

Supplementary Table S3. Chromatographic separation conditions.

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Method	Conditions
UHPLC-DAD	Analytical column
	UFLC Aqueous C18, 2.1 x 100 mm, 3 µm particle size.
	Mobile phase
	A: water acidified with formic acid (0.1% v/v), B: acetonitrile.
	Mobile phase elution
	Gradient.
	0 min: 5% B; 4 min: 5% B; 17 min: 30% B; 18 min: 35% B; 19 min: 50% B; 20 min: 95% B, 21 min: 95% B; 24 min: 50% B; 27 min: 5% B; 37 min: 5% B.
	Gradient program
UHPLC-DAD-FLD	Flow rate
	0.4 mL min ⁻¹
	Detection
	λ=254, 280 and 320 nm.
	Sample volume injection
	0.1 µL
	Column temperature
	30 °C
UHPLC-DAD-FLD	Analytical column
	Kinetex C18, 3.0 x 100 mm, 2.6 µm particle size.
	Mobile phase
	A: water acidified with formic acid (0.1% v/v), B: methanol.
	Mobile phase elution
	Gradient.
	0-1.7 min: 5% B; 1.7-10 min: 30% B; 10-13.5 min: 95% B; 13.5-15 min: 95% B; 15-16 min: 5% B; 16-19 min: 5% B.
	Gradient program
UPLC-MS/MS	Flow rate
	0.8 mL min ⁻¹
	DAD: λ= 254, 280, 320 and 370 nm
	Detection
	FL: excitation wavelength (Ex)= 290 nm; emission (Em) response: 315 nm, 360 and 400 nm.
	Sample volume injection
	1 µL
	Column temperature
UPLC-MS/MS	Analytical column
	BEH C18, 2.1 mm x 50 mm, 1.7 µm particle size.
	Mobile phase
	A: water acidified with formic acid (1% v/v), B: methanol.
	Mobile phase elution
	Gradient.
	0-2 min: 5% B; 6min: 15% B; 10-13 min: 100% B; 13.10-15 min: 5% B.
	Gradient program
UPLC-MS/MS	Flow rate
	0.8 mL min ⁻¹
	DAD: λ= 254, 280, 320 and 370 nm
	Detection
	FL: excitation wavelength (Ex)= 290 nm; emission (Em) response: 315 nm, 360 and 400 nm.
	Sample volume injection
	10 µL
	Column temperature
	35 °C

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