



**Figure S1** Total ion flow chromatogram in negative ion mode and positive ion mode. The multi-reaction monitoring (MRM) mode metabolite detection multippeak diagram shows the substances that can be detected in the sample. Each mass spectrum peak with different colors represents a detected metabolite. The characteristic ions of each substance are screened out through the triple four-stage rod, and the signal strength (CPS) of the characteristic ions is obtained in the detector. The sample of the machine mass spectrometry file is opened with the MultiQuant software to integrate and correct the chromatographic peaks. Each chromatographic peak represents the relative content of the corresponding substance.