

Table S1. The electrospray mode of the analyzed compounds and transition of m/z of precursors to m/z of products.

Analyzed Compound and Electrospray Mode	m/z of Precursor $\rightarrow$ m/z of Product
APAP ESI+	152.0 $\rightarrow$ 110.0
	152.0 $\rightarrow$ 65.0
	152.0 $\rightarrow$ 92.9
NPX ESI-	229.0 $\rightarrow$ 169.1
	229.0 $\rightarrow$ 141.0
IBU ESI-	205.0 $\rightarrow$ 161.1
	205.0 $\rightarrow$ 142.5
	205.0 $\rightarrow$ 103.1
DCF ESI-	293.9 $\rightarrow$ 177.8
	293.9 $\rightarrow$ 249.9
	293.9 $\rightarrow$ 214.0
1-OH-IBU ESI-	221.0 $\rightarrow$ 143.0
	221.0 $\rightarrow$ 159.1
	221.0 $\rightarrow$ 177.0
2-OH-IBU ESI-	221.4 $\rightarrow$ 177.1
	221.4 $\rightarrow$ 116.7
	221.4 $\rightarrow$ 159.0
O-desmethyl-NPX ESI-	215.0 $\rightarrow$ 169.0
	215.0 $\rightarrow$ 142.8
DCF lactam ESI+	277.9 $\rightarrow$ 213.8
	277.9 $\rightarrow$ 180.1
	277.9 $\rightarrow$ 208.0
4-OH-DCF ESI-	309.9 $\rightarrow$ 165.9
	309.9 $\rightarrow$ 229.5
	309.9 $\rightarrow$ 266.0