Table 1. Fragment ions found in positive ionisation mode for detected metabolites.

Compound	***Retention time (min)***	***m/z***	**Mass error (ppm)**	**Elemental composition**	**Fragment ion**	**Formula**	**Mass error (ppm)**
5-MeO-MiPT*	3.24	247.1810	0.0	$C_{15}H_{23}N_2O^+$	174.0916	$C_{11}H_{12}NO^+$	-1.7
					159.0683	$C_{10}H_9NO^{+\cdot}$	-0.6
					143.0733	$C_{10}H_9N^{+\cdot}$	-1.4
					131.0732	$C_9H_9N^{+\cdot}$	-2.3
					86.0972	$C_5H_{12}N^+$	2.3
Metabolite 1	2.94	233.1649	-0.4	$C_{14}H_{21}N_2O^+$	160.0751	$C_{10}H_{10}NO^+$	-3.7
					142.0648	$C_{10}H_8N^+$	-2.5
					132.0799	$C_9H_{10}N^+$	-6.7
					117.0573	$C_8H_7N^{+\cdot}$	-0.1
					115.0536	$C_9H_7^{+\cdot}$	-5.1
					86.0961	$C_5H_{12}N^+$	-4.3
Metabolite 2	4.30	263.1753	-0.4	$C_{15}H_{23}N_2O_2^+$	174.0913	$C_{11}H_{12}NO^+$	-0.3
					159.0685	$C_{10}H_9NO^{+\cdot}$	4.2
					143.0731	$C_{10}H_9N^{+\cdot}$	1.2
					131.0723	$C_9H_9N^{+\cdot}$	-4.8
Metabolite 3	1.30	409.1965	-1.0	$C_{20}H_{29}N_2O_7^+$	336.1061	$C_{16}H_{18}NO_7^+$	-4.9
					233.1637	$C_{14}H_{21}N_2O^+$	-4.8
					160.0750	$C_{10}H_{10}NO^+$	-4.1
					86.0963	$C_5H_{12}N^+$	-1.5
Metabolite 4	1.72	439.2054	-4.9	$C_{21}H_{31}N_2O_8^+$	366.1159	$C_{17}H_{20}NO_8^+$	-6.6
					190.0855	$C_{11}H_{12}NO_2^+$	-4.1
					175.0634	$C_{10}H_9NO_2^{+\cdot}$	-4.1
					158.0592	$C_{10}H_8NO^+$	-5.6
					86.0961	$C_5H_{12}N^+$	-4.4

*: The fragmentation of 5-MeO-MiPT corresponds to the observed in the analysis of *Estrella* sample.