

# Evaluation of the Drug-Induced Liver Injury Potential of Saxagliptin through Reactive Metabolite Identification in Rats

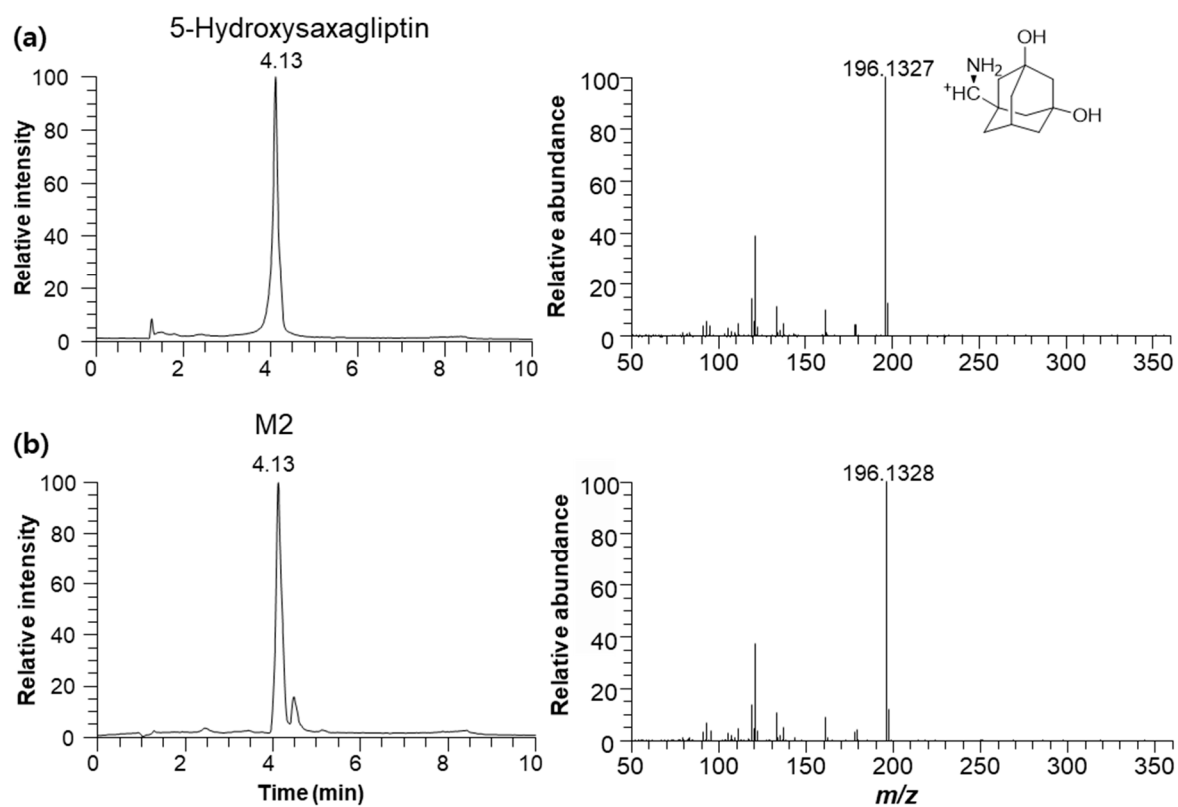
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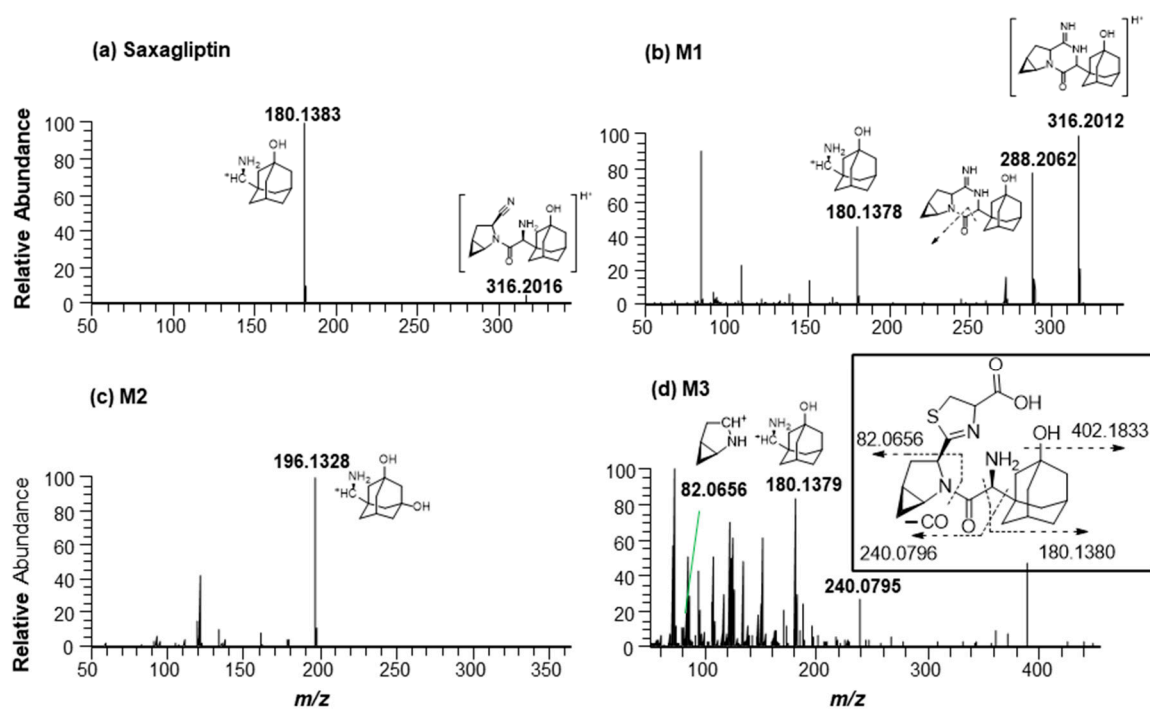
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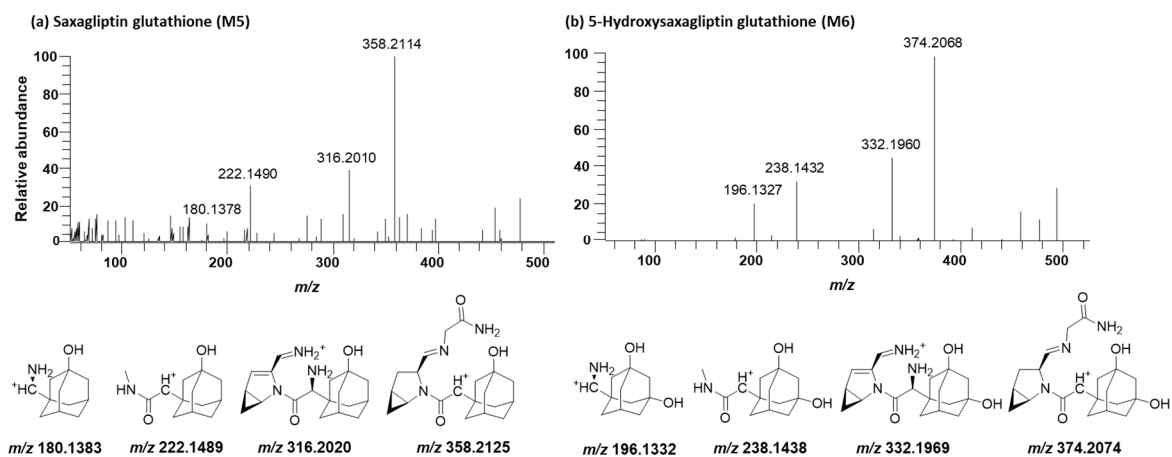
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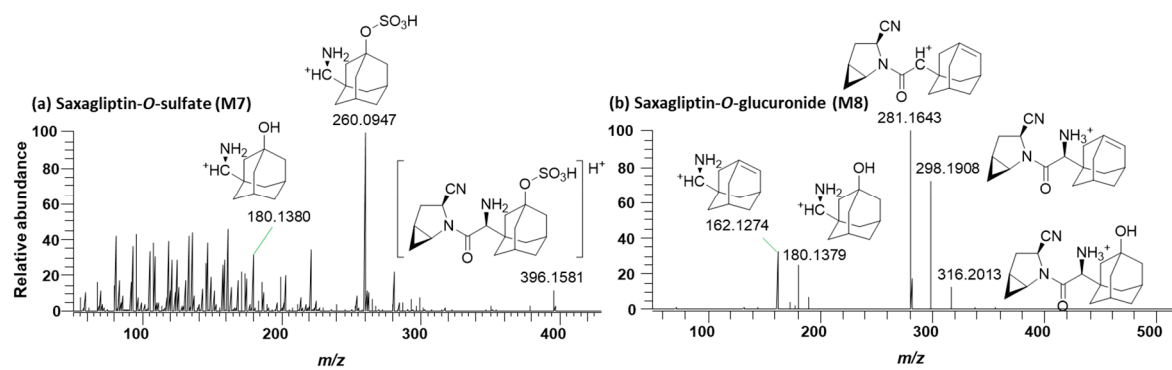
**Figure S1.** Representative extracted ion chromatograms ( $m/z$  332.1969, left panel) and product ion scan mass spectra (right panel) of the authentic 5-hydroxysaxagliptin standard (a) and M2 (b).



**Figure S2.** Product ion scan mass spectra of saxagliptin (P, a,  $m/z$  316.2020), M1 (b,  $m/z$  316.2020), M2 (c,  $m/z$  332.1969), and M3 (d,  $m/z$  420.1952) which were found in bile, plasma, or liver tissues following the intraperitoneal injection of saxagliptin in rats.



**Figure S3.** Product ion scan mass spectra of saxagliptin–cysteinyglycine conjugate (a,  $m/z$  477.2166, M5) and 5-hydroxysaxagliptin–cysteinyglycine conjugate (b,  $m/z$  493.2115, M6) and proposed chemical fragment ion structure.



**Figure S4.** Product ion scan mass spectra of saxagliptin-O-sulfate (a,  $m/z$  396.1588, M7) and saxagliptin-O-glucuronide (b,  $m/z$  492.2340, M8) and the proposed chemical structure of the fragment ions.