

Supplementary Materials

Supplemental Figure 1. PA, HP and DH derivatives of carboxylic acids, aldehydes and ketones. Molecular formula and chemical structures of these derivatives were determined by accurate mass measurement, elemental composition analysis and MS/MS fragmentation. The value of $[M+H]^+$ is the mass-to-charge ratio (m/z) of the protonated derivative. (A) Acetate-PA; (B) HBA-PA; (C) malate-PA; (D) pyruvate-PA; (E) acetate-HP; (F) HBA-HP; (G) malate-HP; (H) pyruvate-HP; (I) acetaldehyde-DH; (J) acetone-DH; (K) pyruvate-DH.

