

Supplementary material V

Table B

Quantifier ions, internal standards and ionization mode applied in analytical methods. Internal standard for PTU was not available.

Compound	Ionization mode	Quantifier ions	IS	Quantifier ions (IS)
TCPy	negative	195.7/35.0	¹³ C ₅ -TCPy	200.7/35.0
3-PBA	negative	213.0/93.0	¹³ C ₆ -3-PBA	219.1/99.0
4F-3-PBA	negative	231.1/93.0	¹³ C ₆ -4F-3-PBA	237.1/98.9
DCCA	negative	207.0/35.0	D ₆ -DCCA	213.0/35.0
CFCA	negative	241.0/205.0	¹³ C ₆ -3-PBA	219.1/99.0
2,4-D	negative	219.1/161.0	D ₃ -2,4-D	224.1/166.0
MCPA	negative	199.1/140.8	D ₃ -MCPA	204.1/146
OH-TBZ	positive	218.0/191.2	[¹³ C ₂][¹⁵ N]-5-OH-TBZ	221.0/194.0
OH-PYM	positive	216.1/107.0	D ₄ -OH-PYM	220.1/111.0
OH-TEB	positive	324.2/124.9	D ₆ -TEB	314.2/72.0
ETU	positive	103.1/60.0	[² H ₄]-ETU	107.1/48.0
PTU	positive	117.1/58.1 117.1/60.1	NA	NA
CCC	positive	122.2/58.1	D ₄ -CCC	126.2/58.1
MQ	positive	114.3/98.3	D ₁₆ -MQ	130.0/110.0