

Table S1. Chromatographic profiles used in the HPLC/FT-HRMS FS and SIM mode analyses.

Mode	Step	Time (min)	% CH ₃ CN (0.1% formic acid)	% H ₂ O (0.1% formic acid)
FS ^a	1	0	30	70
	2	5	80	20
	3	7	95	5
	4	12	95	5
	5	13	30	70
	6	16	30	70
	7	18	90	10
SIM ^b	1	0	0	100
	2	1	0	100
	3	1.5	50	50
	4	5.5	90	10
	5	8	99	1
	6	13	99	1
	7	13.2	0	100
	8	18	0	100

^aFlow rate of 80 μ L/min.^bFlow rate of 350 μ L/min.