

ELECTRONIC SUPPLEMENTARY MATERIAL

ANALYTICAL STRATEGY TO INVESTIGATE 3,4-METHYLENEDIOXYPYROVALERONE (MDPV) METABOLITES IN CONSUMERS' URINE BY HIGH RESOLUTION MASS SPECTROMETRY

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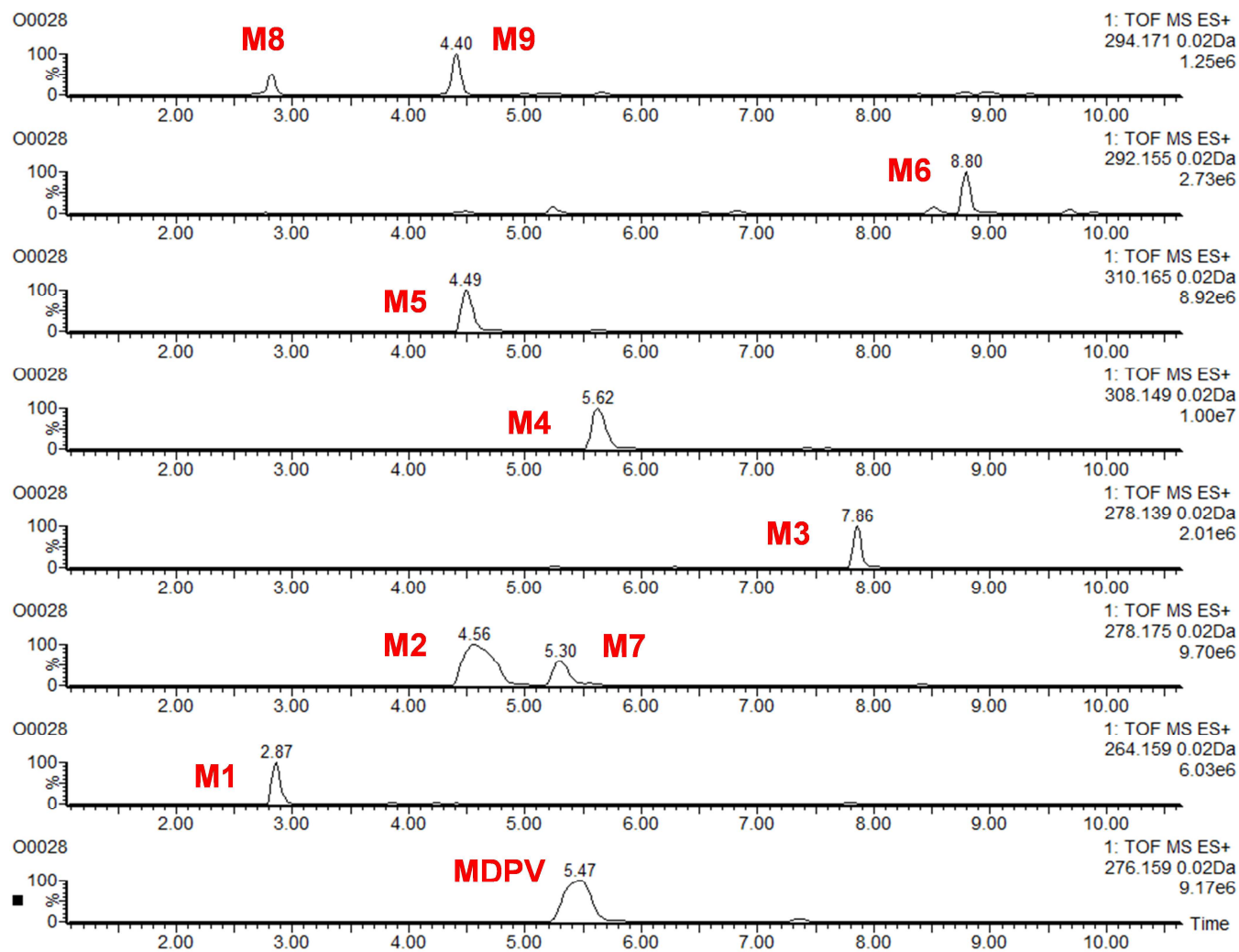


Fig S.1. Extracted Ion Chromatograms (XICs) for all detected metabolites.

Metabolite M1

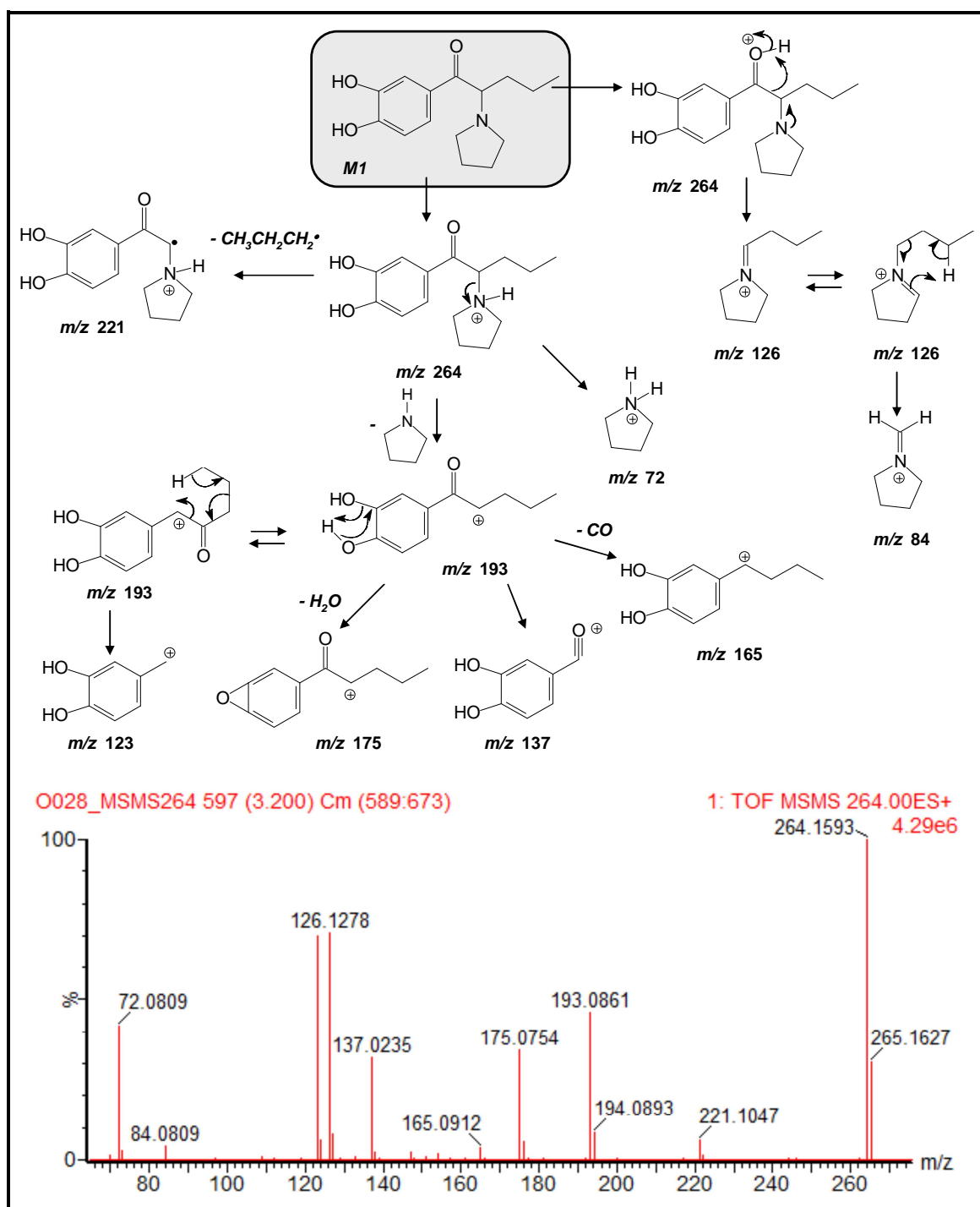


Figure S.2. Product ion spectrum of M1 (20 eV) and proposed fragmentation pathway.

Metabolite M2

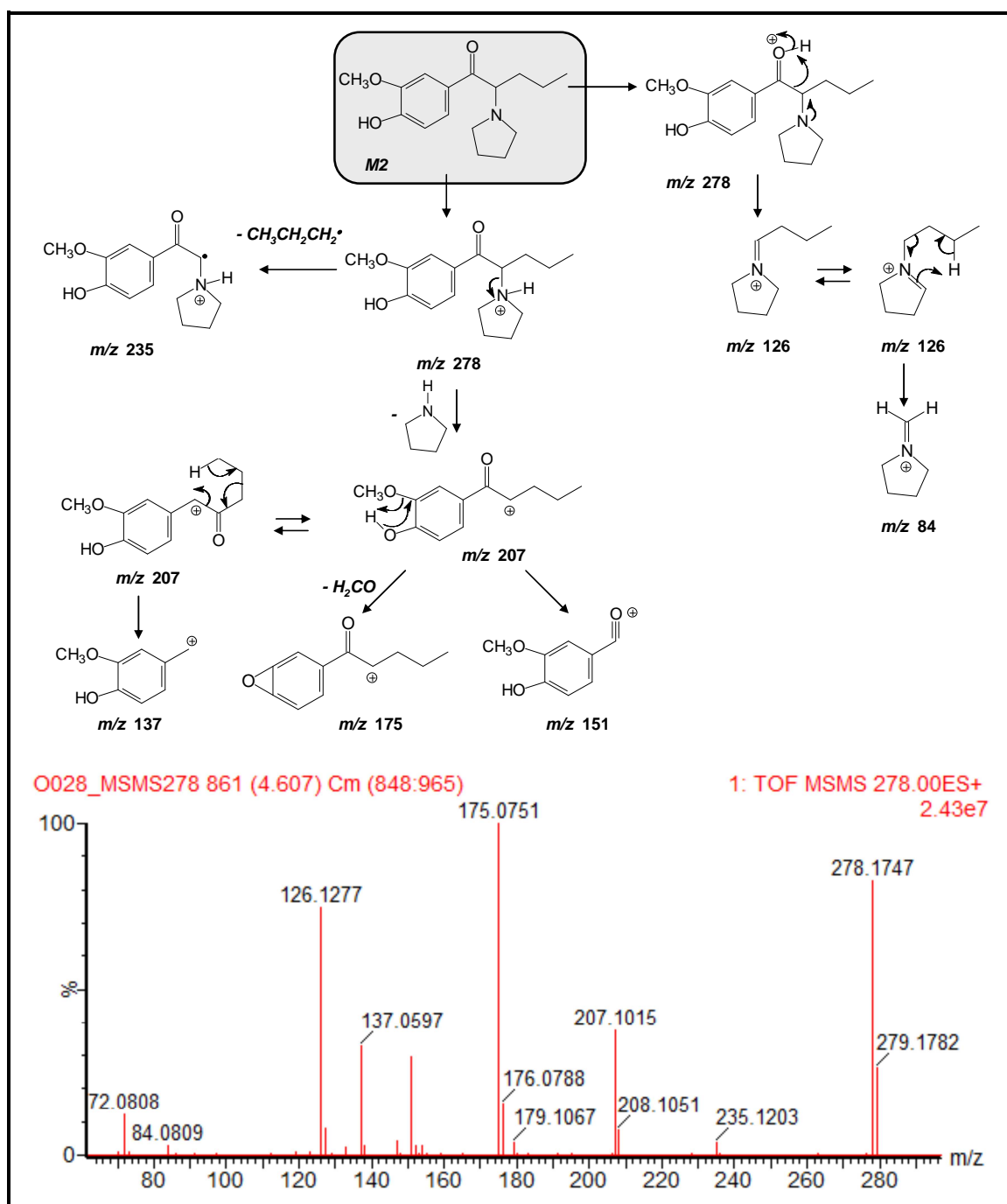


Figure S.3. Product ion spectrum of M2 (20 eV) and proposed fragmentation pathway.

Metabolite M3

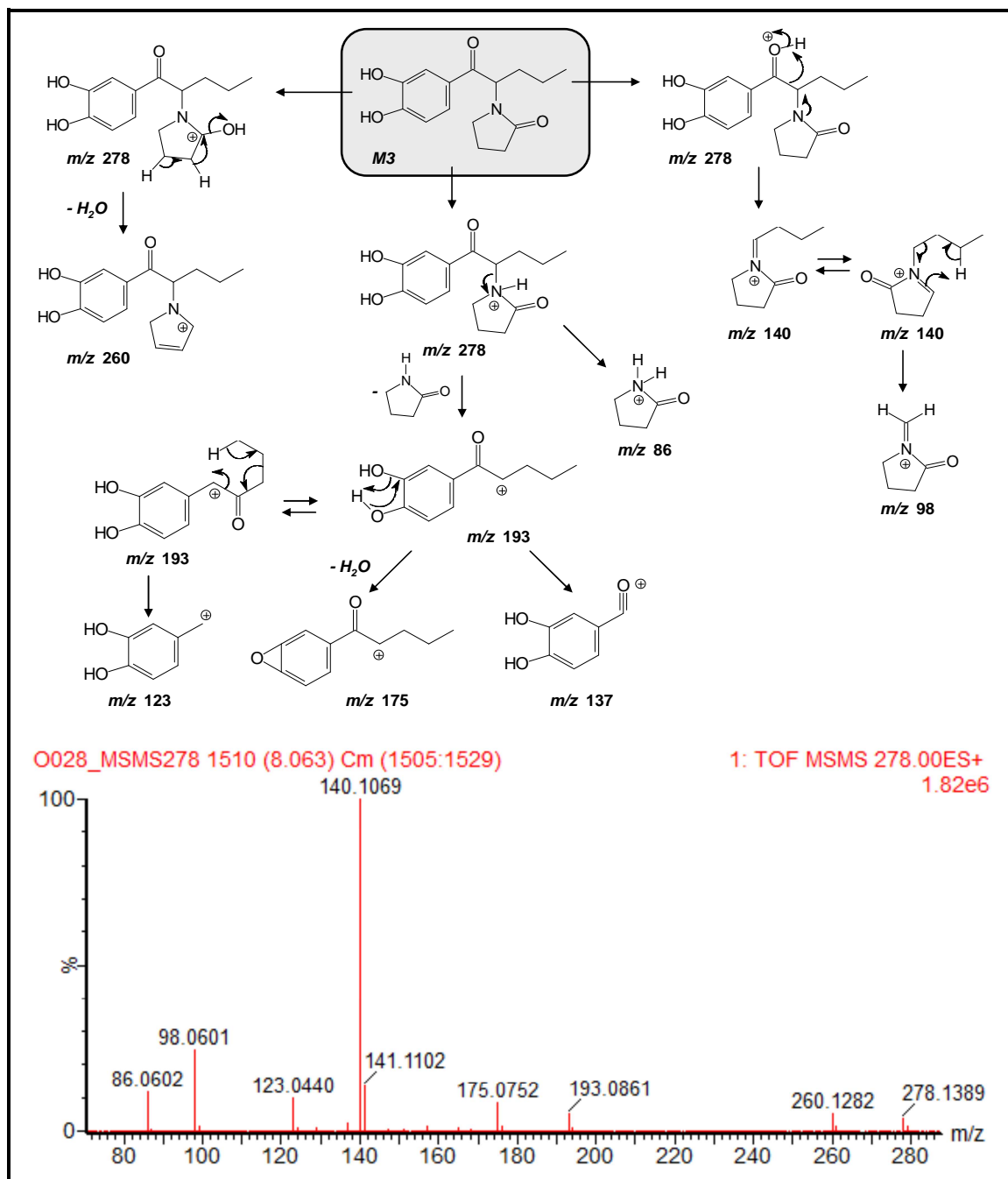
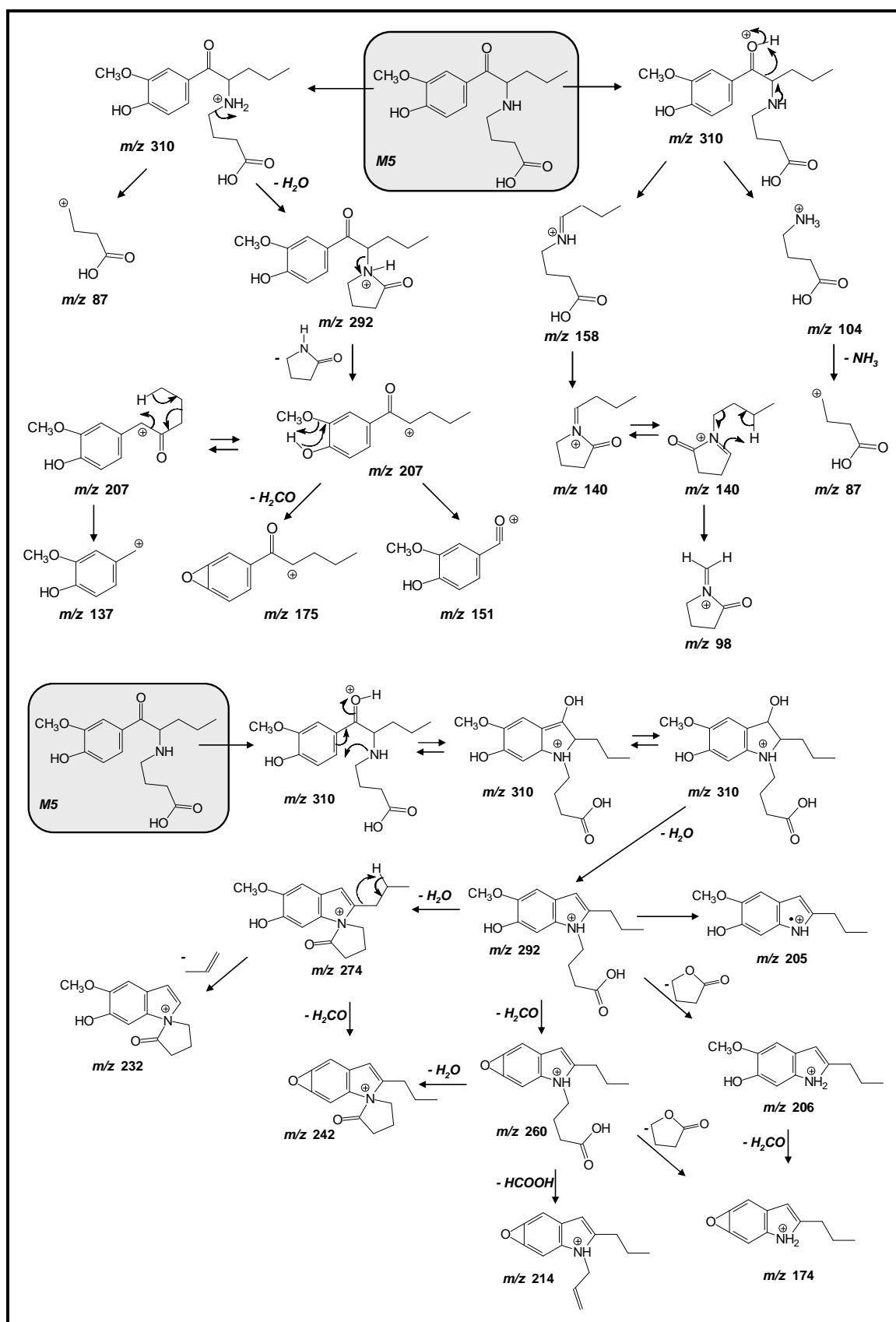


Figure S.4. Product ion spectrum of M3 (20 eV) and proposed fragmentation pathway.

Metabolite M5



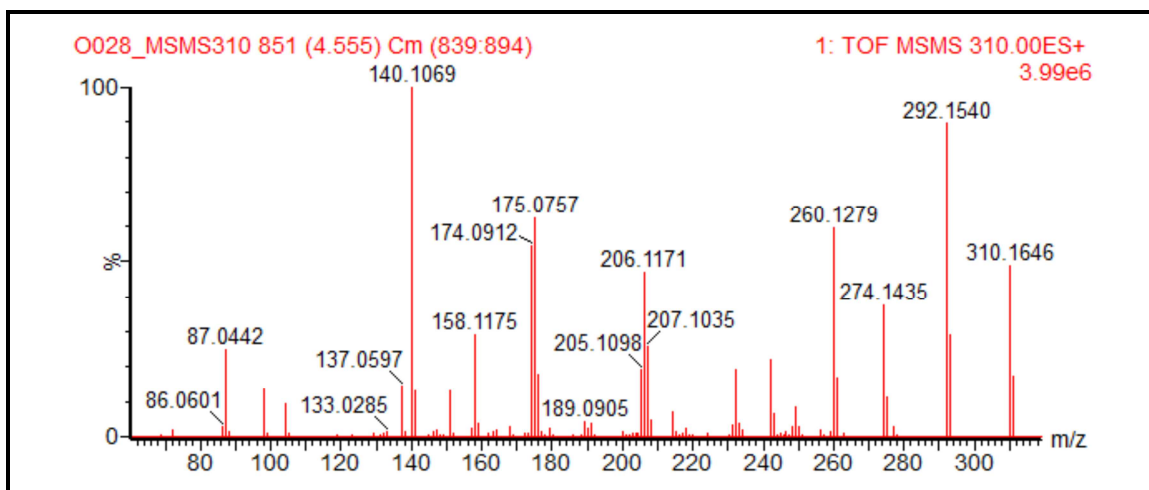


Figure S.5. Product ion spectrum of M5 (20 eV) and proposed fragmentation pathway.

Metabolite M6

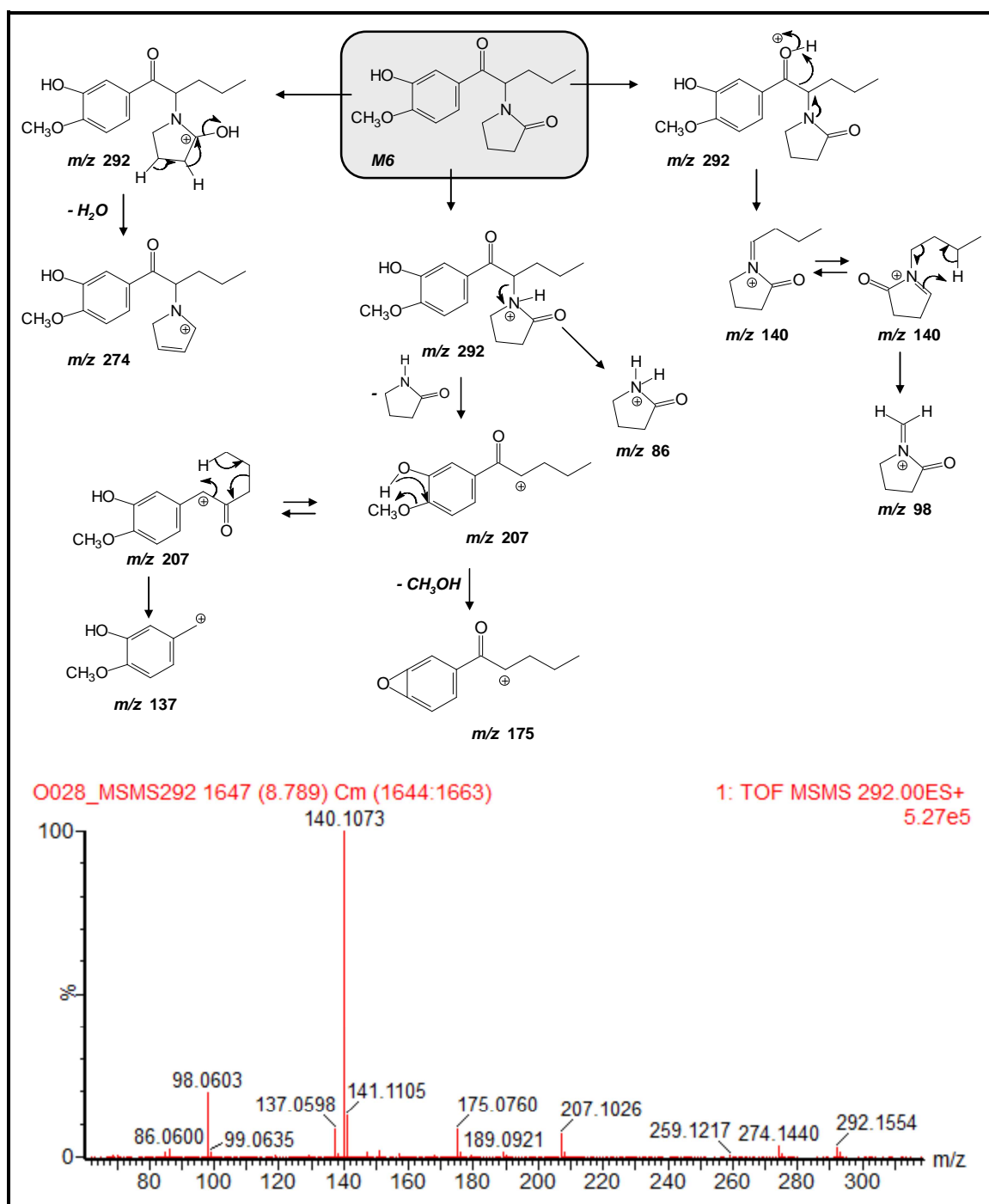


Figure S.6. Product ion spectrum of M6 (20 eV) and proposed fragmentation pathway.

Metabolite M7

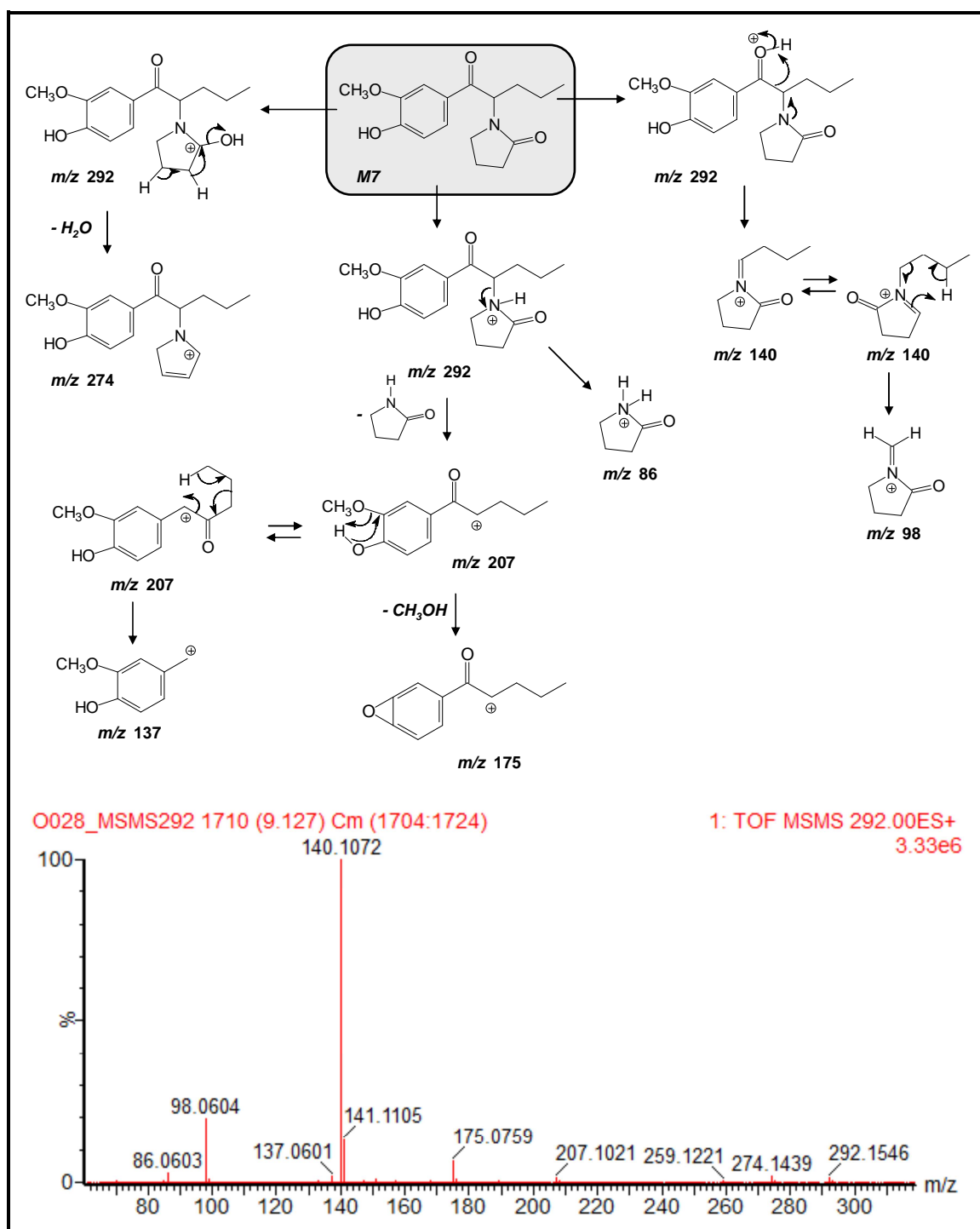


Figure S.7. Product ion spectrum of M7 (20 eV) and proposed fragmentation pathway.

Metabolite M8

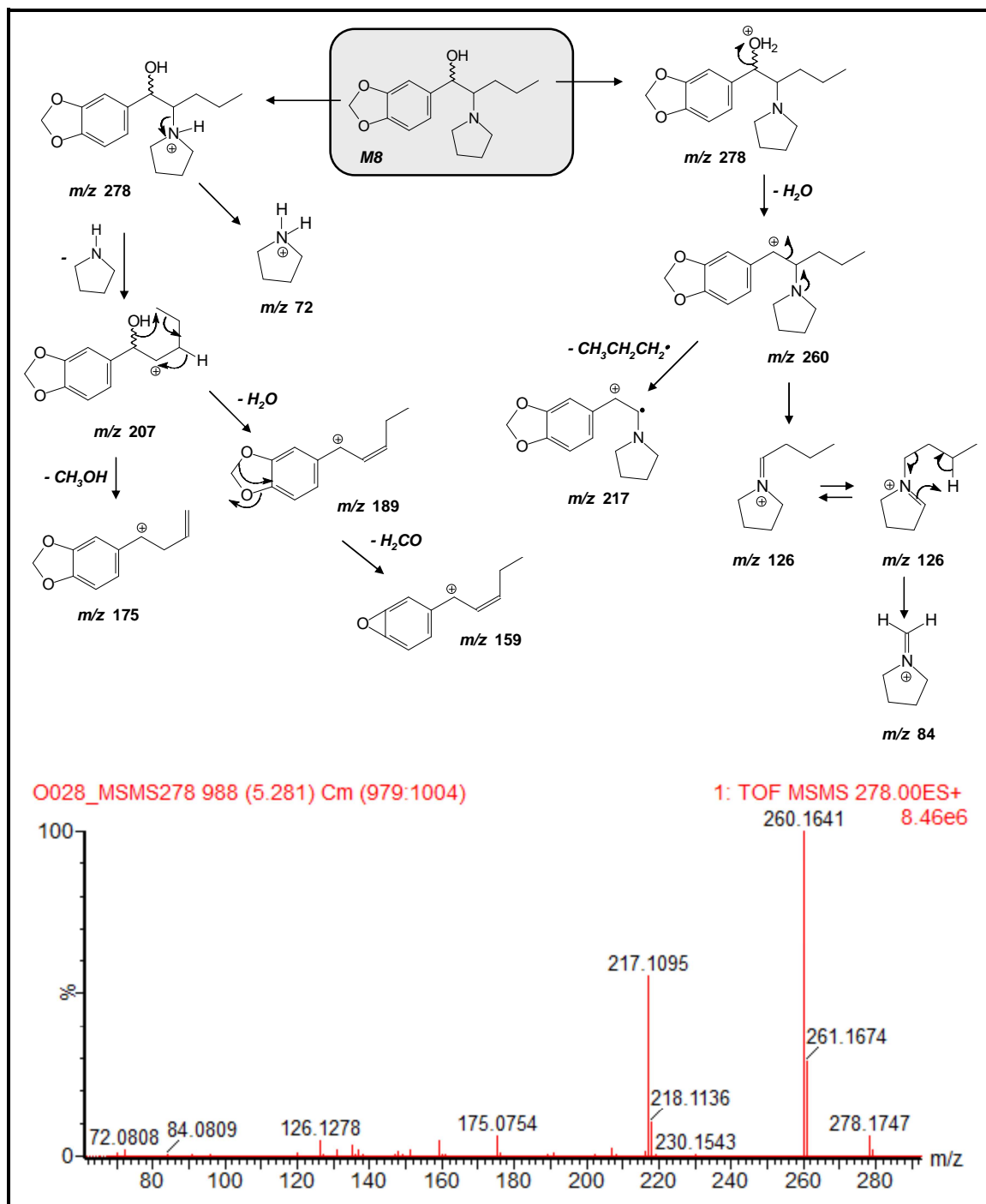
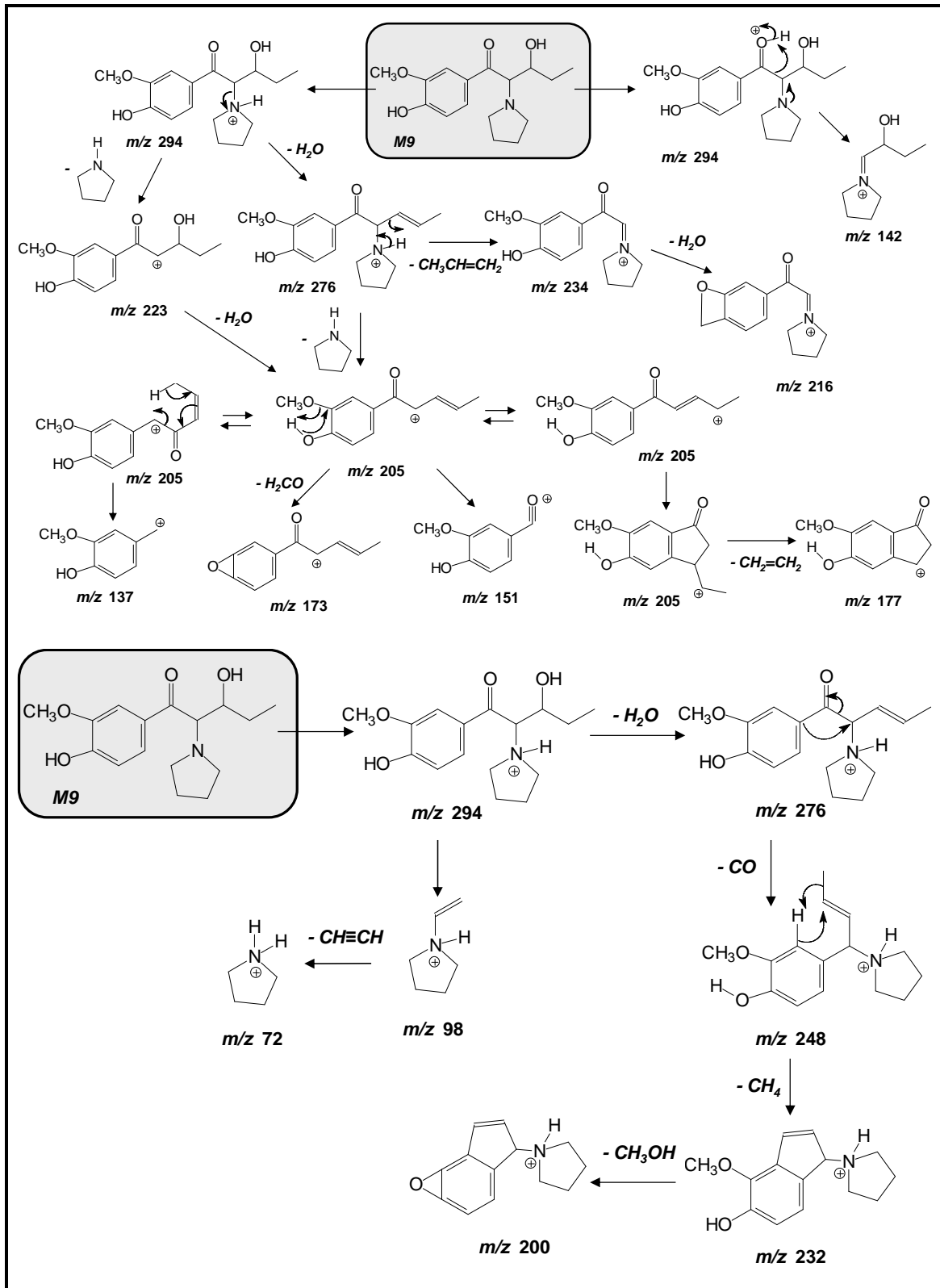


Figure S.8. Product ion spectrum of M8 (20 eV) and proposed fragmentation pathway.

Metabolite M9



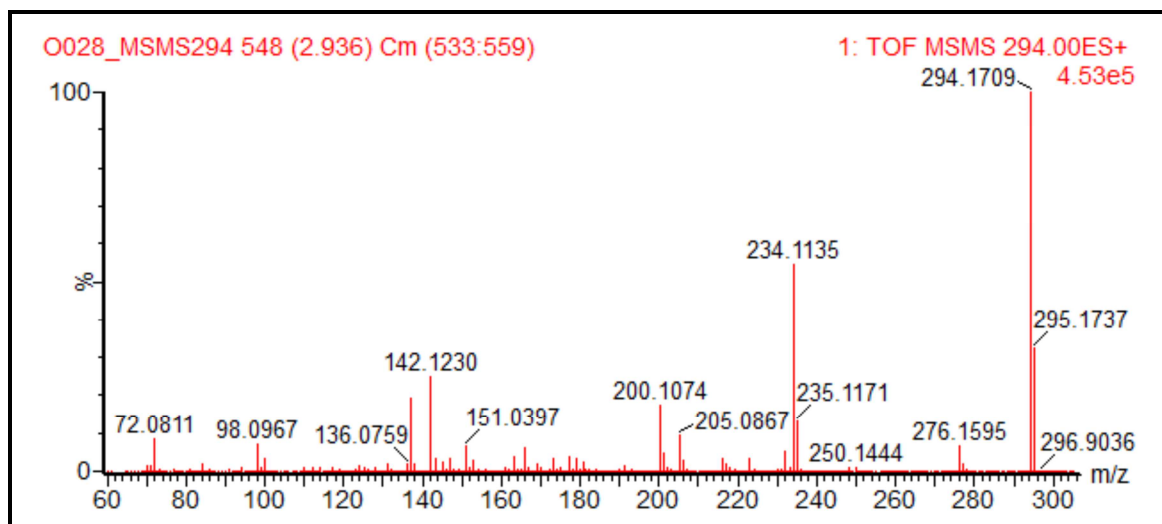


Figure S.9. Product ion spectrum of M9 (20 eV) and proposed fragmentation pathway. Only fragmentation corresponding to one of the two possible candidates (concretely, **1-(4-hydroxy-3-methoxyphenyl)-3-hydroxy-2-(1-pyrrolidinyl)pentan-1-one**) is shown, but the implied pathways for both candidates will be “identical”.

Metabolite M10

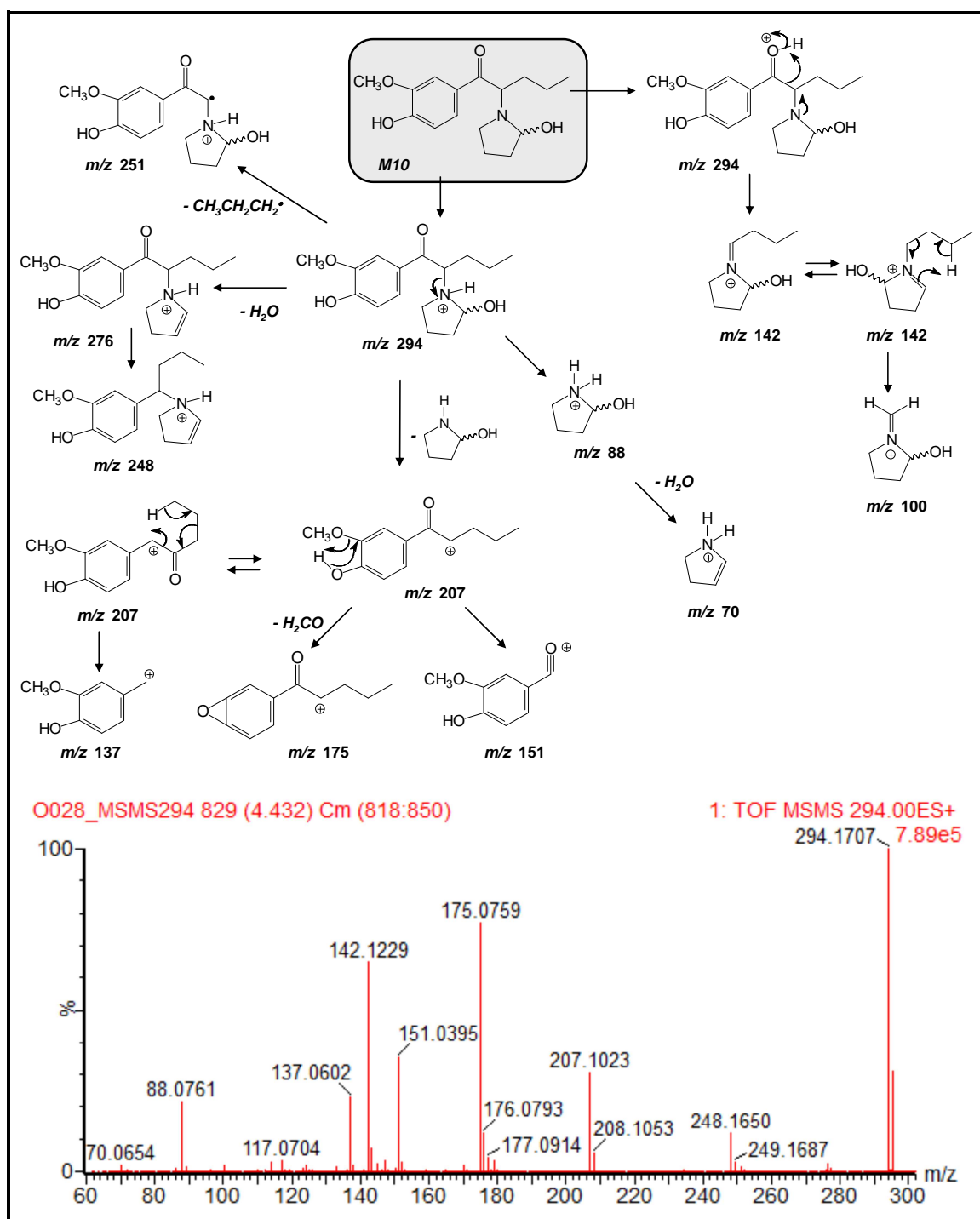


Figure S.10. Product ion spectrum of M10 (20 eV) and proposed fragmentation pathway. Only fragmentation corresponding to the most feasible candidate (concretely **1-(4-hydroxy-3-methoxyphenyl)-2-(2-hydroxypyrrolidinyl)pentan-1-one** is shown, but the implied pathways for both candidates will be “identical”.