(1) PCA was performed on the data acquired in positive ion mode, and score plot was as the following Figure-1.

It is clear that, data acquired in positive ion mode has poor classification ability on various groups. All the scatter points overlapped.
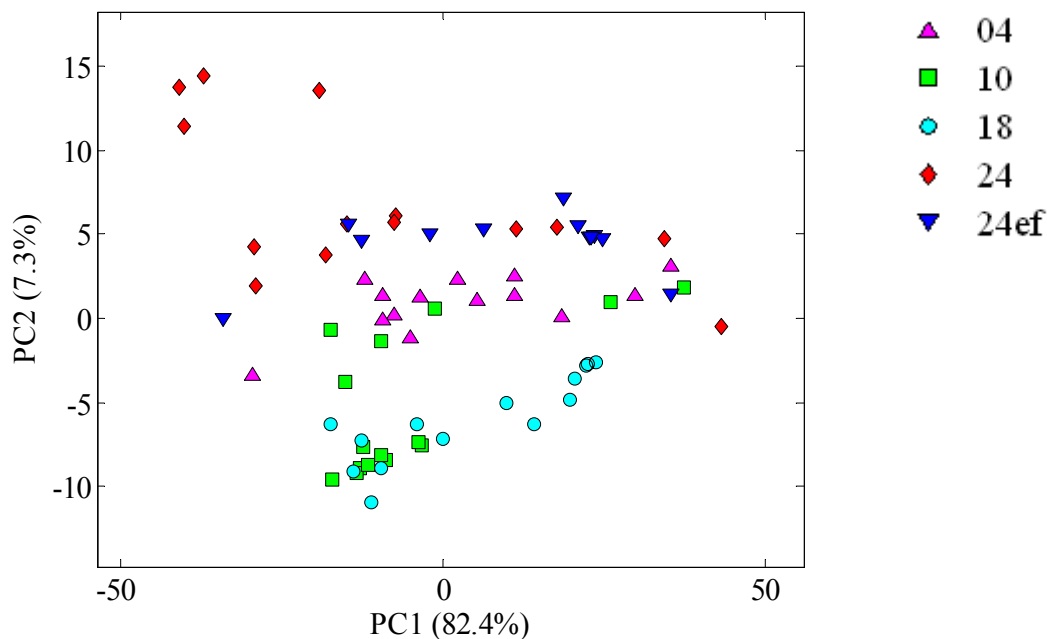

Figure-1

(2) PCA was performed on the data acquired in negative ion mode, and score plot was shown as Figure-2.

Data acquired in negative ion mode has good classification ability on various groups. All the scatter points from five groups can be clearly classified as distinct from each other.
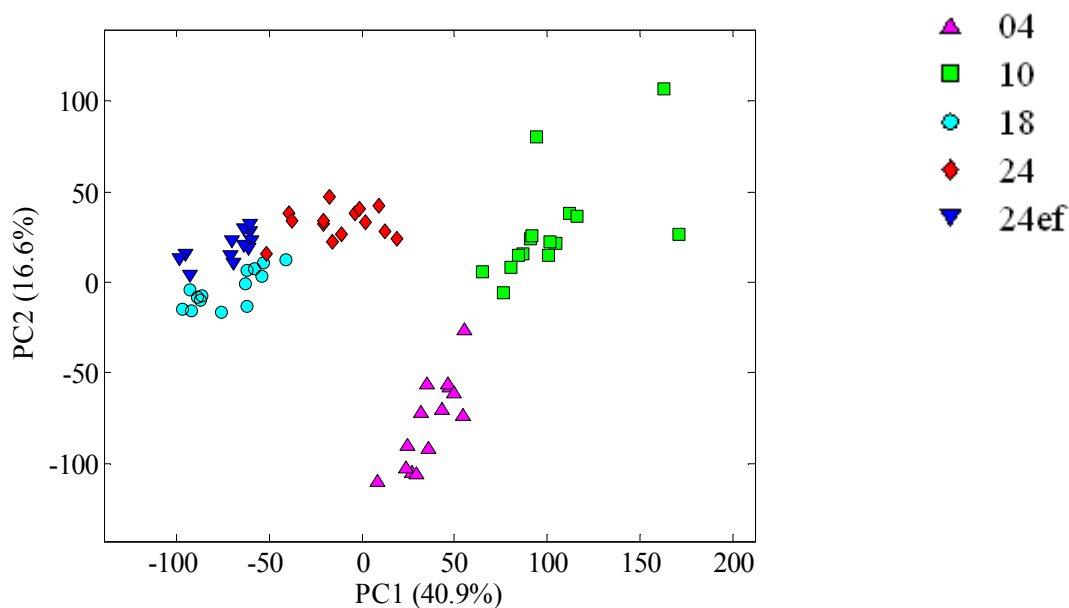

Figure-2

(3) Two sets of data acquired in positive ion mode and in negative ion mode were combined together, and then PCA was performed on the combined data. Score plot was shown as Figure-3.

Compared with Figure-1 and Figure-2, it is clear that the combined data shows much better classification ability than data in positive mode; however, its classification ability is inferior to data in negative mode.
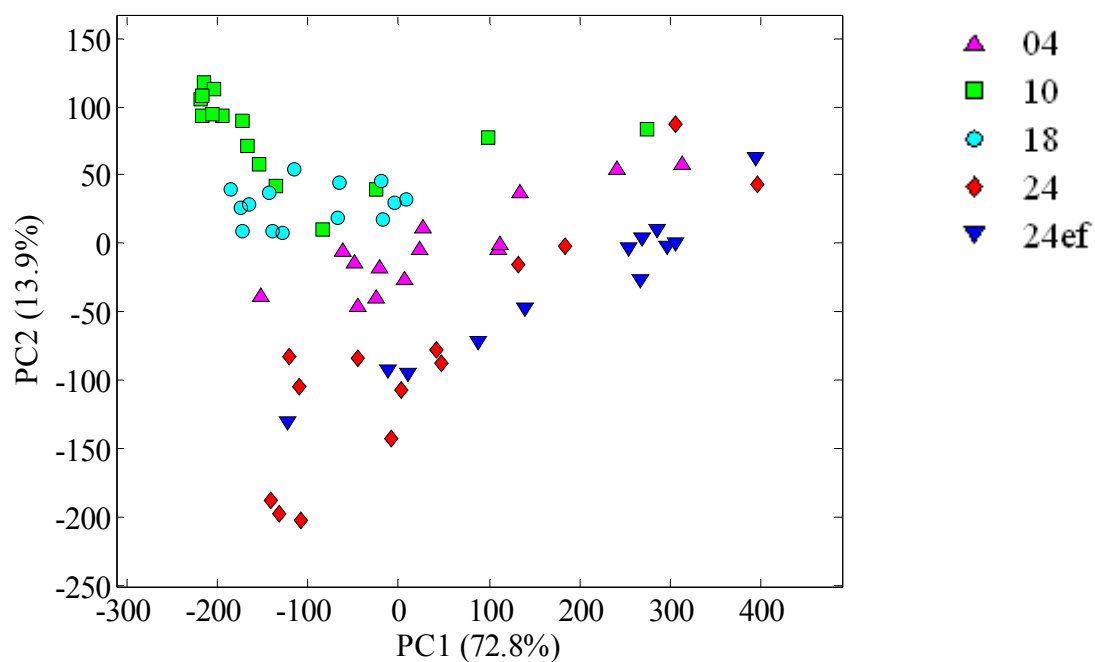

Figure-3