

Supplementary Materials

Two-Step Derivatization of Amino Acids for Stable-Isotope Dilution GC-MS Analysis: Long-Term Stability of Methyl Ester-Pentafluoropropionic Derivatives in Toluene Extracts

Svetlana Baskal, Alexander Bollenbach and Dimitrios Tsikas *

Institute of Toxicology, Core Unit Proteomics, Hannover Medical School;
baskal.svetlana@mh-hannover.de (S.B.); bollenbach.alex@gmail.com (A.B.)

* Correspondence: Tsikas.dimitros@mh-hannover.de

Table S1. Mean peak area ratio (coefficient of variation, CV) of endogenous amino acids in the seven human urine samples to the respective internal standard as measured by GC-MS analysis of 1- μ L aliquots of the toluene extracts stored and room temperature for several days.

Amino acid	Mean peak area ratio (CV, %)						
Urine No.	#29	#364	#367	#377	#382	#388	#390
Ala	0.306 (6.3)	1.10 (2.4)	0.14 (4.3)	0.45 (1.2)	0.28 (1.8)	0.407 (3.2)	0.242 (4.9)
Thr	0.692 (9.3)	0.884 (7.5)	0.292 (4.1)	0.727 (7.3)	0.718 (6.2)	0.568 (6.0)	0.469 (5.4)
Gly	0.56 (4.9)	0.84 (0.48)	0.18 (4.1)	0.78 (0.6)	0.426 (3.5)	0.64 (2.9)	0.39 (2.6)
Val	0.846 (12.6)	1.523 (12.9)	0.601 (4.9)	0.888 (12.6)	0.695 (10.7)	0.903 (9.8)	0.746 (5.3)
Ser	0.804 (4.3)	1.17 (3.1)	0.301 (3.3)	0.851 (6.9)	0.768 (3.4)	0.852 (3.7)	0.499 (5.3)
Leu/Ile	0.380 (1.8)	1.169 (1.7)	0.392 (2.6)	0.622 (5.6)	0.530 (1.1)	0.516 (1.8)	0.371 (3.8)
Asn/Asp	1.619 (5.1)	3.594 (6.2)	1.311 (28.3)	3.202 (11.1)	2.373 (6.2)	2.585 (6.2)	1.936 (6.5)
Pro	0.047 (3.6)	0.105 (4.9)	0.085 (4.5)	0.073 (2.4)	0.096 (2.8)	0.076 (3.9)	0.077 (1.3)
Gln/Glu	2.434 (6.8)	5.248 (10.3)	1.881 (13.2)	3.782 (12.6)	2.486 (16.0)	3.512 (19.7)	2.331 (14.5)
Met	1.881 (9.4)	2.053 (14.5)	1.255 (8.7)	2.005 (10.2)	1.445 (13.6)	1.800 (15.8)	1.486 (12.5)
Orn/Cit	0.858 (1.5)	1.791 (2.0)	0.555 (2.1)	1.288 (4.5)	1.038 (2.0)	1.049 (1.0)	1.104 (1.3)
Phe	0.317 (1.1)	0.861 (6.1)	0.159 (5.6)	0.354 (12.1)	0.262 (5.8)	0.304 (2.5)	0.225 (7.3)
Tyr	0.766 (1.6)	1.619 (1.5)	0.390 (1.5)	0.804 (3.3)	0.843 (0.7)	0.738 (2.7)	0.524 (1.0)
Lys	0.499 (2.49)	2.034 (0.9)	0.314 (3.8)	0.943 (3.8)	0.639 (3.8)	0.872 (3.2)	0.533 (3.0)
Arg	0.263 (1.0)	0.934 (1.3)	0.418 (1.9)	0.316 (1.6)	0.477 (0.9)	0.315 (1.3)	0.321 (1.9)
hArg	0.100 (5.1)	0.408 (7.6)	0.055 (6.5)	0.068 (7.9)	0.151 (9.1)	0.120 (5.3)	0.049 (6.9)
Trp	0.306 (6.3)	1.102 (2.4)	0.141 (4.3)	0.454 (1.2)	0.277 (1.8)	0.407 (3.2)	0.242 (4.9)

Figure S1. Plots of the peak area of urinary amino acids (upper panel), of the peak area of their internal standards (middle panel), and of the peak area ratio of the amino acids to their internal standards (lower panel) in seven 24-h collected urine samples against the storage time of the toluene extracts (day 1, 2, 8, 15). Note the decadic logarithm scale on the y axes in the left and middle panels.













