



Method name	LC-MS/MS-ESI(+)-11 (corresponds to QuPpe M10)							
Instrument	LC-MS/MS							
Chromatographic method	LC							
Extraction method	QuPpe							
Clean-up	no							
Use of AP (analyte protectant)	no							
Internal standard	respective IL-IS							
Instrument parameters								
Ionisation mode	ESI(+)							
Column	Waters APPC, 130Å, 5 µm, 2.1 mm x 100 mm							
Pre-column	Waters APPC Van Guard Cartridge, 130Å, 5µm, 2.1 mm X 5 mm							
Column temperature (°C)	50							
Eluent A1	1.2% formic acid in water							
Eluent B1	0.5% formic acid in ACN							
Gradient	%A	Flow [mL/min]		Time [min]				
	10	0.5		0				
	10	0.5		0.5				
	80	0.5		1.5				
	90	0.5		4.5				
	90	0.5		5				
	10	0.5		5.5				
	10	0.5		10				
Injection volume (µL)	2							
Acquired mass transitions	Target		Qualifier 1		Qualifier 2		Qualifier 3	
	Q1 (m/z)	Q3 (m/z)	Q1 (m/z)	Q3 (m/z)	Q1 (m/z)	Q3 (m/z)	Q1 (m/z)	Q3 (m/z)
Triazole-alanine	157	88	157	70	157	42		
Triazole-alanine ¹³ C ₂ ¹⁵ N ₃ (IL-IS)	162	75						
Triazole-acetic acid	128	70	128	43	128	73		
Triazole-acetic acid ¹³ C ₂ ¹⁵ N ₃ (IL-IS)	133	75						
Triazole-lactic acid	158	70	158	43	158	112		
Triazole-lactic acid ¹³ C ₂ ¹⁵ N ₃ (IL-IS)	163	75						