

Supplementary Table S1. The detailed ion source conditions of quadrupole time-of-flight mass spectrometry.

Parameters	ESI+
Sample temperature	10 °C
Column temperature	50 °C
Analysis mode	sensitivity
Capillary voltage	3000 V
Ion source temperature	120 °C
Desolvation temperature	500 °C
Cone gas flow	50 L/h
Desolvation gas flow	900 L/h