Article

Dilute-and-shoot-liquid chromatography-quadrupole time of flight-mass spectrometry for pteridine profiling in human urine and its association with different pathologies

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Supplementary material

Table S1. Calibration lines data obtained in the presence and absence of matrix

Compound	Aqueous		Urine			Matrix effect
	Slope ± SD, (mL ng^{-1})	R^2	Slope ± SD, (mL ng^{-1})	R^2	S$_{y/x}$[a]	MF (RSD)[b]
7,8-DHNEO	0.097 ± 0.003	0.996	0.021 ± 0.003	0.992	0.046	0.25 (4.2)
MON	0.051 ± 0.002	0.995	0.016 ± 0.0006	0.994	0.078	0.30 (5.6)
NEO	0.035 ± 0.0008	0.997	0.023 ± 0.0002	0.997	0.028	0.69 (4.8)
6,7-DMPT	0.013 ± 0.0004	0.996	0.0035 ± 0.0003	0.990	0.004	0.28 (3.3)
7,8-DHBIO	0.028 ± 0.001	0.993	0.0042 ± 0.0006	0.992	0.005	0.12 (3.8)
6-BIO	0.033 ± 0.0005	0.993	0.018 ± 0.0003	0.998	0.042	0.54 (5.9)
LEU	0.051 ± 0.0005	0.999	0.0098 ± 0.0003	0.992	0.046	0.17 (3.7)
PT	0.14 ± 0.001	0.999	0.047 ± 0.001	0.996	0.160	0.31 (6.2)
6-OHMPT	0.037 ± 0.001	0.995	0.0096 ± 0.0003	0.992	0.044	0.30 (5.7)
7,8-DHXAN	0.0035 ± 0.0001	0.995	0.0006 ± 0.00009	0.994	0.002	0.15 (4.2)
LU	0.016 ± 0.0002	0.998	0.0012 ± 0.00005	0.996	0.007	0.09 (4.4)
6-HLU	0.0034 ± 0.0001	0.994	0.0005 ± 0.00005	0.998	0.001	0.13 (5.1)
7-HLU	0.015 ± 0.0002	0.998	0.0024 ± 0.00008	0.992	0.012	0.14 (4.6)

[a] S$_{y/x}$ is the standard error of estimate of the regression line.

[b] RSD obtained from the comparison of aqueous slopes with those obtained for urine samples

Table S2. Mean concentration values found for each QC level with their 95% confidence intervals

Compound	QC$_1$	QC$_2$	QC$_3$
7,8-DHNEO	46.7 ± 2.53	309 ± 14.3	586 ± 23.7
MON	47.9 ± 3.04	282 ± 15.4	622 ± 25.3
NEO	44.2 ± 3.34	305 ± 14.0	606 ± 24.3
6,7-DMPT	45.2 ± 3.26	302 ± 15.6	603 ± 26.4
7,8-DHBIO	44.7 ± 4.22	303 ± 20.9	604 ± 29.1
6-BIO	43.4 ± 3.50	309 ± 18.2	590 ± 27.5
LEU	43.3 ± 3.33	291 ± 18.8	615 ± 28.1
PT	49.7 ± 3.78	264 ± 16.9	552 ± 25.6
6-OHMPT	46.6 ± 4.01	291 ± 17.4	613 ± 25.1
7,8-DHXAN	44.9 ± 4.12	301 ± 16.6	599 ± 23.7
LU	44.6 ± 3.87	303 ± 18.0	595 ± 25.2
6-HLU	44.9 ± 4.07	300 ± 18.8	600 ± 29.0
7-HLU	44.4 ± 3.52	306 ± 17.7	593 ± 26.9

QC$_1$= 45 ng mL^{-1}, QC$_2$= 300 ng mL^{-1} and QC$_3$= 600 ng mL^{-1}