

SUPPORTING INFORMATION

Analysis of neurochemicals by capillary electrophoresis in athlete's urine and a pilot study of their changes responding to sport fatigue

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Figure Captions

Fig. S1. Electropherograms of 11 mixtures at different BGE pH .

Fig. S2. Electropherograms of 11 mixtures at different separation voltage.

Fig. S3. Electropherograms of 11 mixtures at different injection time.

Table Legend

Table. S1. Representative neurochemicals and their physicochemical characteristics

Table. S2. Comparison of this method with the reported methods for determination of the target neurochemicals in urine samples.

Table. S3. Under the different physiological conditions, changes in the content of six neurochemicals

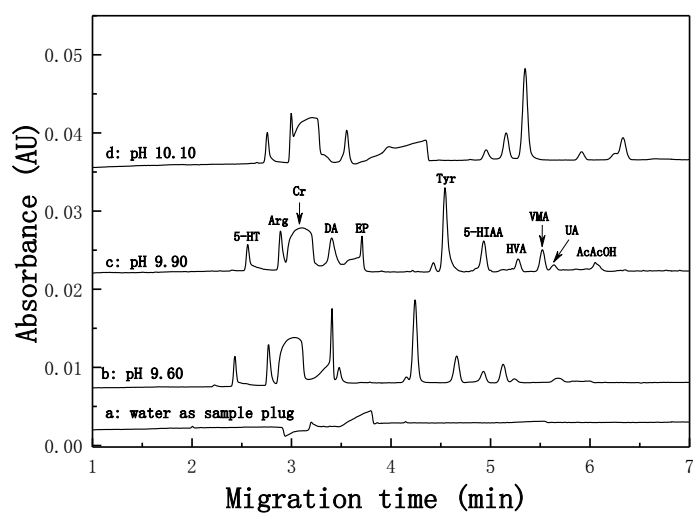


Fig. S1. Electropherograms of 11 mixtures at different BGE pH . BGE was 12.5 mmol/L $\text{Na}_2\text{B}_4\text{O}_7$, whose pH was adjusted by 0.1mo l /L NaOH. The concentrations of 5-HT, Arg, Cre, DA, EP, Tyr, 5-HIAA, HVA, VMA, UA, AcAcOH were at 10.0, 50.0, 120.0, 10.0, 5.0, 20.0, 8.0, 2.0, 5.0, 1.5, 100.0 $\mu\text{mol/ L}$, respectively. Detection wavelength: 200 nm. Injection: 0.5 psi at 20 s. Separation voltage: +25 kV.

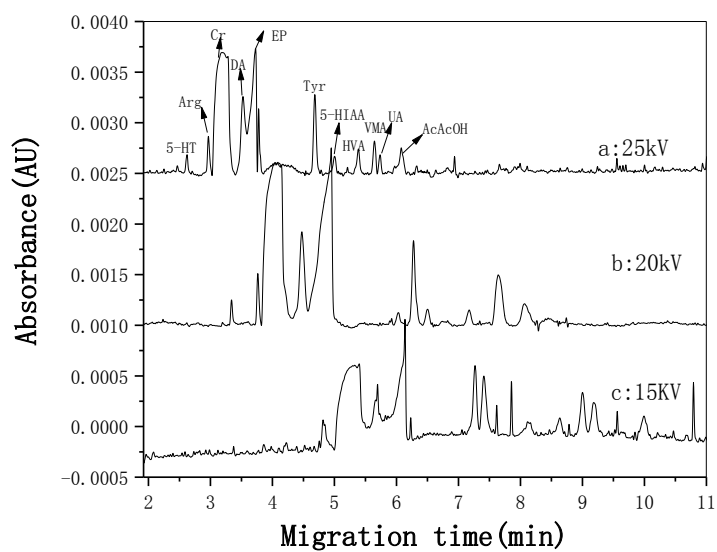


Fig. S2. Electropherograms of 11 mixtures at different separation voltage. BGE was 12.5 mmol / L $\text{Na}_2\text{B}_4\text{O}_7$, pH : 9.90. (a) 25 kV, (b) 20 kV, (c) 15 kV. The concentrations of 5-HT, Arg, Cre, DA, EP, Tyr, 5-HIAA, HVA, VMA, UA, AcAcOH were at 0.8, 4.0, 75.0, 2.7,1.2, 1.6, 0.6, 0.16, 0.4, 0.64, 1.6 $\mu\text{mol}/\text{L}$, respectively. Detection wavelength: 200 nm. Injection: 0.5 psi at 20 s. Separation voltage: +25 kV.

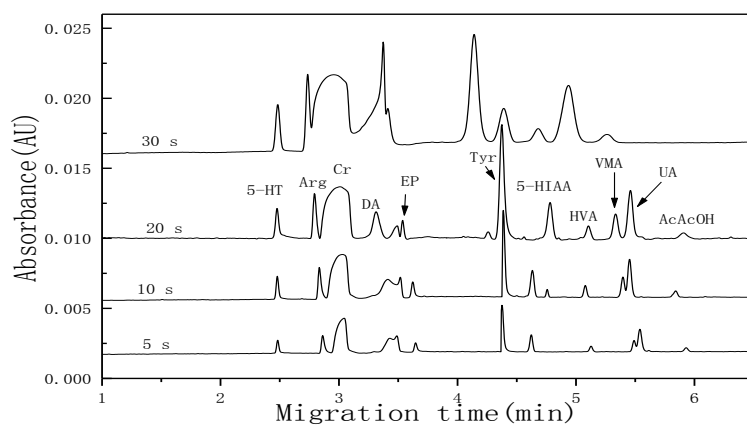


Fig.S3 Electropherograms of 11 mixtures at different injection time. Injection: 0.5 psi from 5 s to 30s. BGE was 12.5 mmol/L $\text{Na}_2\text{B}_4\text{O}_7$, pH = 9.9. The concentrations of 5-HT, Arg, Cre, DA, EP, Tyr, 5-HIAA, HVA, VMA, UA, AcAcOH were at 10.0, 50.0, 120.0, 10.0, 5.0, 20.0, 8.0, 2.0, 5.0, 1.5, 100.0 $\mu\text{mol/L}$. respectively. Other conditions are were as described in optimization of CE conditions.

Table. S1. Representative neurochemicals and their physicochemical characteristics

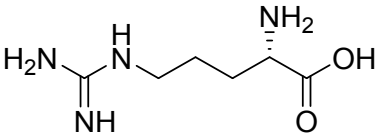
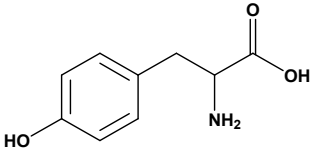
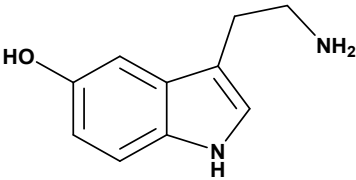
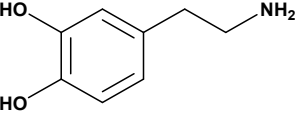
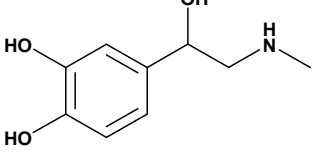
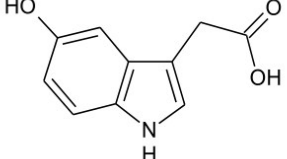
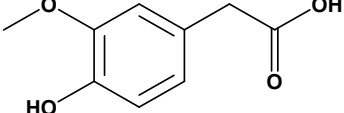
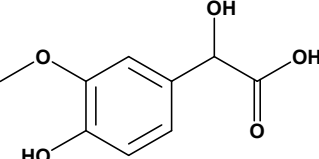
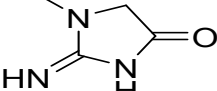
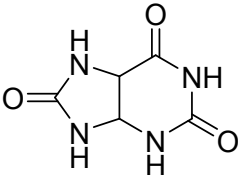
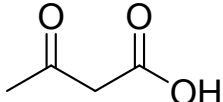
Neurochemicals	Structures	Molar mass (g/mol)	pK a*
Arginine (Arg)		174.2	2.17;9.04;12.5
Tyrosine (Tyr)		181.19	5.65
Serotonin (5-HT)		212.68	9.8;11.1
Dopamine (DA)		153.18	8.9;10.6;13.1
Epinephrine (EP)		183.2	8.66;9.95
5-hydroxy-3-indoleacetic acid (5-HIAA)		191.18	ND*
Homovanillic acid (HVA)		182.17	4.41;10.52
vanilla mandelic acid (VMA)		198.17	3.41
Creatinine(Cre)		113.12	4.84;9.20

Table. S1. Representative neurochemicals and their physicochemical characteristics

Neurochemicals	Structures	Molar mass (g /mol)	pK a*
Uric acid(UA)		168.11	3.89;5.75;10.3
Acetoacetic acid(AcAcOH)		118.09	3.58

pKa* values obtained from chemicalize.com; ND* = Not defined

Table S2**Comparison of this method with the reported methods for determination of the target neurochemicals in urine samples.**

Analytical methods	Analytes	LODs (ng/mL)	Refs.
GC-MS/MS	Tyr, Trp, Glu	0.02 ~ 11.10	[31]
GC-MS	DOPAC, VMA, DOMA	0.02 ~ 4.7	[32]
GC-MS/MS-MRM	HVA, MHPG, DOPAC, VMA, 5-HIAA, DA	0.17 ~ 0.60	[33]
GC-MS	HVA, DOPAC, DA, VMA, NMN, NEP, EP, L-DOPA,	0.05 ~ 6.24	[34]
CE-UV	HA, Cad, PEA, TA Try, DA, 5-HT	61-411	[38]
CE-LINF	TA, 5-HT, DA, E, VMA, 5-HIAA	2.33×10^{-3} -3.92	[39]
tITP-CZE	DA, TA, Try, 5-HT	4.41-11.48	[40]
MEKC-LIF	Cad, His, Spd, Tyr	111.15-1741	[44]
MEKC-LIF	1,6-Diaminohexane, 2- phenylethylamine, Cad, His, Put, Spd, Spm, TA, Tyr	0.0735-48.57	[46]

CZE-LIF	5-HT, DA, DOPA, E, NE	0.0918-0.2693	[47]
CE-UV	TA, 5-HT , 3-MT HMBA , NMN, DA	4.307-31.248	[48]
	Trp, 5-HIAA, VMA		
	5-HT, Arg, Cre	0.504-169.68	
CE-UV	DA, EP, Tyr 5-HIAA,HVA,VMA UA, AcAcOH		In this work

Table. S3. Under the different physiological conditions, changes in the content of six neurochemicals

Volunteer information		Biomarker compounds						
(age(Y, year), mental physiology , RPE value)		Arg ($\mu\text{mol/L}$)	DA ($\mu\text{mol/L}$)	Cre (mmol/L)	HVA ($\mu\text{mol/L}$)	VMA ($\mu\text{mol/L}$)	UA (mmol/L)	
NO.1	normal	6	477.2	27.35	8.84	72.75	95.65	0.44
	fatigue	18	281.2	NF	8.41	74.60	58.30	0.39
	relaxed	14	423.0	25.35	10.76	51.60	84.85	0.39
NO.2	normal	11	285.4	15.65	7.43	51.10	37.80	0.55
	fatigue	19	210.2	14.25	7.83	55.05	49.90	0.67
	relaxed	10	277.5	23.55	8.48	64.40	78.05	0.52
NO.3	normal	13	294.0	20.85	12.36	48.60	95.05	1.02
	fatigue	18	111.2	17.30	5.04	65.30	144.7	0.59
	relaxed	15	247.0	13.35	11.89	39.10	98.60	0.34
NO.4	normal	12	208.6	18.00	9.74	29.15	67.90	1.01
	fatigue	18	109.7	13.75	6.77	31.95	56.55	0.61
	relaxed	17	105.8	13.55	6.68	NF	56.15	0.72
NO.5	normal	7	124.4	16.40	9.68	27.60	73.95	1.00
	fatigue	14	111.2	19.70	7.61	28.40	74.20	0.36
	relaxed	9	174.6	22.35	7.04	30.70	69.95	0.59