

Supplemental Information:

Main ion trap instrumental conditions for the analysis of proline derivatives by ESI-MS/MS in positive ionization mode.

Compound	Cut-off mass	Ion trap conditions		
		Amplitude (volt)	Scan range	Scan speed (m/z/s)
Pro ^a	50	0.9	65-120	1650
HyPro ^b	50	0.9	65-135	1650
NmePro ^c	70	1.30	50-135	1650
ProBet ^d	50	0.9	80-150	1650
HypBet ^e	50	1.10	80-165	1650

^a Pro: L-proline. ^b HyPro: 4-hydroxy-L-proline. ^c NmePro: *N*-methyl-L-proline. ^d ProBet: *N,N*-dimethylproline. ^e HypBet: 4-hydroxy-L-prolinebetaine