

### **SWATH parameters for un-targeted analysis**

For ESI(+), the SWATH parameters were MS<sup>1</sup> accumulation time, 100 ms; MS<sup>1</sup> mass range, m/z 100–1700; MS<sup>2</sup> accumulation time, 10 ms; collision energy, 45 eV; collision energy spread, 15 eV; cycle time, 550 ms; Q<sub>1</sub> window, 20 Da; SWATH mass range, m/z 300–1100; number of SWATH experiments, 40; MS<sup>2</sup> mass range: m/z 100–1100. Other parameters were curtain gas, 35; ion source gas 1, 60; ion source gas 2, 60; temperature, 350°C; ion spray voltage floating, 4.5 kV; declustering potential, 80 V. For ESI(–), the SWATH parameters were MS<sup>1</sup> accumulation time, 100 ms; MS<sup>1</sup> mass range, m/z 100–1700; MS<sup>2</sup> accumulation time, 10 ms; collision energy, -45 eV; collision energy spread, 15 eV; cycle time, 550 ms; Q<sub>1</sub> window, 20 Da; SWATH mass range, m/z 220–1020; number of SWATH experiments, 40; MS<sup>2</sup> mass range: m/z 100–1000. Other parameters were curtain gas, 35; ion source gas 1, 60; ion source gas 2, 60; temperature, 350°C; ion spray voltage floating, -4.5 kV; declustering potential, -80 V.