Fig. S1. The screening of potential phthalides by polygonal MMDF. (A) Scatter diagram of predicted metabolites of phthalides. (B) Construction of original MMDF windows connected by seven outermost datapoints (dotted line) and final MMDF window connected by shifted datapoints (full line). (C) 2801 SM-LC related ions screened by background subtraction. (D) 217 phthalides-related ions by polygonal MMDF.