b> | 1.378 | 7.24  | 384.253 |                                | UN9                |
| <b>29</b> | 4.709 | 11.77 | 520.341 |                                | LPC (18:2)         |
| <b>30</b> | 2.905 | 12.27 | 496.339 | 184.07                         | LPC(16:0)          |
| <b>31</b> | 1.801 | 12.67 | 546.357 | 184.07                         | LPC(20:3)          |
| <b>32</b> | 5.963 | 12.76 | 496.339 |                                | LPC(16:0)          |
| <b>33</b> | 1.497 | 12.77 | 991.670 |                                | dimer of LPC(16:0) |
| <b>34</b> | 1.759 | 12.9  | 522.355 | 184.07, 104                    | LPC(18:1)          |
| <b>35</b> | 1.216 | 13.27 | 480.308 | 480.31, 462.30, 339.29, 308.30 | LPE(18:1)          |
| <b>36</b> | 3.946 | 13.31 | 522.355 | 184.07, 104                    | LPC(18:1)          |
| <b>37</b> | 1.386 | 13.40 | 480.308 |                                | LPC(15:1)          |
| <b>38</b> | 2.556 | 13.64 | 522.355 | 184.07, 104                    | LPC(18:1)          |
| <b>39</b> | 4.054 | 15.41 | 524.371 |                                | LPC (18:0)         |
| <b>40</b> | 1.059 | 20.08 | 310.31  | 310.31, 293.28, 275.27         | Oleoyl ethyl amide |
| <b>41</b> | 1.318 | 22.58 | 816.059 |                                | Isotope of 815.557 |
| <b>42</b> | 1.368 | 22.59 | 815.557 |                                | UN10               |
| <b>43</b> | 1.074 | 23.30 | 842.101 |                                | PE (44:8)          |
| <b>44</b> | 1.216 | 23.30 | 844.58  |                                | PE (44:8)          |
| <b>45</b> | 1.175 | 23.31 | 845.081 |                                | Iso of PE (44:8)   |

\*: metabolites validated by authentic standard compounds, UN: unknow, metabolites that unable to assign an unambiguous structure, -: metabolites not detected.