

**Table S1. Main biotransformation reactions found in AP-237 *in vitro* experiments with associated loss of mass or gain of mass for the parent molecule.**

<b>Biotransformation</b>	<b>Delta <i>m/z</i></b>
dehydrogenation	-2.015
oxidation / reduction	±15.995
Hydrolysis	-18.011
oxidation + deacetylation	+26.016
2 x oxidation	+31.990
deacetylation / acetylation	±42.011