

## Supplementary Materials

### **Exploring the isomeric precursors of olive oil major secoiridoids: an insight into olive leaves and drupes by liquid-chromatography and Fourier-transform tandem mass spectrometry**

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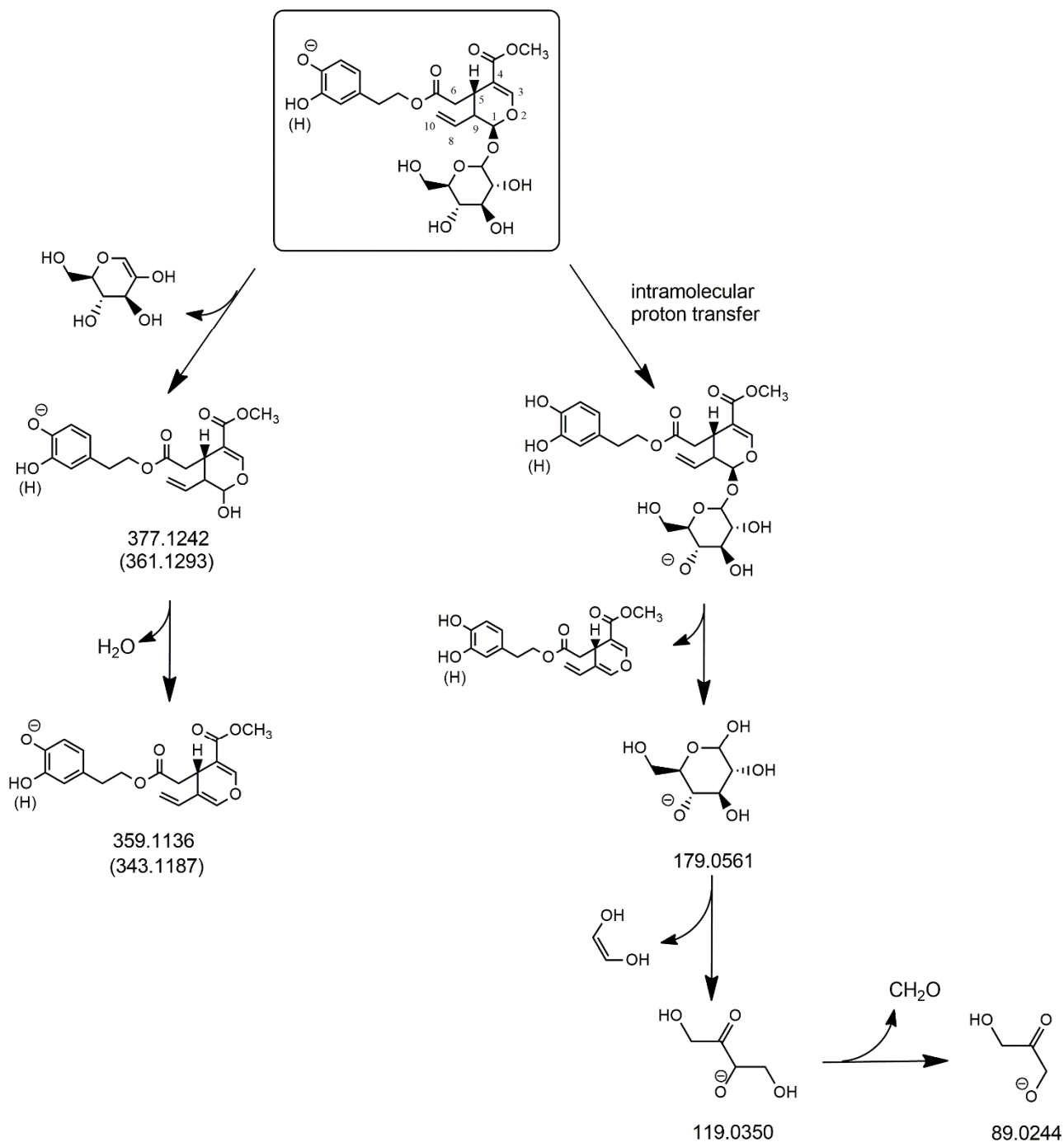
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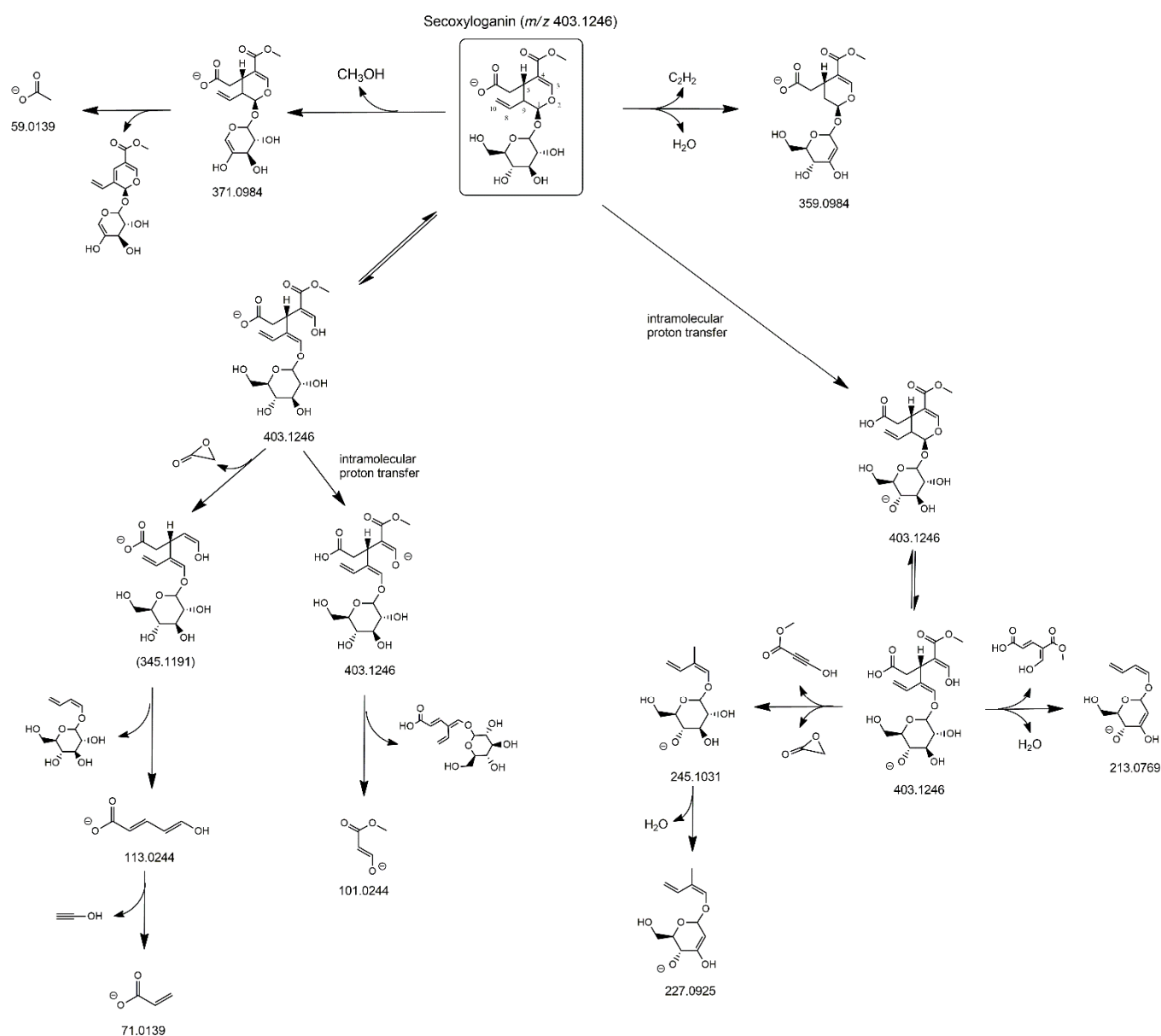
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Oleuroside,  $m/z$  539.1770  
(Ligstroside positional  
isomer,  $m/z$  523.1821)



**Figure S1.** Fragmentation pathways hypothesized for the  $[M-H]^-$  ions of oleuroside and of ligstroside positional isomers detected in olive leaves/drupes extracts, all including a C<sup>10</sup>=C<sup>8</sup> bond in their structures.  $m/z$  ratios reported in parentheses are referred to product ions of ligstroside positional isomers, in which a H atom replaces the OH group in the *meta* position of the phenyl ring.



**Figure S2.** Fragmentation pathways hypothesized for the  $[\text{M}-\text{H}]^-$  ions of secoxyloganin detected in extracts of olive leaves/drupes. Intramolecular proton transfers have been hypothesised to explain the displacement of negative charge from the  $\text{COOH}$  group to an enolic or a glucose  $\text{OH}$  group (only one of the possible charging sites is shown in the latter case), required to explain the generation of some product ions.