Table S1. Optimized MRM parameters of the QqQ-MS determination of ibuprofen and its metabolites

Compound	Retention time (min)	Ion polarity	Precursor ion (m/z)	MRM 1 (quantification)	MRM 2 (confirmation)	CE (V)
Ibuprofen	8.80	Negative	205	205>205	205>161	0/4
1-hydroxyibuprofen	7.84	Positive	240	240>205	240>163	8/20
2-hydroxyibuprofen	7.64	Positive	240	240>205	240>107	12/36
Carboxyibuprofen	7.63	Positive	254	254>219	254>117	8/48

CE: collision energy; MRM: Multiple Reaction Monitoring