Supporting information

Untargeted metabolomics of colonic digests reveals kynurenine pathway metabolites, dityrosine and 3-dehydroxycarnitine as red versus white meat discriminating metabolites

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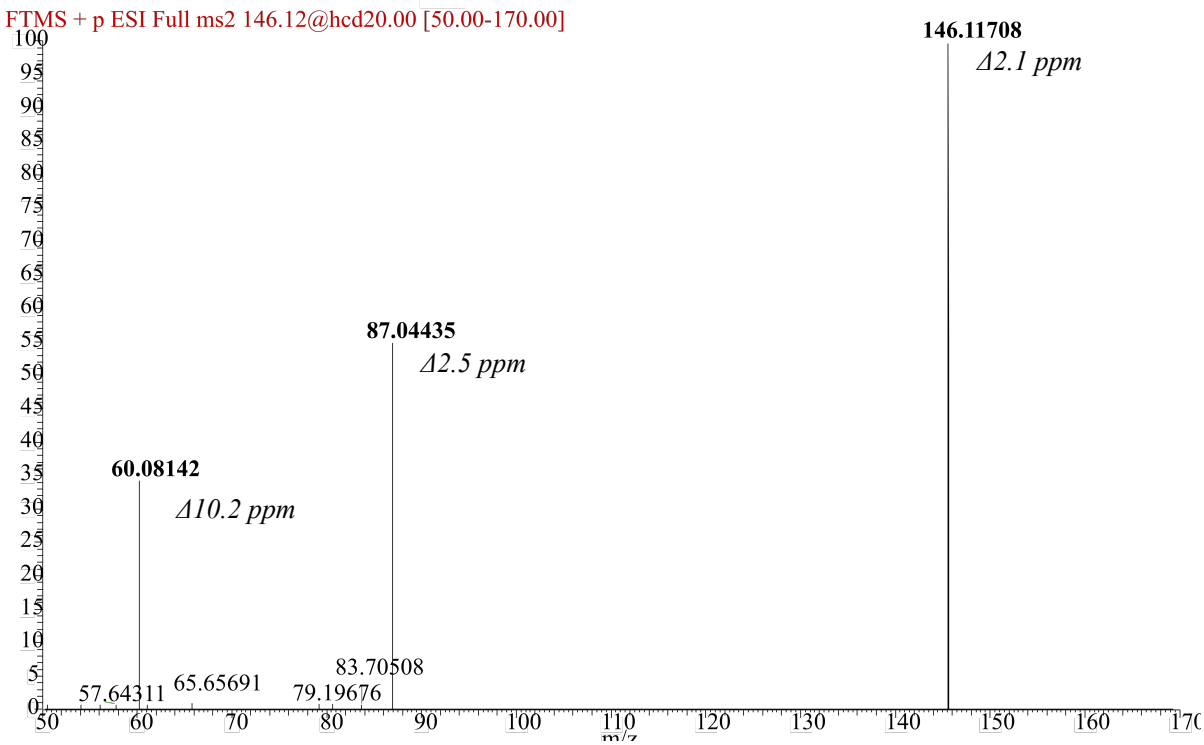
Figure S1. MS/MS data (+ ionization mode) used for identification of 3-dehydroxycarnitine. MS/MS fragmentation data (PRM) of *m/z* 146.11708.



m/z: 146.11756
Chemical Formula: $C_7H_{16}NO_2^+$

m/z: 87.04406
Chemical Formula: $C_4H_7O_2$

m/z: 60.08078
Chemical Formula: $C_3H_{10}N^+$

Figure S2. MS/MS data (+ ionization mode) used for identification of kynurenic acid.

MS/MS fragmentation data (PRM) of *m/z* 190.04919.

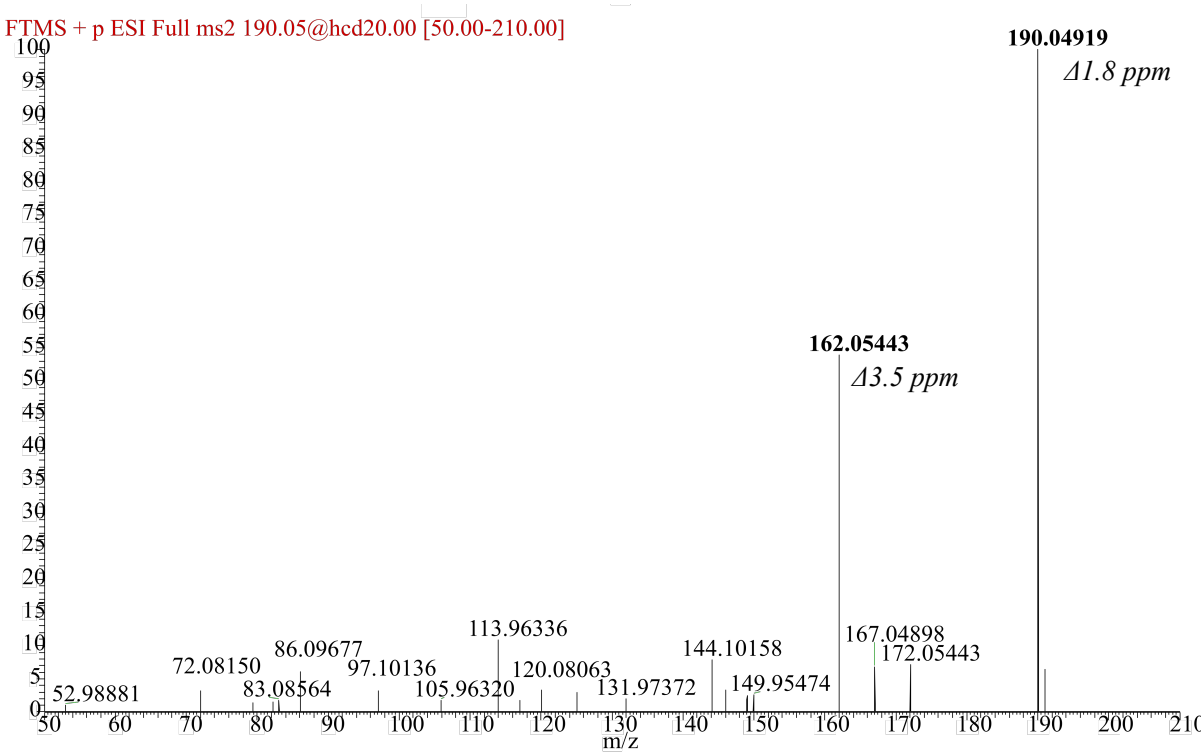


Figure S3. MS/MS data (+ ionization mode) used for identification of L-kynurenine. MS/MS fragmentation data (PRM) of *m/z* 209.09186.

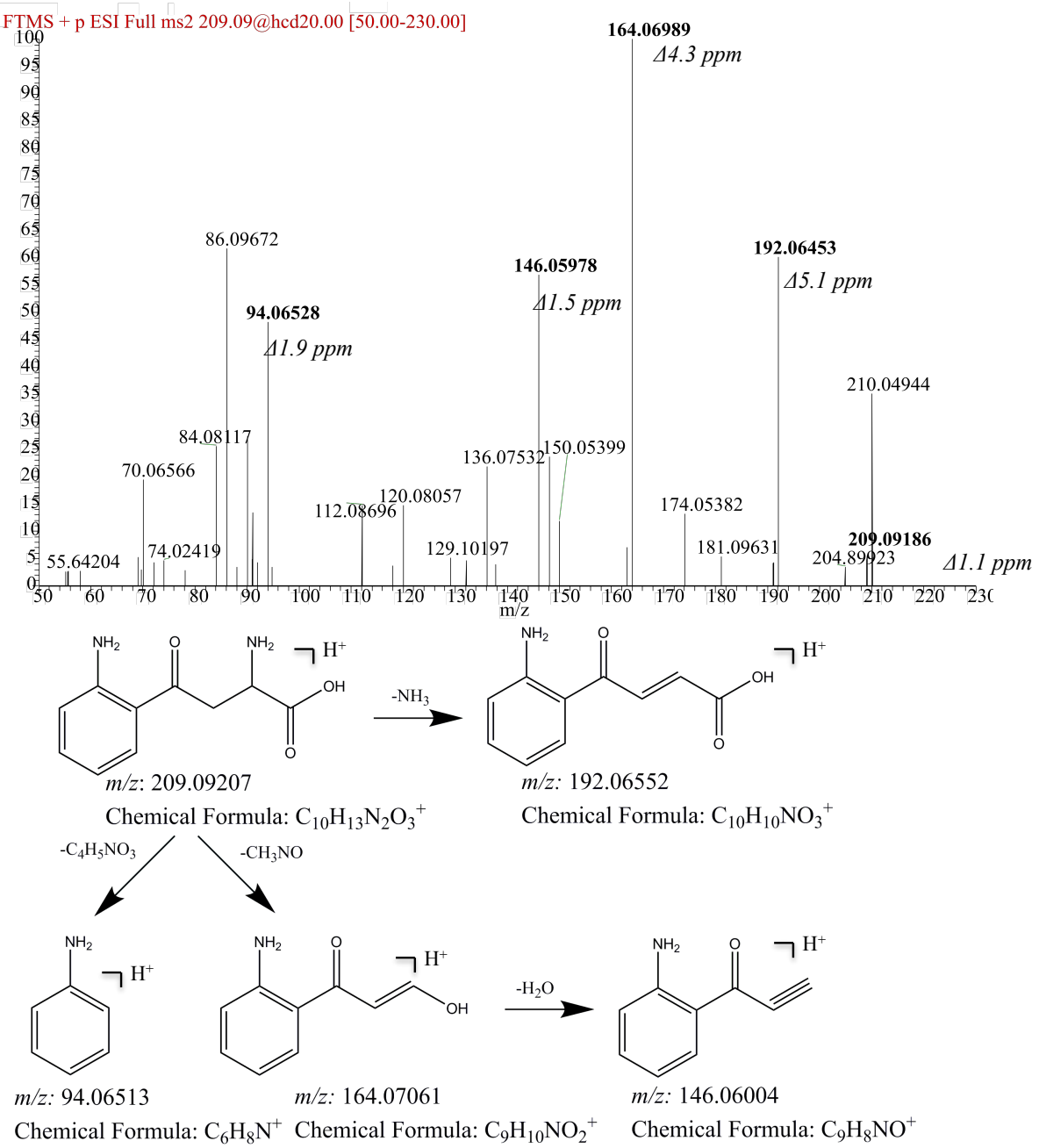


Figure S4. MS/MS data (+ ionization mode) used for identification of N'-formylkynurenine. MS/MS fragmentation data (PRM) of *m/z* 237.08652.

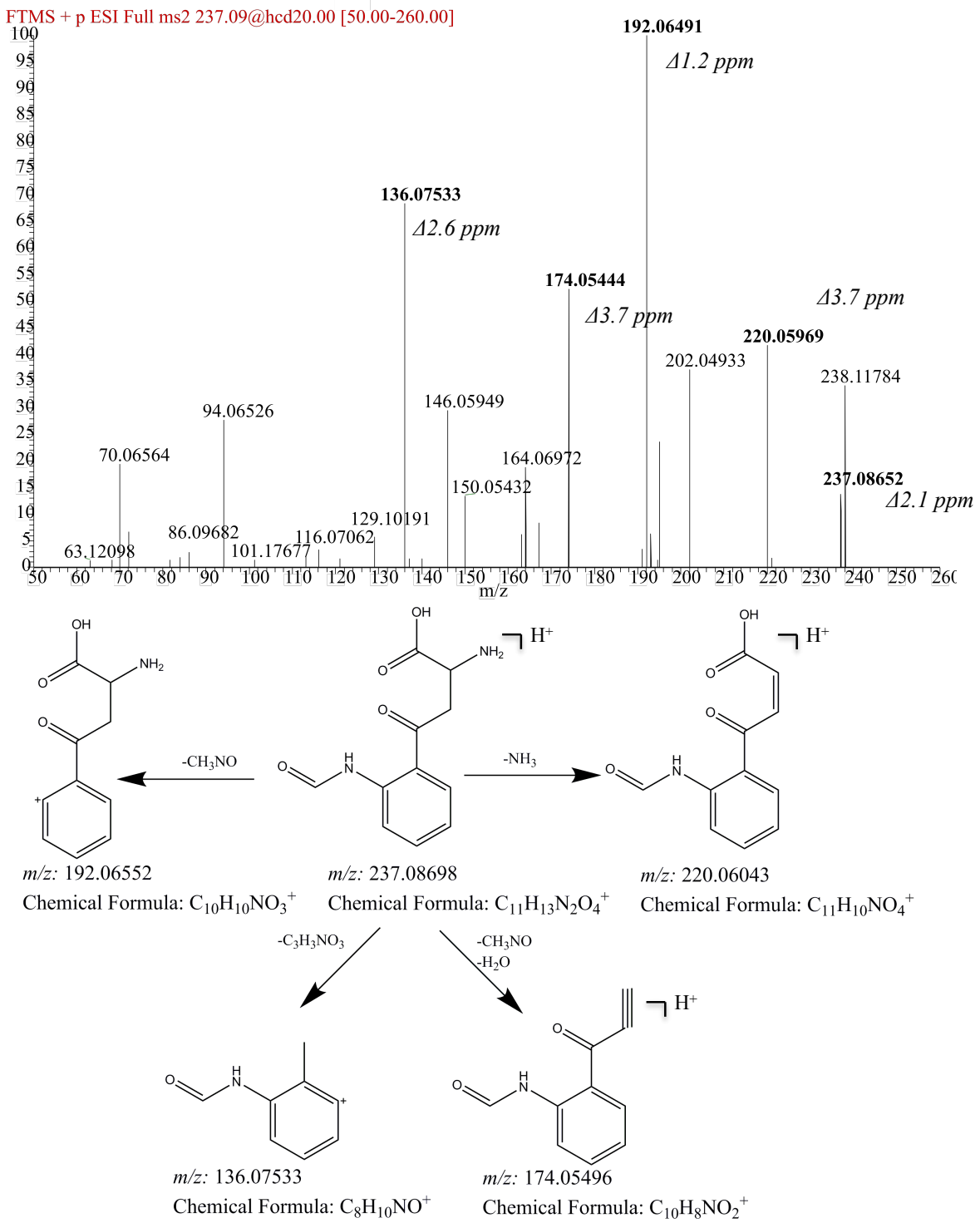
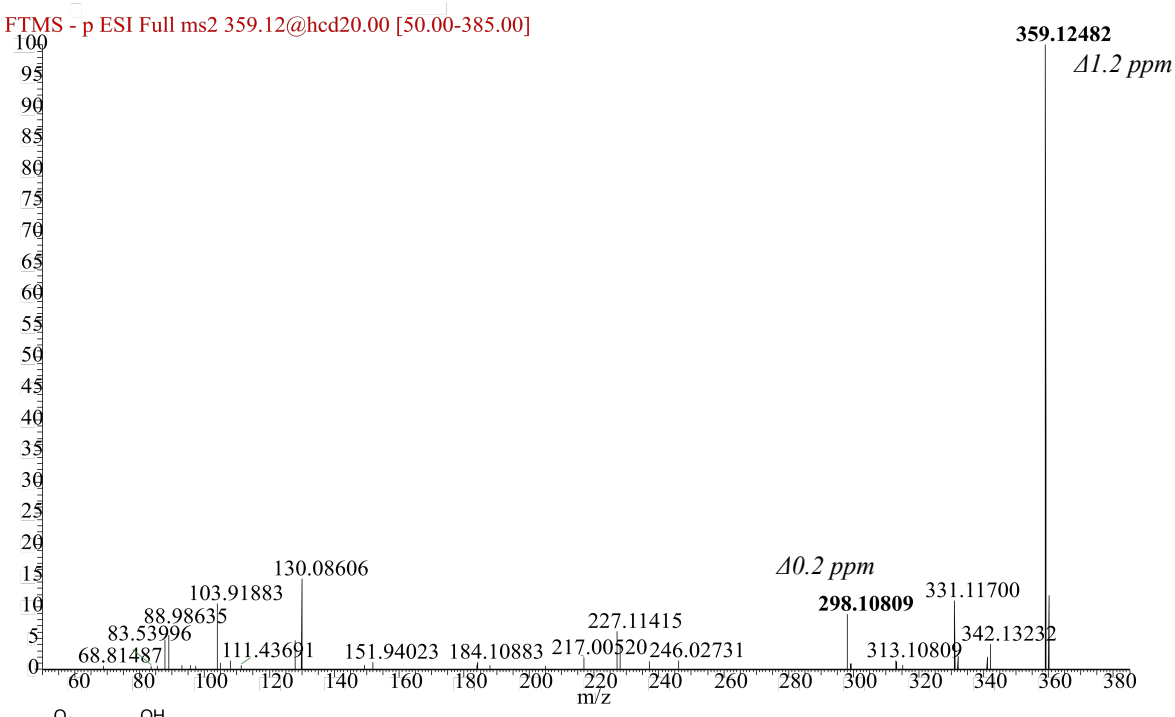


Figure S5. MS/MS data (- ionization mode) used for identification of dityrosine.

MS/MS fragmentation data (PRM) of *m/z* 359.12482.



m/z: 359.12486
Chemical Formula: $C_{18}H_{19}N_2O_6^-$

m/z: 298.10848
Chemical Formula: $C_{17}H_{16}NO_4^-$