

**Supplemental Data to Gas-phase rearrangement of the O-glucuronide of  
Vildagliptin forms product ion fragments suggesting wrongly an N-glucuronide**

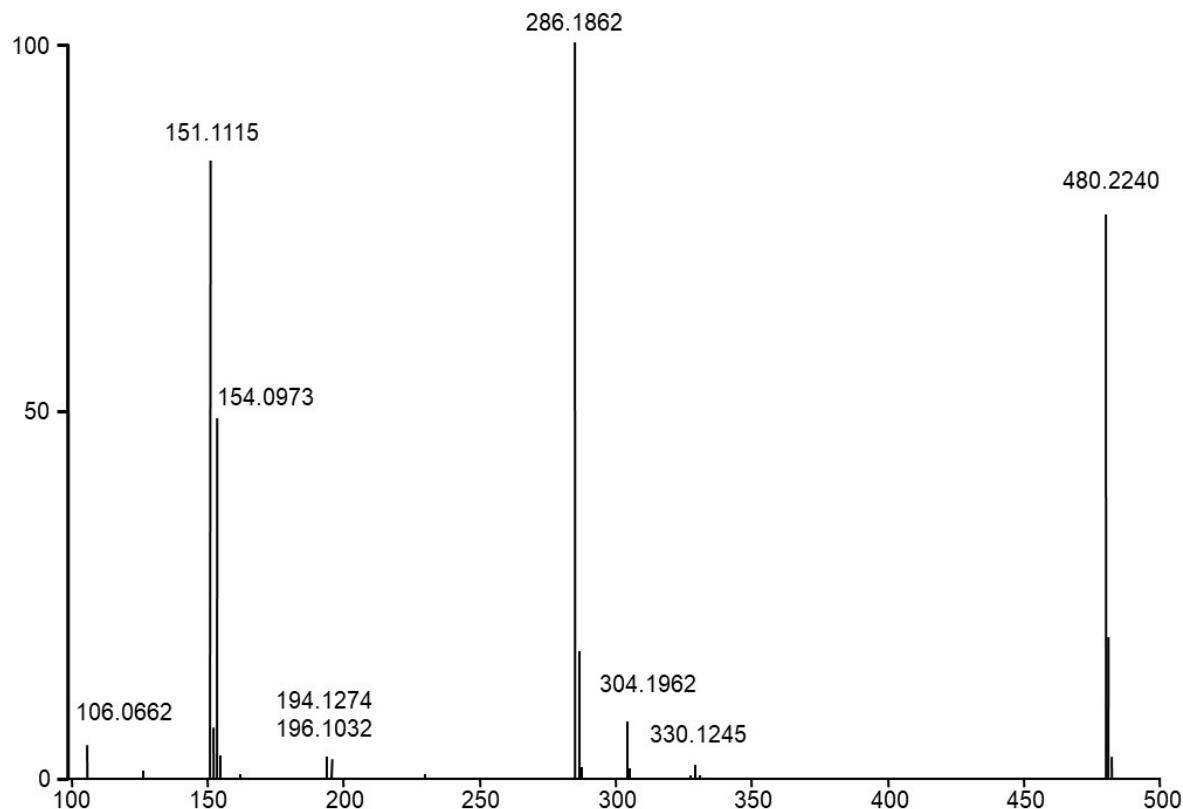
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**Content**

1.  $\text{MS}^{\text{E}}$  spectrum of Vildagliptin O-glucuronide on an Q-TOF-type MS
2. Ratio of m/z 286.2 and 330.2 upon variation of the activation time and different collision energies

**Supplemental Figure 1:**  $\text{MS}^{\text{E}}$  spectrum of Vildagliptin O-glucuronide on a Q-TOF-type MS utilizing a collision energy ramped from 20 to 40 eV



**Supplemental Table 1:** Ratio of intensities  $m/z$  330.2 divided by  $m/z$  286.2 upon variation of the activation time and CID or HCD activation with 15 % or 30 % collision energies

Activation Type	CID 15 %	CID 30 %	HCD 15 %	HCD 30 %
<b>Normalized collision energy</b>				
<b>Activation time</b>				
(ms)				
2	0.39 %	0.71 %	6.8 %	6.4 %
4	0.85 %	0.78 %	6.6 %	6.5 %
10 <sup>a)</sup>	0.93 %	0.92 %	6.8 %	6.4 %
200	1.27 %	1.22 %	6.6 %	6.6 %
2000	1.35 %	1.22 %	n.d.	n.d.

a) 10 ms is the default value