Electronic Supplementary Material (ESI) for Analyst.

Supplementary information

Baseline separation of amino acid biomarkers of hepatocellular carcinoma by polyvinylpyrrolidone-filled capillary electrophoresis with light-emitting doide-induced fluorescence in the presence of mixed micelles

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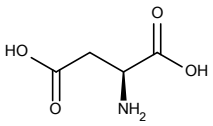
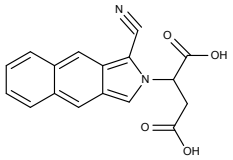
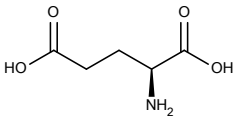
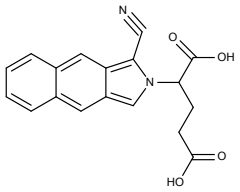
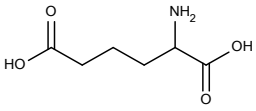
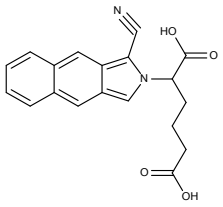
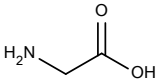
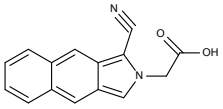
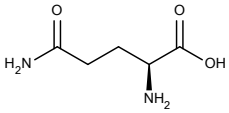
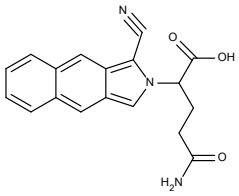
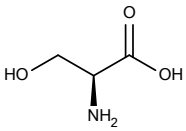
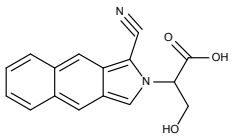
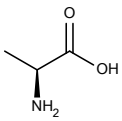
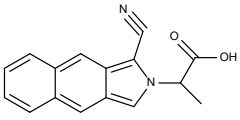
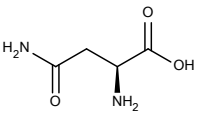
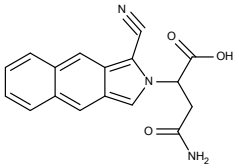
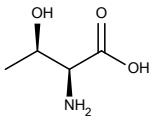
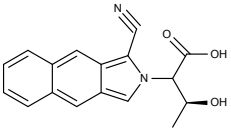
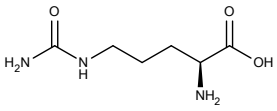
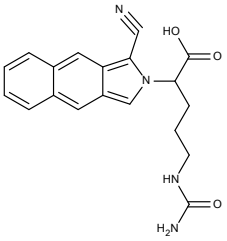
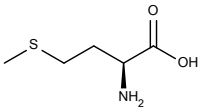
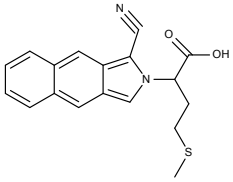
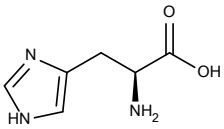
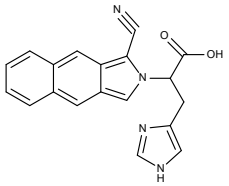
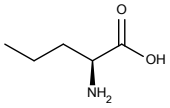
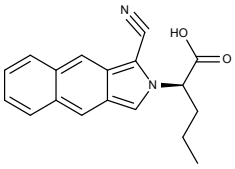
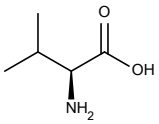
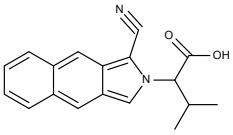
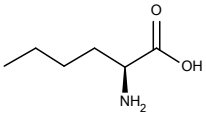
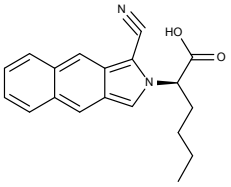
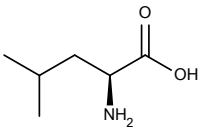
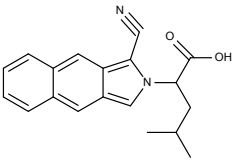
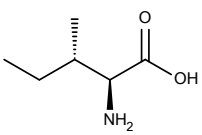
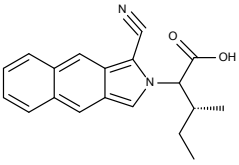
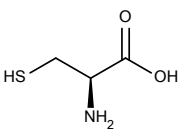
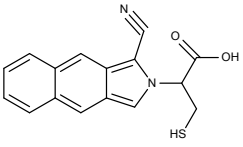
Table S1. The structure, Mw, logP and net charge of AAs and AA derivatives.

Name	Structure of AA	logP	Net charge at pH 7.0	Structure of AA-CBIs	Mw	logP	Net charge at pH 7.0
Aspartic acid		-1.22	-0.990		309	2.44	-1.998
Glutamic acid		-0.93	-1.002		322	2.73	-2.000
α-Aminoadipic acid (I.S.)		-0.49	-1.002		336	3.17	-1.999
Glycine		-1.15	-0.006		250	2.51	-1.000
Glutamine		-1.74	-0.005		321	1.92	-1.000
Serine		-1.63	-0.012		280	2.03	-1.000
Alanine		-0.58	-0.003		264	3.08	-1.000
Asparagine		-2.03	-0.036		308	1.63	-1.000
Threonine		-1.21	-0.010		294	2.45	-1.000

Citrulline		-1.67	-0.006		350	1.99	-1.000
Methionine		0.07	-0.003		324	3.73	-1.000
Histidine		-1.01	0.115		330	2.65	-0.740
Norvaline		0.39	-0.003		292	4.05	-1.000
Valine		0.31	-0.002		292	3.97	-1.000
Norleucine		0.83	-0.003		306	4.49	-1.000
Leucine		0.68	-0.003		306	4.33	-1.000
Isoleucine		0.75	-0.002		306	4.41	-1.000
Cysteine		-0.53	-0.010		296	3.31	-1.001

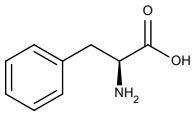
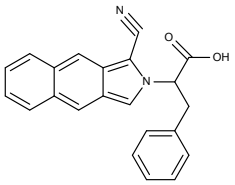
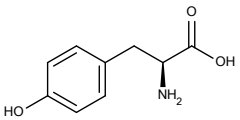
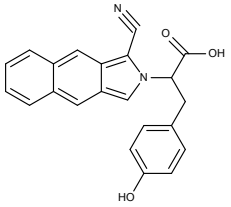
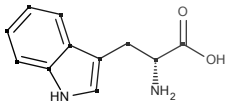
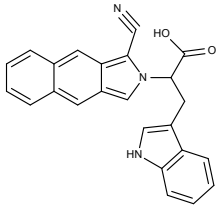
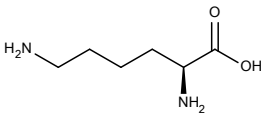
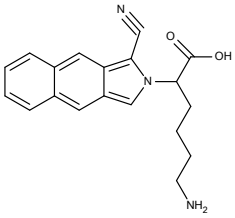
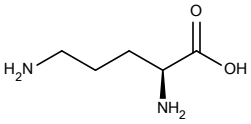
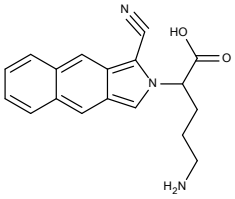
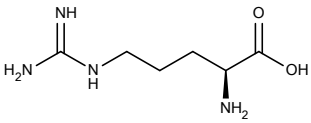
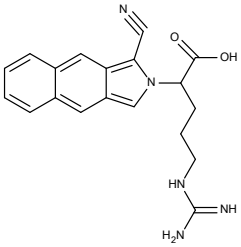
Phenylalanine		1.08	-0.004		340	4.73	-1.000
Tyrosine		0.77	-0.010		356	4.43	-1.003
Tryptophan		1.18	-0.004		377	4.83	-1.000
Lysine		-0.71	0.996		322	2.95	-0.001 (-0.111 at pH 9.3)
Ornithine		-1.16	0.996		307	2.50	-0.001 (-0.111 at pH 9.3)
Arginine		-1.49	0.996		350	2.17	0.000 (-0.002 at pH 9.3)

Figure S1. The hydrogen bonding formation between PVP and the aromatic AAs (Trp and Tyr).

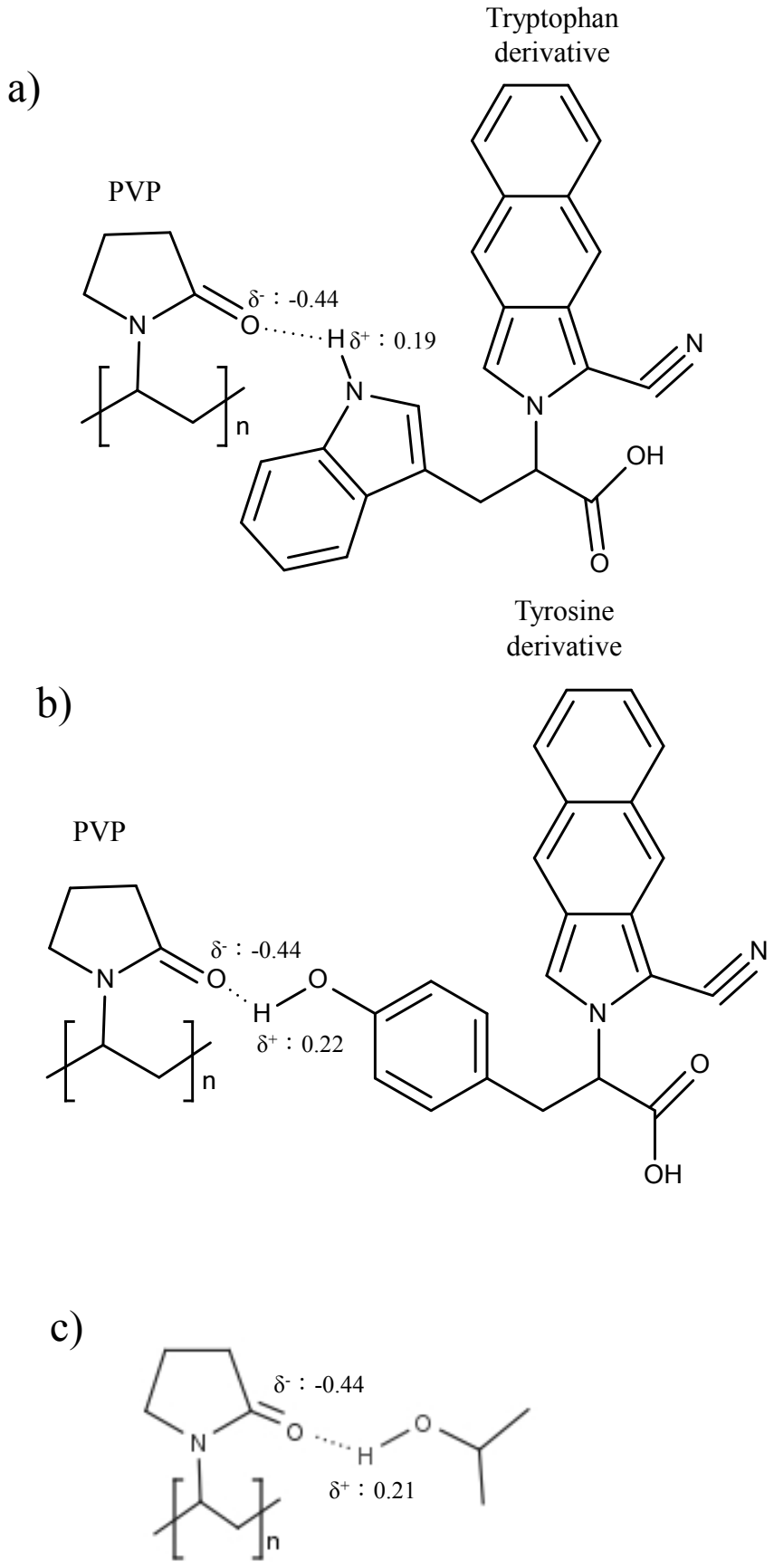


Figure S2. The impact of SDS on the separation of AA-CBIs by PVP in the absence of IP. The separations were completed using a) 5% PVP containing b) 10 mM, c) 20 mM and d) 30 mM SDS.

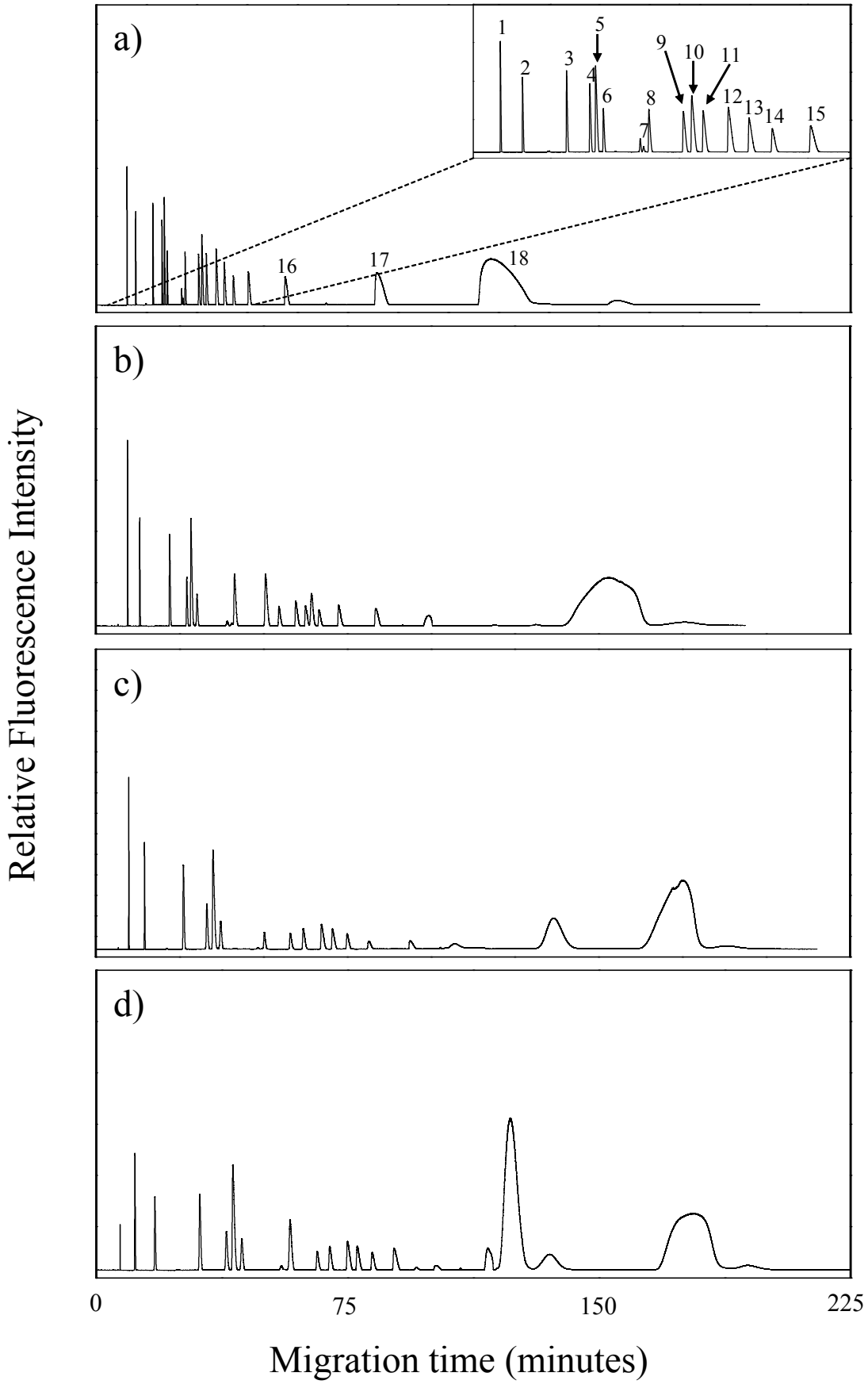


Figure S3. The matrix effect of the plasma on the derivatization and electrophoretic separation. The samples of a) untreated plasma, b) protein-removed plasma and c) ten-fold dilution of protein-removed plasma were utilized in the NDA derivatization.

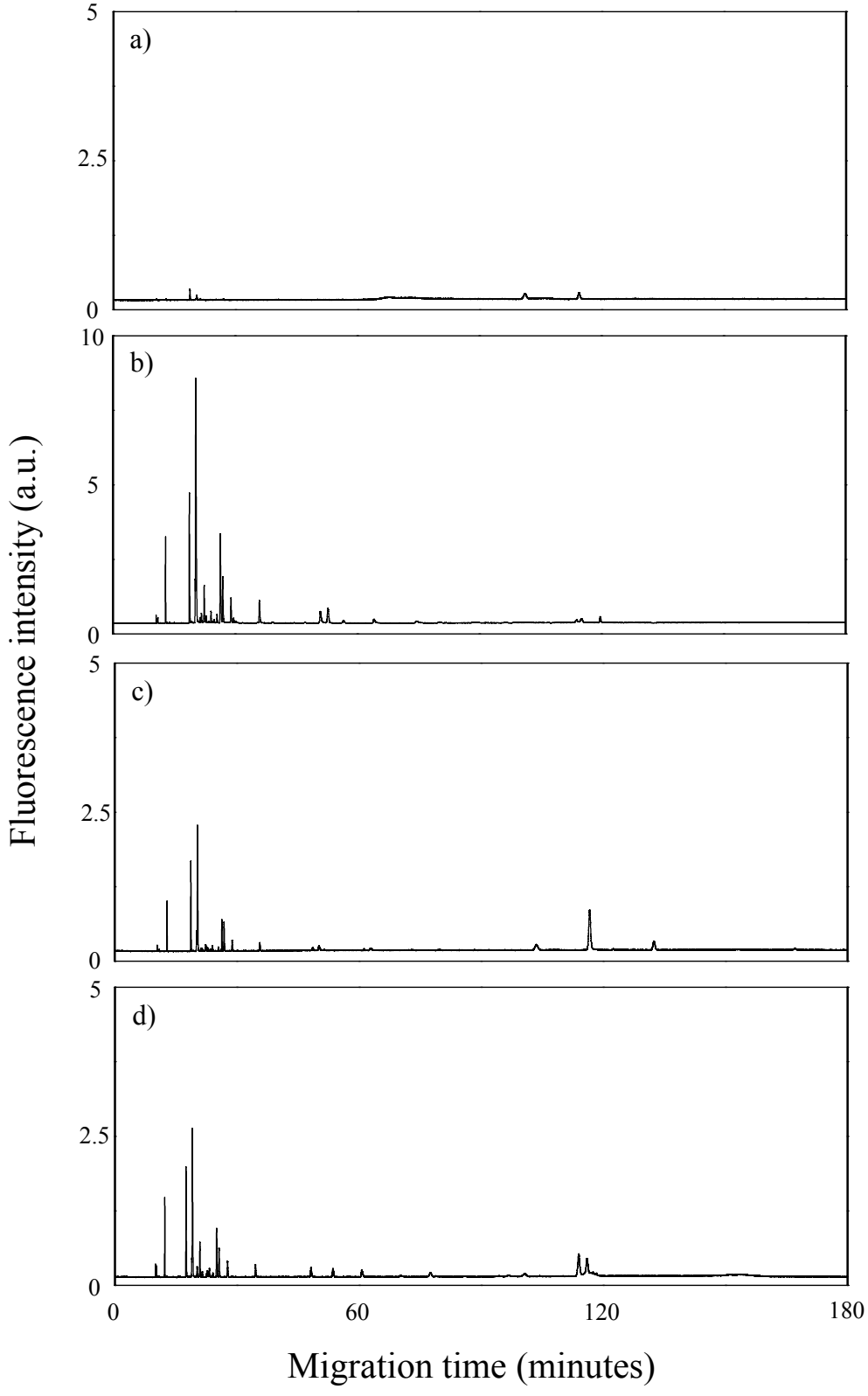


Figure S4. The stability of AA-CBIs of NDA. An AA-CBI sample was utilized to establish the stability of AA-CBIs of NDA by allowing the sample to stand at -20ºC for a) 0, b) 4, c) 8 and d) 12 h after NDA derivatization.

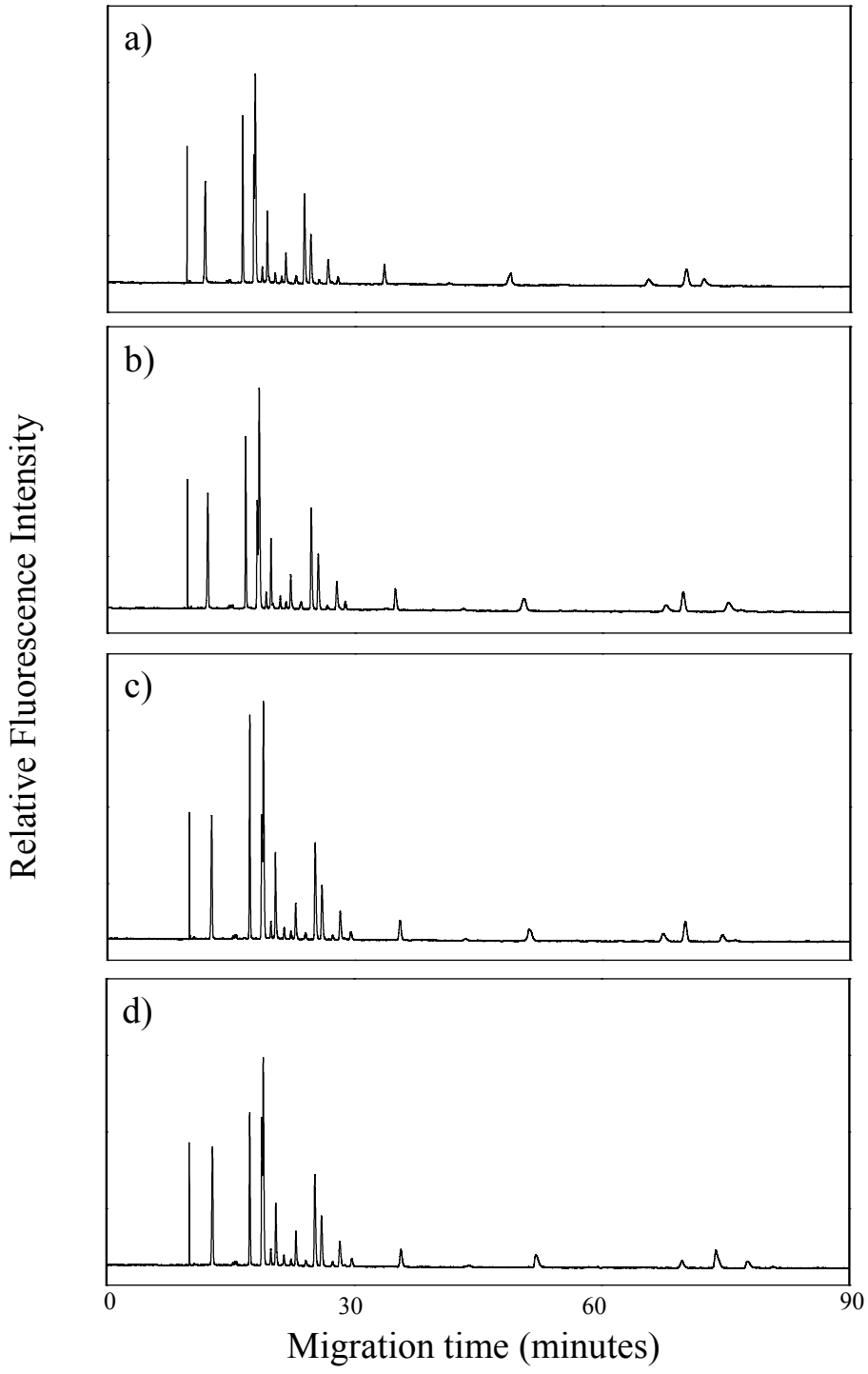


Figure S5. The reproducibility of AA derivatization by NDA and separation by PVP-filled capillary electrophoresis. The experiments were performed by five independent derivatizations of a standard AA mixture followed by electrophoretic separation using 5% PVP in the presence of IP (20%) and SDS (20 mM). α-Aminoadipic acid was spiked into the plasma as the internal standard.