Fragmentation profiles of the two unknown features to be monitored in future studies as well as methacholine as shown in Table 2.

The fragment masses and intensities were extracted from the aggregated .mgf file computed by MZmine and used in the network analysis.

ID8605 selected based on fold change	ID5593 selected based on significant p values before FDR correction	Methacholine selected based on significant p values before FDR correction
BEGIN IONS FEATURE_ID=8605 PEPMASS=1014.4892 SCANS=8605 RTINSECONDS=398.449 CHARGE=1+ MSLEVEL=2 99.4840 5.0E3 130.2113 4.7E3 178.2334 6.2E3 498.1496 2.9E5 557.1633 3.9E5 616.1768 1.3E6 END IONS	BEGIN IONS FEATURE_ID=5593 PEPMASS=231.1701 SCANS=5593 RTINSECONDS=166.747 CHARGE=1+ MSLEVEL=2 72.0808 4.2E4 84.9599 4.4E3 103.8799 2.1E3 144.7223 2.3E3 END IONS	BEGIN IONS FEATURE_ID=159 PEPMASS=160.1332 SCANS=159 RTINSECONDS=26.97 CHARGE=1+ MSLEVEL=2 55.0546 2.1E5 59.0493 5.7E4 60.0810 6.1E5 101.0598 1.9E6 131.9749 2.3E4 END IONS