

1 **Supplementary Information**

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3 **Proposal of 5-methoxy-*N*-methyl-*N*-isopropyltryptamine consumption**
4 **biomarkers through identification of *in vivo* metabolites from mice.**

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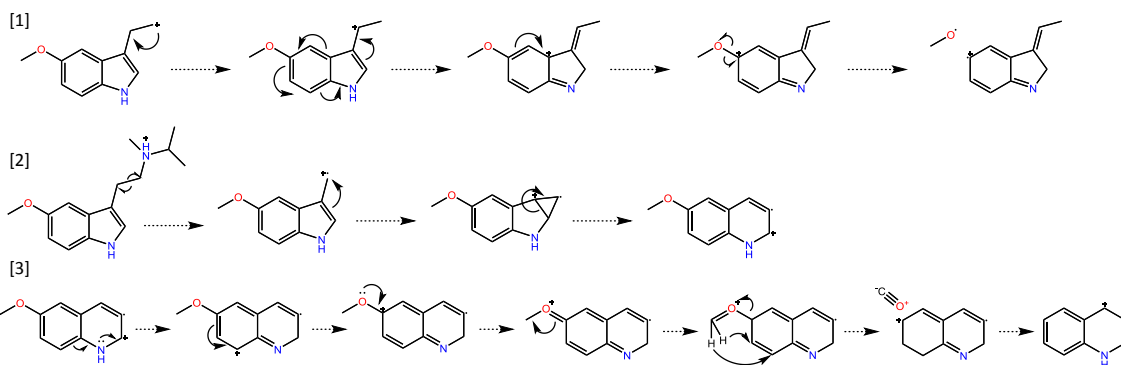
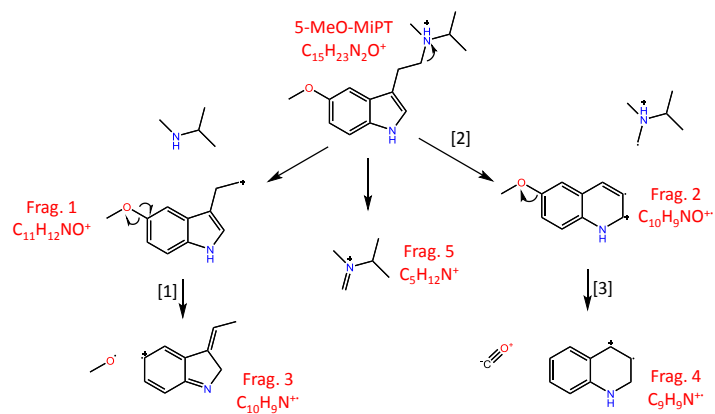
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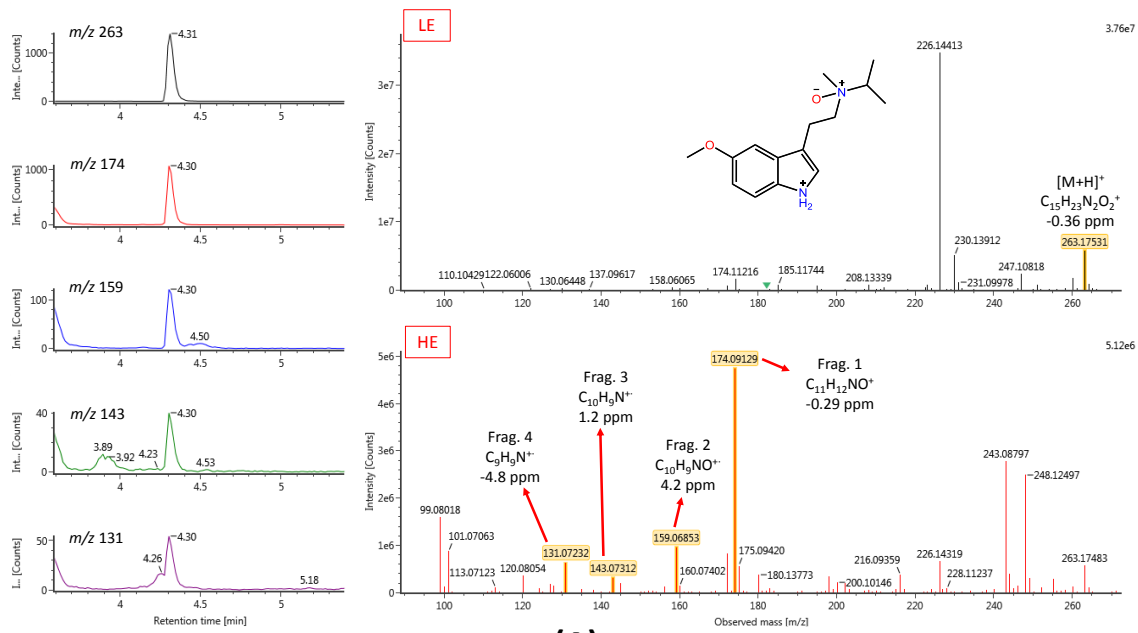
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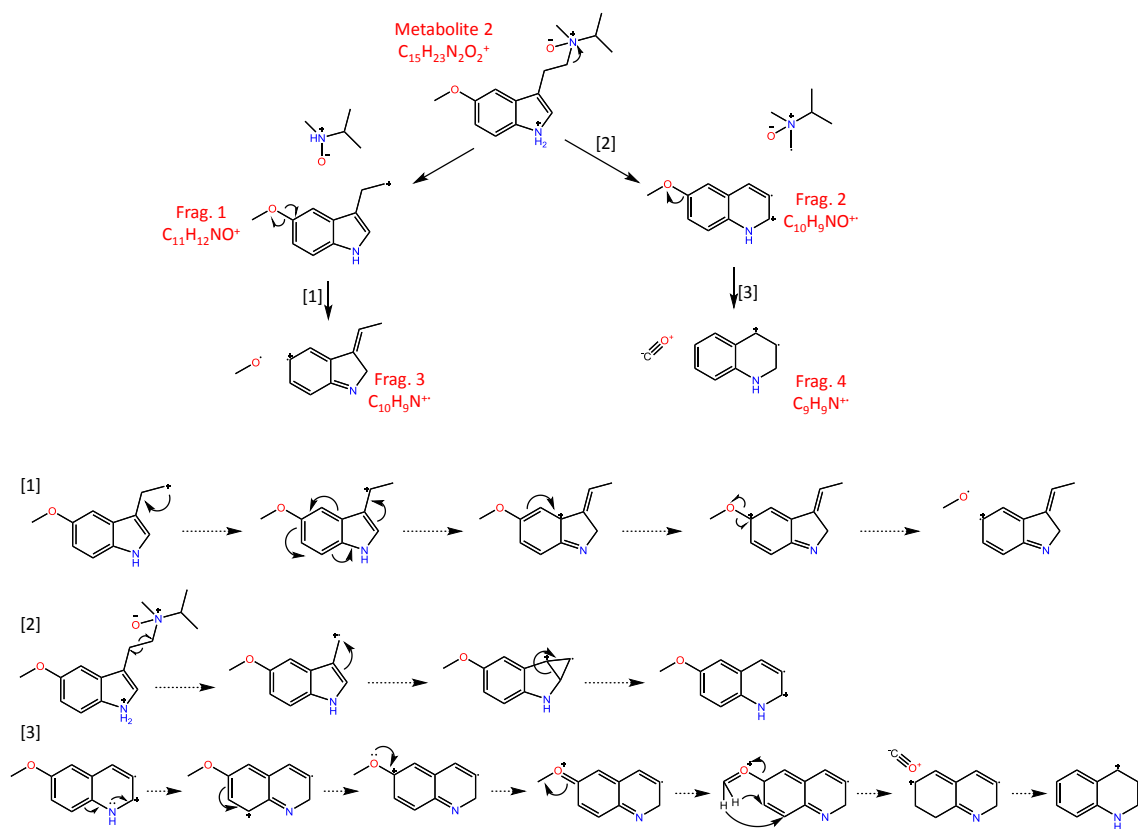


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SI.1. Proposed fragmentation pathway for 5-MeO-MiPT



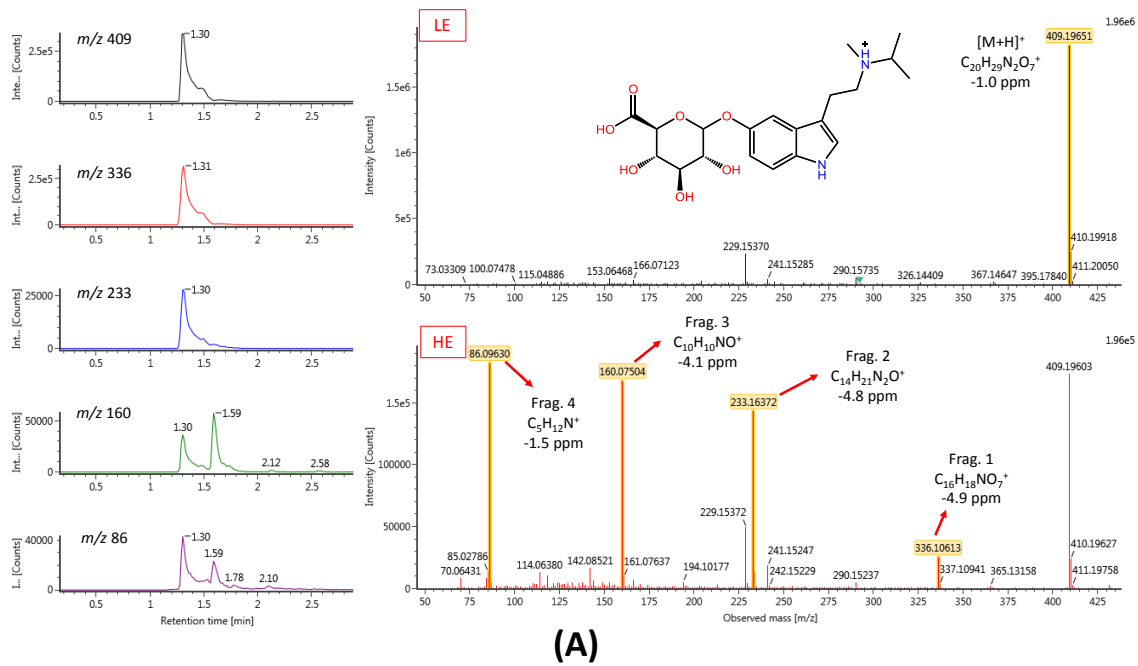
(A)



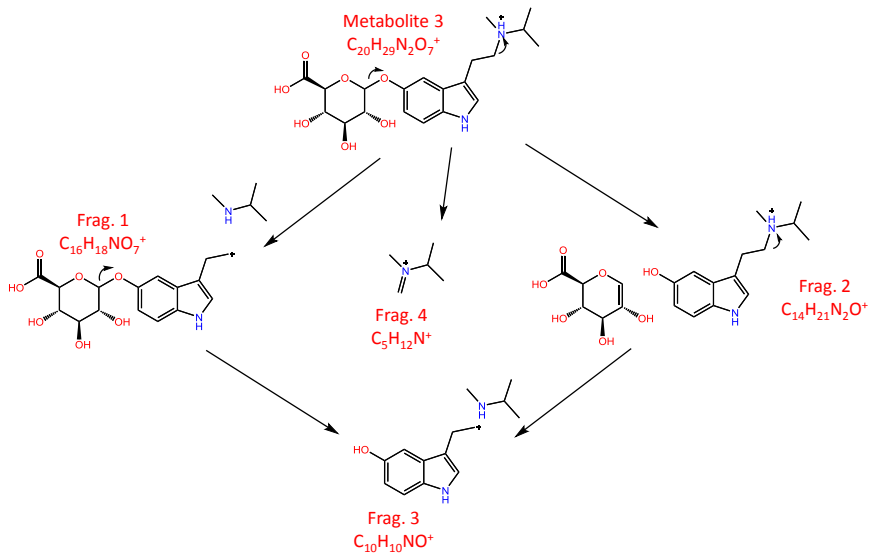
(B)

SI.2. (A) LE and HE spectra of Metabolite 2 (right) and XICs with a ± 20 mDa mass window (left); (B) proposed fragmentation pathway for Metabolite 2

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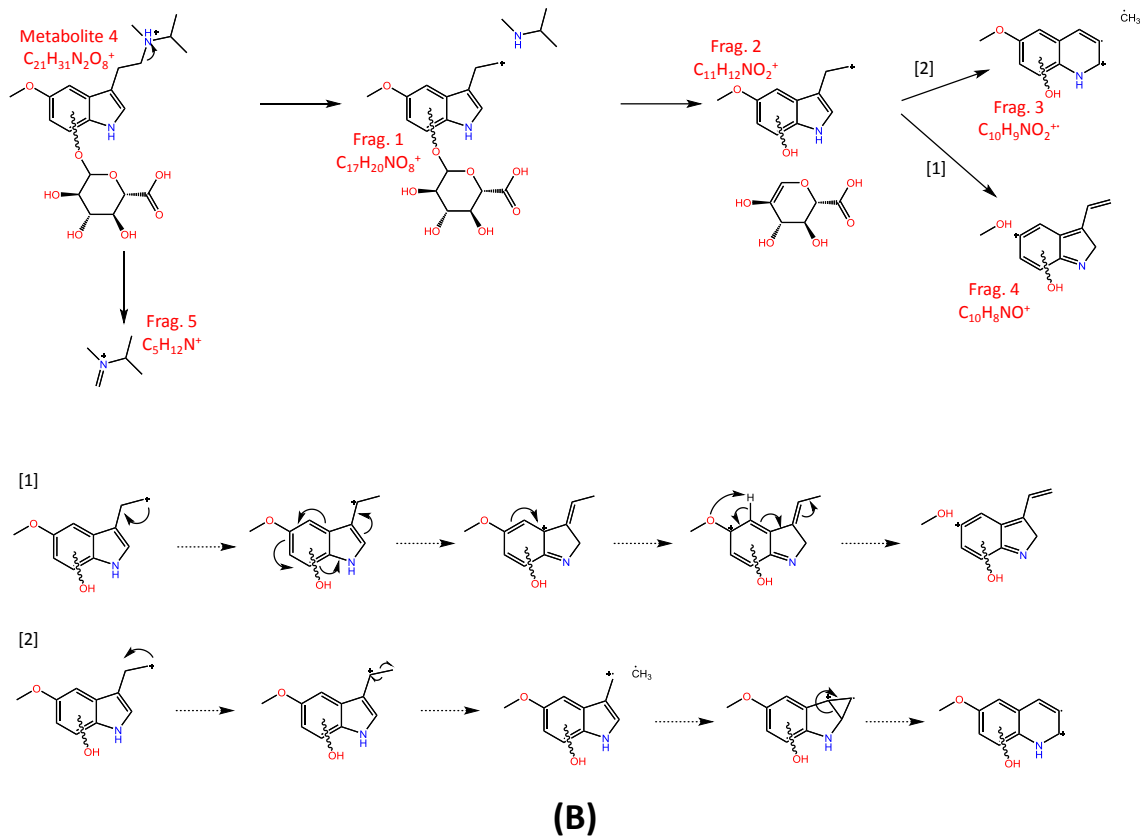
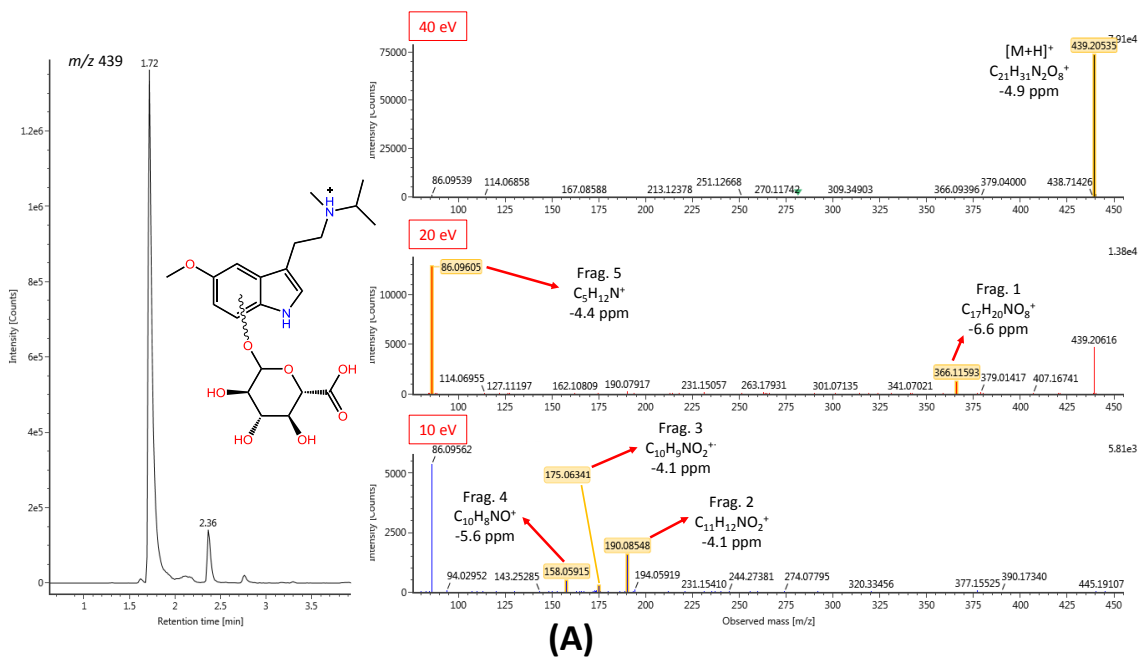
(A)



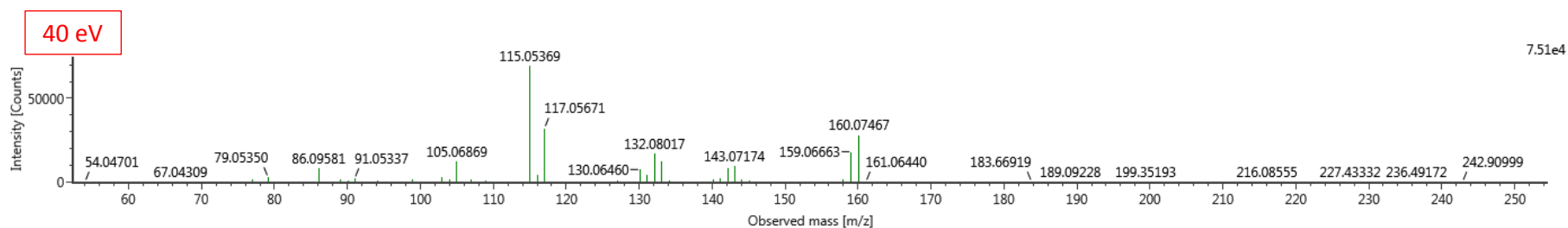
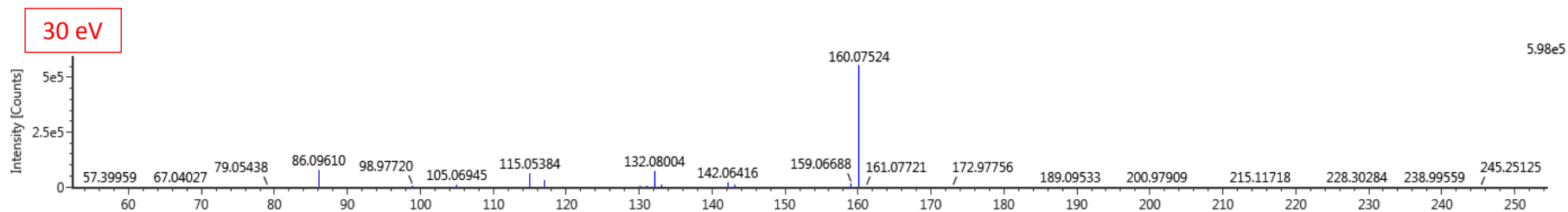
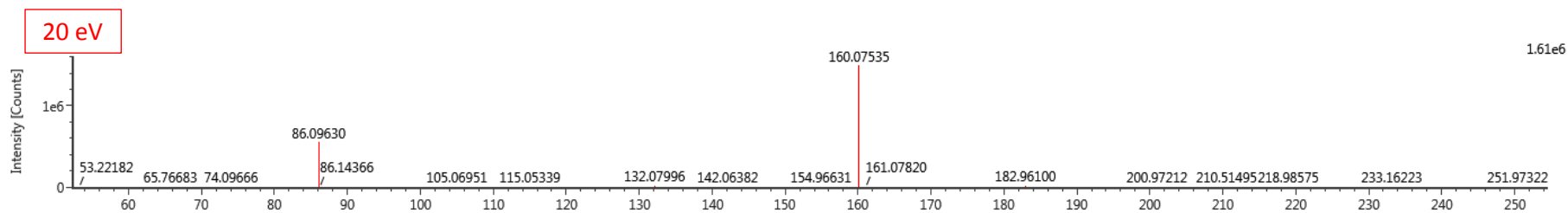
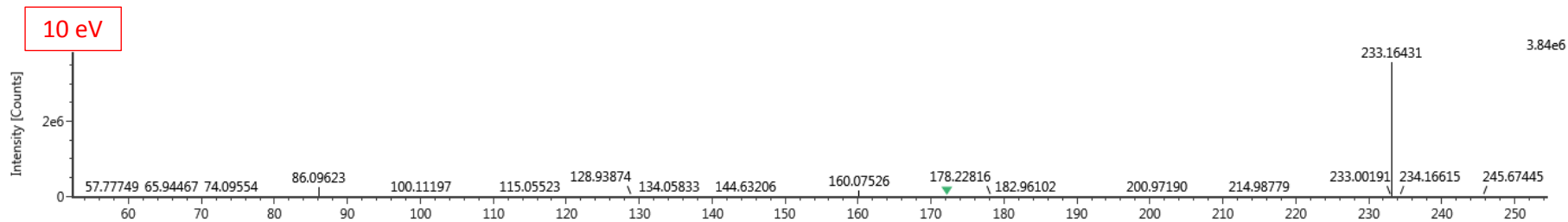
(B)

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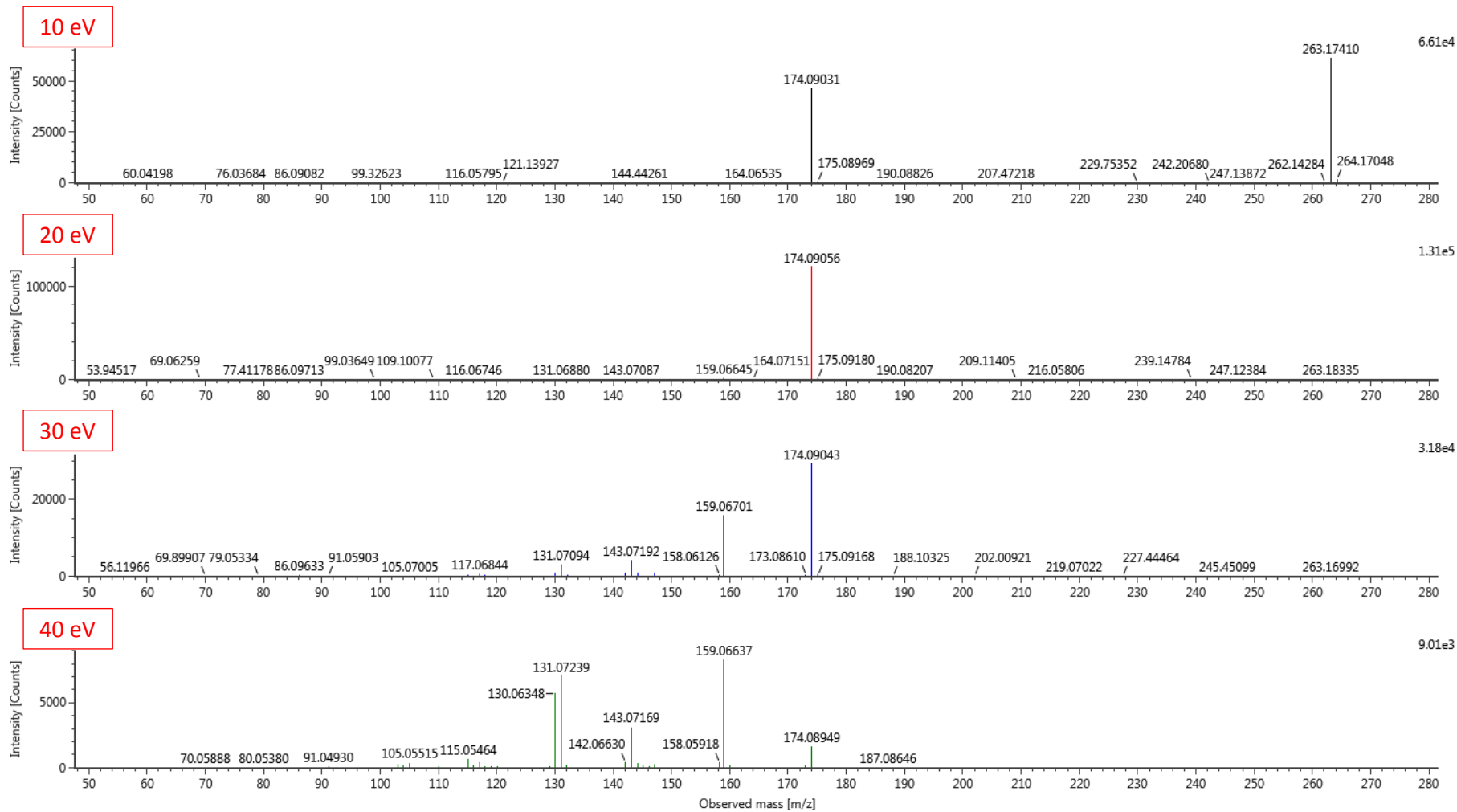
SI.3. (A) LE and HE spectra of Metabolite 3 (right) and XICs with a ± 20 mDa mass window (left); (B) proposed fragmentation pathway for Metabolite 3



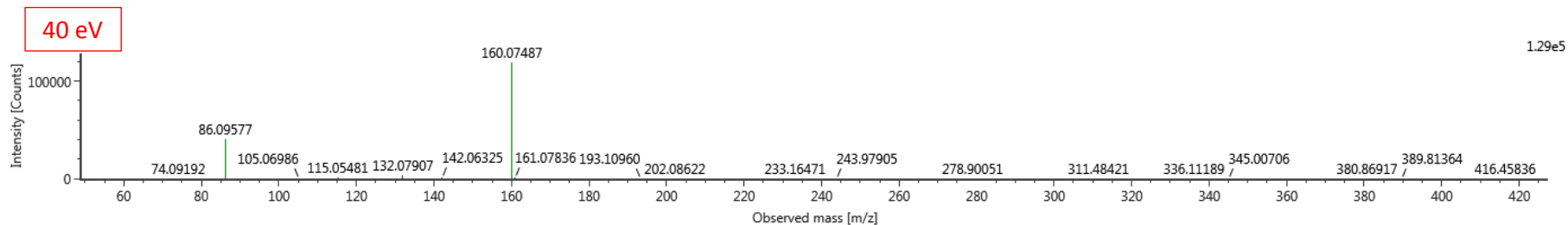
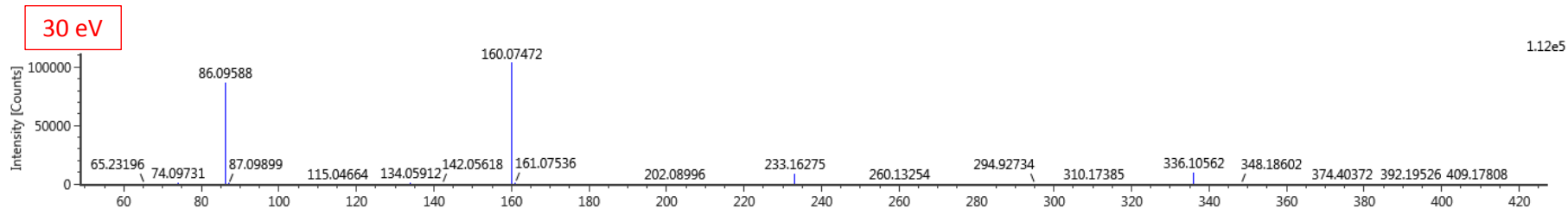
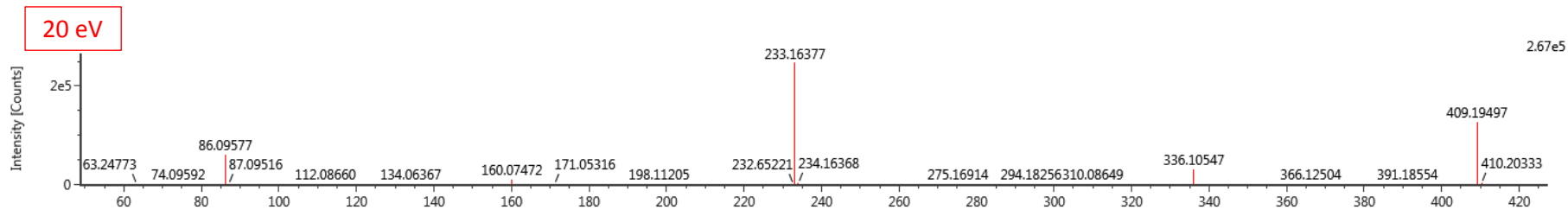
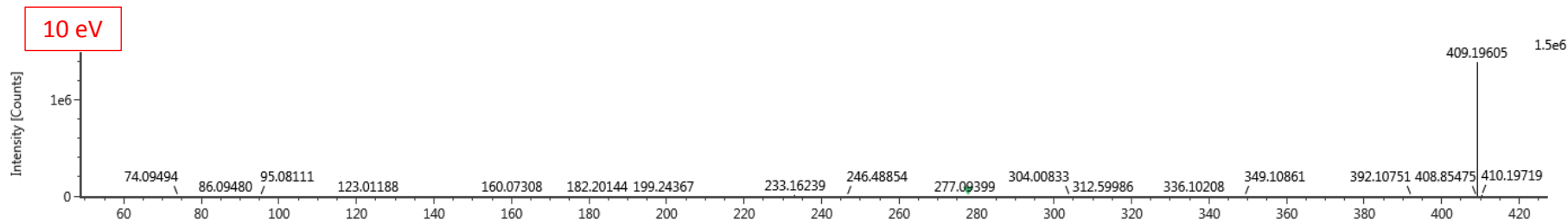
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 29 **SI.4. (A)** MS/MS spectra acquired at 10, 20 and 40 eV for Metabolite 4 (right) and XIC
 30 of the $[M+H]^+$ in the LE function with a ± 20 mDa mass window; **(B)** proposed
 31 fragmentation pathway for Metabolite 4
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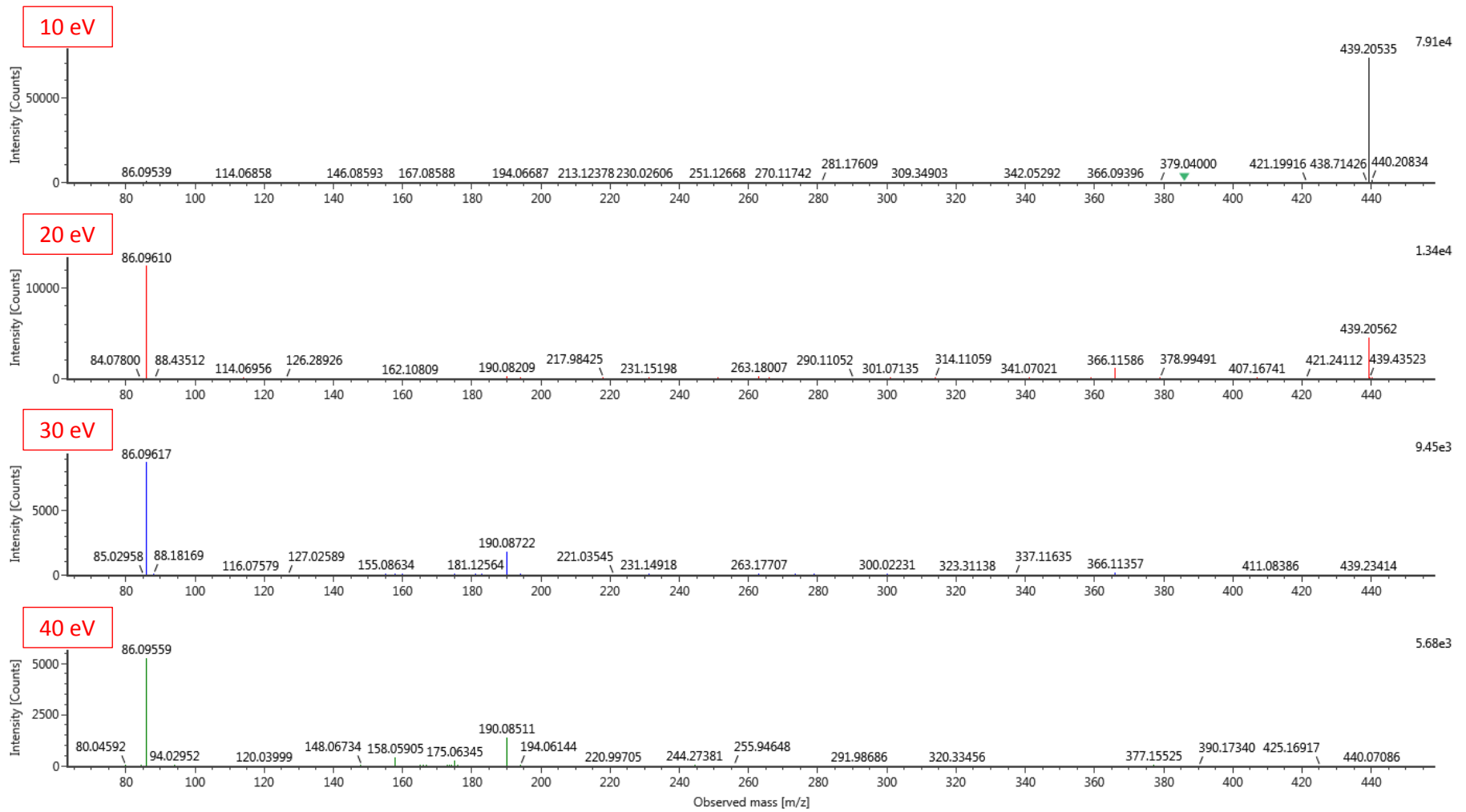
SI.5. MS/MS spectra collected at 10, 20, 30 and 40 eV for Metabolite 1.



SI.6. MS/MS spectra collected at 10, 20, 30 and 40 eV for Metabolite 2.



SI.7. MS/MS spectra collected at 10, 20, 30 and 40 eV for Metabolite 3.



SI.8. MS/MS spectra collected at 10, 20, 30 and 40 eV for Metabolite 4.