Parameters for the testing data:

(1) Reaction search settings:

positive: TRUE

M’: 340.16746

Threshold: 10

Magnum: 5

(2) Pair peaking settings:

Mass difference: 6.037

Pair peaking mass accuracy: 10

Pair peaking retention time: 0.06

Pair peaking mean: 1.25

Adduct mass accuracy: 10