

## Supplement of:

### A six-metabolite panel as potential blood-based biomarkers for Parkinson's disease.

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**Supplementary Table 1.** Mean metabolite concentrations (pmol\* $\mu\text{L}^{-1}$ ) with standard deviations (SD) and results of pairwise comparison prior and after the adjustment for age and sex. Additional data to

Table 1.

Metabolite	Mean (SD); in picomoles/ $\mu\text{L}$				Unadjusted for confounders p-values			Adjusted for confounders p-values
	CN (n = 93)	naive-iPD (n = 7)	iPD (n = 103)	AD (n = 28)	naive-iPD vs iPD	naive-iPD vs CN	iPD vs AD	iPD vs AD
2-Ambut	22.03 (6.72)	24.34 (9.77)	20.7 (5.33)	20.49 (8.59)	0.37	0.51	0.38	0.27
3-AA	0.04 (0.01)	0.03 (0.01)	0.04 (0.02)	0.03 (0.01)	0.55	0.32	<b>6.20E-05</b>	0.002
3-HK	0.04 (0.02)	0.05 (0.06)	0.05 (0.04)	0.03 (0.01)	0.22	0.98	<b>0</b>	<b>1.05E-03</b>
4-OH-Pro	11.37 (5.01)	13.97 (6.83)	12.16 (4.94)	12.41 (5.35)	0.48	0.28	0.93	0.51
Ala	414.07 (81.01)	438.91 (119.44)	432.91 (90.87)	407.2 (80.2)	0.96	0.67	0.18	0.02
Arg	81.5 (20.04)	76.93 (24.66)	73.81 (15.54)	85.11 (19.45)	0.97	0.56	0.02	0.27
Asn	41.65 (6.23)	42.59 (7.95)	42.59 (6.61)	38.65 (4.35)	0.91	0.81	<b>4.46E-04</b>	0.01
Asp	9.69 (5.32)	10.81 (5.71)	12.57 (4.99)	9.83 (3.82)	0.42	0.96	0.02	0.002
$\beta$ -ala	4.52 (1.59)	4.69 (1.96)	5.19 (1.64)	4.41 (1.8)	0.41	0.85	0.02	0.01
Cad	0.2 (0.09)	0.13 (0.07)	0.17 (0.08)	0.22 (0.1)	0.25	0.04	0.002	0.01
Citrulline	34.61 (8.12)	32.03 (7.7)	33.06 (7.22)	37.06 (9.57)	0.67	0.41	0.10	0.81
Cys	177.14 (28.59)	160.55 (29.36)	157.78 (27.56)	191.13 (22.99)	0.84	0.23	<b>0</b>	<b>9.83E-04</b>
GABA	0.32 (0.17)	0.34 (0.19)	0.31 (0.17)	0.35 (0.16)	0.56	0.75	0.11	0.94
Gln	710.1 (81.81)	729.43 (140.56)	690.75 (80.77)	711.35 (65.59)	0.58	0.81	0.17	0.19
Glu	45.94 (20.46)	52.99 (13.61)	54.88 (20.47)	38.74 (15.61)	0.91	0.12	<b>7.40E-05</b>	<b>1.76E-04</b>
Gly	274.57 (67.96)	268.57 (63.31)	298.52 (86.63)	294.61 (61.72)	0.38	0.84	0.49	0.69
His	70.47 (12.75)	75.28 (8.27)	70.58 (11.31)	69.25 (11.27)	0.10	0.10	0.60	0.87
Homoserine	0.37 (0.14)	0.42 (0.11)	0.43 (0.13)	0.42 (0.15)	0.90	0.12	0.50	0.32
Ile	78.89 (14.87)	81.76 (11.6)	83.54 (17.3)	74.58 (19.6)	0.72	0.64	0.01	0.05
L-KYN	3.02 (0.78)	2.45 (0.7)	2.59 (0.7)	2.69 (0.94)	0.58	0.09	0.83	0.64
Leu	156.23 (28.16)	167.94 (29.47)	165.33 (34.58)	139.5 (25.99)	0.31	0.18	<b>1.76E-04</b>	0.01
Lys	229.23 (33.62)	219.13 (10.11)	222.4 (36.23)	214.97 (35.57)	0.72	0.15	0.26	0.05
Met	29.94 (4.36)	30.21 (3.13)	30.62 (5.23)	27.73 (4.29)	0.75	0.83	0.005	0.04
N-acetyl-phenylalanine	0.03 (0.01)	0.02 (0)	0.03 (0.01)	0.02 (0.01)	0.75	0.71	<b>2.30E-05</b>	0.0016
Orn	63.82 (16.44)	66.93 (26.17)	74.95 (16.14)	61.41 (12.1)	0.32	0.88	<b>7.30E-05</b>	<b>3.03E-04</b>
Phe	79.92 (9.29)	80.7 (10.2)	83.44 (11.08)	75.63 (8.83)	0.48	0.85	<b>1.75E-04</b>	0.002
Pro	228.05 (54.83)	274.65 (98.72)	246.8 (76.35)	259.25 (83.25)	0.43	0.22	0.49	0.42
Put	0.28 (0.15)	0.23 (0.07)	0.24 (0.18)	0.29 (0.15)	0.42	0.44	0.02	0.06
Sarco	1.8 (0.63)	2.08 (0.89)	1.83 (0.61)	1.7 (0.66)	0.60	0.59	0.23	0.52
Ser	89.3 (17.26)	86.46 (16.05)	92.55 (18.43)	91.36 (16.96)	0.96	0.70	0.69	0.61
Serotonin	0.39 (0.22)	0.34 (0.21)	0.43 (0.32)	0.33 (0.24)	0.72	0.62	0.14	0.22
Tau	111.79 (31.34)	124.97 (35.26)	124.91 (32.11)	121.06 (28.68)	0.80	0.49	0.32	0.09
Thr	125.32 (23.7)	122.05 (20.64)	137.59 (31.11)	122.77 (26.25)	0.15	0.77	0.02	0.06
Trp	75.04 (13.19)	78.18 (10.4)	74.46 (12.72)	65.49 (12.27)	0.19	0.20	0.002	0.07
Tryptamine	0.02 (0.01)	0.02 (0.01)	0.02 (0.01)	0.02 (0.01)	0.92	0.91	0.01	0.02
Tyr	86.02 (14.66)	88.82 (7.86)	102.73 (25.51)	78.74 (15.1)	0.01	0.28	<b>0</b>	<b>8.40E-05</b>
Val	276.45 (47.38)	292.45 (31.63)	283.03 (53.43)	248.16 (46.45)	0.20	0.13	<b>1.40E-03</b>	0.02

**Supplementary Table 2. Age and gender effects of tested cohort.** Possible effects were tested via Pearson's correlation and Independent Samples t-test. Interactions between disease state (CN vs iPD participants) and age/gender were tested for each metabolite/amino acid via Generalized Linear Modelling (GLM) to determine whether either confounder had a significant effect on metabolite via disease state.

Metabolite	Mean (SD)	Mean (SD)	T-test	Pearson's R correlation coefficient with age	p-value	Interaction CN/iPD*Age	Interaction CN/iPD*Sex
	Males	Females	p-value			p-value	p-value
Ala	6.03 (0.21)	6.02 (0.19)	0.683	0.029	0.664	0.181	0.266
2-Ambut	3.02 (0.28)	3 (0.3)	0.600	-0.044	0.507	0.005	0.444
Arg	4.32 (0.23)	4.36 (0.22)	0.225	0.253	<0.001	0.675	0.417
Asn	3.75 (0.13)	3.68 (0.14)	<0.001	-0.094	0.155	0.463	0.022
Asp	2.22 (0.57)	2.36 (0.46)	0.034	-0.120	0.069	0.449	0.715
β-ala	1.59 (0.3)	1.4 (0.36)	<0.001	0.043	0.518	0.095	0.006
Cad	-1.78 (0.45)	-1.78 (0.51)	0.977	0.221	<0.001	0.272	0.576
Citrulline	3.5 (0.22)	3.52 (0.23)	0.473	0.319	<0.001	0.799	0.969
Cys	5.1 (0.19)	5.14 (0.18)	0.145	0.500	<0.001	0.158	0.915
GABA	-1.31 (0.57)	-1.23 (0.57)	0.329	0.186	0.005	0.619	0.754
Gln	6.56 (0.11)	6.53 (0.11)	0.018	0.084	0.202	0.483	0.076
Glu	3.85 (0.42)	3.77 (0.41)	0.178	-0.120	0.070	0.045	0.960
Gly	5.59 (0.2)	5.68 (0.29)	0.010	0.049	0.460	0.659	0.255
His	4.27 (0.15)	4.21 (0.18)	0.009	-0.095	0.151	0.477	0.012
Homoserine	-0.96 (0.37)	-1.01 (0.4)	0.414	-0.037	0.578	0.291	0.684
3-AA	-3.27 (0.43)	-3.49 (0.44)	<0.001	-0.130	0.048	0.438	0.396
4-OH-Pro	2.47 (0.39)	2.3 (0.39)	<0.001	0.072	0.276	0.037	0.203
3-HK	-3.36 (0.54)	-3.46 (0.57)	0.184	-0.116	0.080	0.078	0.659
Ile	4.43 (0.2)	4.29 (0.19)	<0.001	-0.115	0.080	0.964	0.239
Kyn	1 (0.27)	0.97 (0.28)	0.426	0.306	<0.001	0.060	0.124
Leu	5.11 (0.19)	4.97 (0.17)	<0.001	-0.256	<0.001	0.335	0.082
Lys	5.4 (0.15)	5.4 (0.16)	0.841	0.053	0.419	0.197	0.018
Met	3.43 (0.15)	3.33 (0.15)	<0.001	-0.133	0.043	0.639	0.023
N-Acetyl-phenylalanine	-3.65 (0.45)	-3.83 (0.45)	0.003	-0.101	0.126	0.562	0.700
Orn	4.22 (0.25)	4.17 (0.26)	0.208	-0.039	0.554	0.354	0.069
Phe	4.41 (0.12)	4.36 (0.13)	0.002	-0.201	0.002	0.873	0.072
Pro	5.5 (0.27)	5.38 (0.25)	<0.001	-0.023	0.732	0.062	0.290
Put	-1.49 (0.61)	-1.5 (0.71)	0.952	0.097	0.143	0.541	0.172
Sarco	0.6 (0.3)	0.44 (0.33)	<0.001	-0.131	0.047	0.150	0.947
Ser	4.5 (0.19)	4.49 (0.22)	0.860	-0.004	0.952	0.406	0.244
Serotonin	-1.13 (0.82)	-1.35 (1.12)	0.108	0.012	0.852	0.525	0.747
Tau	4.72 (0.28)	4.81 (0.23)	0.006	-0.110	0.097	0.418	0.951
Thr	4.88 (0.2)	4.81 (0.23)	0.025	-0.082	0.217	0.379	0.160
Trp	4.33 (0.17)	4.22 (0.19)	<0.001	-0.164	0.013	0.776	0.296
Typtamine	-3.86 (0.45)	-4.06 (0.49)	0.002	-0.044	0.508	0.535	0.315
Tyr	4.53 (0.22)	4.47 (0.22)	0.037	-0.112	0.088	0.030	0.231
Val	5.65 (0.18)	5.56 (0.18)	<0.001	-0.197	0.003	0.163	0.757

**Supplementary Table 3. Mean ratios/interaction levels between CN and iPD groups.** To assess the interrelationships between metabolites, all possible metabolite ratios and interactions were calculated for assessment between the CN and treated iPD groups.

Metabolite	N		Mean (SD)				unadjusted for confounders p-values		Adjusted for confounders p-values					
	CN	iPD	naive-iPD	iPD	AD	naive-iPD vs iPD	naive-iPD vs CN	iPD vs CN	iPD vs AD					
Homoserine*Orn	93	7	23.77 (11.96)	28.84 (15.45)	31.98 (11.89)	26.15 (11.49)	0.515	0.310	1.00E-06	0.262	3.17E-02	0.239	1.74E-02	
	93	7	297.95 (156.41)	336.65 (251.12)	398.66 (181.81)	259.8 (103.45)	0.324	0.845	7.00E-06	0.336	4.50E-05	0.783	8.30E-05	
	93	7	845.07 (479.13)	974.6 (531.85)	1278.56 (593.25)	772.85 (346.92)	0.295	0.770	1.00E-06	0.947	2.50E-05	1.90E-05	0.855	5.30E-05
Asp*Thr	93	7	4001.77 (2008.08)	4756.41 (1511.22)	5695.77 (2774.62)	3036.21 (1297.06)	0.430	0.109	1.00E-06	0.013	0.00E+00	2.10E-05	0.338	6.00E-06
	93	7	646.85 (407.25)	780.03 (542.86)	951.5 (464.85)	611.64 (277.79)	0.349	0.852	2.00E-06	0.626	5.10E-04	4.10E-05	0.799	1.80E-04
	93	7	3.42 (1.97)	4.82 (3.49)	5.03 (2.33)	4.12 (2.28)	0.558	0.434	0.00E+00	0.091	4.59E-02	4.30E-05	0.151	2.22E-02
Asp/L-KYN	93	7	3036.22 (1674.92)	3564.5 (1613.55)	4207.2 (2027.61)	2423.13 (1117.07)	0.463	0.277	3.00E-06	0.123	6.00E-06	4.90E-05	0.194	2.70E-05
	93	7	3.72 (2.8)	4.27 (2.24)	5.28 (2.56)	4.36 (2.89)	0.412	0.399	7.00E-06	0.137	8.83E-02	8.70E-05	0.239	1.10E-02
	93	7	17.14 (11.2)	21.68 (5.6)	23.5 (12.31)	16.13 (8.18)	0.923	0.010	8.00E-06	0.973	2.37E-03	1.03E-04	0.971	1.08E-03
Homoserine*Asp	93	7	45.39 (30.63)	57.03 (43.98)	66.15 (37.25)	40.47 (19.1)	0.406	0.848	1.20E-05	0.877	3.12E-04	1.15E-04	0.793	1.45E-04
	93	7	1.72 (1.09)	1.99 (1.01)	2.24 (1.09)	1.78 (0.85)	0.592	0.296	7.00E-05	0.520	4.29E-02	1.56E-04	0.300	9.20E-03
	93	7	217.91 (145.68)	253.6 (126.92)	292.63 (173.49)	159.33 (73.78)	0.590	0.324	4.50E-05	0.062	2.00E-06	1.67E-04	0.234	3.40E-05
Gln*β-ala	93	7	12.39 (15.1)	10.22 (7.07)	7.19 (4.72)	10.28 (5.39)	0.321	0.657	2.00E-06	0.734	1.27E-03	1.82E-04	0.884	9.75E-04
	93	7	0.06 (0.03)	0.07 (0.03)	0.08 (0.04)	0.05 (0.02)	0.361	0.589	1.00E-06	0.979	3.40E-05	2.59E-04	0.930	1.39E-04
	93	7	0.48 (0.28)	0.48 (0.3)	0.64 (0.32)	0.56 (0.29)	0.228	0.907	6.30E-05	0.070	2.32E-01	3.16E-04	0.182	1.16E-01
Asp/Z-Ambut	93	7	503 (480.26)	619.4 (398.59)	723.85 (477.04)	405.28 (280.77)	0.535	0.525	3.10E-05	0.684	3.46E-04	3.74E-04	0.611	1.21E-04
	93	7	0.04 (0.02)	0.05 (0.03)	0.06 (0.02)	0.05 (0.02)	0.447	0.780	3.40E-05	0.134	4.70E-02	5.19E-04	0.361	2.27E-02
	93	7	1258.72 (763.75)	1328.03 (714.45)	1725.4 (802.02)	1214.27 (599.01)	0.305	0.922	3.80E-05	0.605	2.78E-03	5.49E-04	0.714	1.46E-03
Asp*Thr	93	7	2.28 (1.29)	1.92 (1.18)	3.46 (2.14)	1.58 (0.69)	0.066	0.480	3.90E-05	0.005	0.00E+00	6.31E-04	0.017	4.29E-04
	93	7	111.76 (150.06)	103.34 (90.43)	70.03 (51.09)	85.93 (43.33)	0.442	0.787	8.50E-05	0.449	1.21E-02	7.27E-04	0.781	1.83E-03
	93	7	5818.59 (2990.61)	6358.46 (1537.65)	7709.95 (3964.18)	4873.56 (2521.66)	0.351	0.138	4.50E-05	0.113	7.70E-05	7.56E-04	0.176	2.68E-04
Orn*hydroxyanthranilic.acid	93	7	2.27 (0.99)	2.18 (0.99)	3.16 (1.59)	1.71 (0.73)	0.087	0.968	8.70E-05	0.010	1.00E-06	8.94E-04	0.061	1.33E-04
	93	7	0.37 (0.37)	0.32 (0.21)	0.57 (0.37)	0.24 (0.12)	0.155	0.712	3.00E-05	0.156	1.00E-06	9.15E-04	0.174	3.70E-04
	93	7	3.12 (1.81)	2.46 (1.15)	4.71 (3.07)	2.03 (0.89)	0.028	0.404	5.50E-05	0.001	0.00E+00	1.03E-03	0.005	2.08E-04
Tyr*Pro	93	7	2244.92 (1282.91)	2912.11 (2002.8)	3027.73 (1527.01)	2406.65 (1020.46)	0.643	0.491	6.50E-05	0.141	5.33E-02	1.03E-03	0.225	9.96E-03
	93	7	2.27 (1.24)	1.92 (0.43)	2.93 (1.29)	1.55 (0.61)	0.005	0.646	6.90E-05	0.002	0.00E+00	1.08E-03	0.021	1.20E-05
	93	7	68.22 (188.83)	56.24 (39.63)	100.4 (148.22)	43.58 (30.65)	0.339	0.738	6.90E-05	0.931	1.43E-03	1.29E-03	0.953	3.25E-03
Asp*Put	93	7	0.35 (0.24)	0.38 (0.29)	0.52 (0.34)	0.25 (0.12)	0.258	0.942	4.90E-05	0.197	2.00E-06	1.29E-03	0.358	1.10E-04
	93	7	1.82 (1.94)	1.48 (0.74)	2.41 (1.41)	1.04 (0.7)	0.113	0.966	8.60E-05	0.005	0.00E+00	1.45E-03	0.010	4.30E-05
	93	7	423.33 (376.29)	588.37 (285.68)	549.44 (297.14)	319.84 (107.77)	0.584	0.052	3.90E-05	0.113	1.00E-06	1.63E-03	0.297	3.41E-04
Asp*N-Acetyl-phenylalanine	93	7	0.26 (0.21)	0.24 (0.15)	0.37 (0.21)	0.2 (0.12)	0.175	0.911	5.30E-05	0.325	8.20E-05	1.76E-03	0.394	1.61E-04
	93	7	104.79 (62.17)	98.49 (35.21)	76.58 (47.88)	115.67 (44.81)	0.034	0.978	4.00E-06	0.135	3.00E-06	1.78E-03	0.157	6.85E-03
	93	7	69.69 (84.73)	97.8 (71.97)	90.49 (58.89)	50.45 (24.12)	0.992	0.196	6.60E-05	0.769	3.10E-05	2.37E-03	0.745	3.51E-04
Asp/Citrulline	93	7	0.29 (0.17)	0.35 (0.21)	0.4 (0.19)	0.28 (0.14)	0.479	0.672	7.80E-05	0.863	4.67E-03	3.99E-03	0.915	6.26E-03

**Supplementary Table 4. Mean ratios/interaction levels between AD and iPD. Same assessment as in Supplementary Table 2.**

Metabolite	N	CN	Mean (SD)					unadjusted for confounders p-values					Adjusted for confounders p-values				
			naive-PD	iPD	AD	naive-PD vs iP	CN AD vs CN iPD	AD vs iPD	AD vs iPD	AD vs iPD	AD vs iPD	AD vs iPD	AD vs iPD	AD vs iPD			
Gln-Tyr	93	7	103	28	4001.77 (2008.08)	4756.41 (1511.22)	5695.77 (2774.62)	3026.21 (1297.06)	0.429841	0.109172	1.00E-06	0.133031	0	2.10E-05	0.038469	6.00E-06	
Cad/N-Acetyl-phenylalanine	93	7	103	28	9.67 (6.2)	7.01 (5.54)	7.22 (5.23)	12.1 (5.69)	0.953762	0.283706	0.004548	0.00478	0	0.078795	0.057181	0.000458	
Phe <sup>3</sup> -HK	93	7	103	28	2.9 (1.67)	2.22 (0.96)	3.82 (2.19)	1.95 (0.8)	0.040634	0.297522	0.003536	0.001294	0	0.031236	0.008569	0.001205	
Asn <sup>3</sup> -HK	93	7	103	28	1.5 (0.87)	1.17 (0.58)	1.91 (1.06)	0.99 (0.4)	0.05412	0.319379	0.006118	0.000479	0	0.040923	0.006613	0.000204	
Gly <sup>3</sup> -HK	93	7	103	28	25848.96 (14397.63)	29390.23 (12533.15)	21150.56 (13713.42)	31747.96 (12096.33)	0.053147	0.344501	0.003957	0.00322	0	0.025656	0.008913	0.00334	
Tyr <sup>3</sup> -HK	93	7	103	28	2.69 (1.54)	2.15 (0.92)	3.38 (1.92)	1.69 (0.79)	0.063877	0.391153	0.017027	0.001162	0	0.129541	0.001766	0.001963	
Tyr <sup>3</sup> -HK	93	7	103	28	3.12 (1.81)	2.48 (1.15)	4.71 (3.07)	2.03 (0.89)	0.027519	0.403836	0.005405	0.000946	0	0.001027	0.004079	0.002028	
Val <sup>3</sup> -HK	93	7	103	28	10.08 (6.25)	7.99 (3.4)	12.85 (7.47)	6.47 (3.14)	0.065714	0.421249	0.008483	0.000597	0	0.070434	0.0041	0.001032	
Leu <sup>3</sup> -HK	93	7	103	28	5.72 (3.64)	4.53 (1.8)	7.52 (4.55)	3.64 (1.79)	0.052989	0.442073	0.004011	0.000537	0	0.055787	0.005586	0.000906	
β-ala <sup>3</sup> -HK	93	7	103	28	0.17 (0.13)	0.13 (0.07)	0.23 (0.15)	0.11 (0.06)	0.06062	0.067234	0.000287	0.000623	0	0.001676	0.037271	0.000164	
Orn <sup>3</sup> -HK	93	7	103	28	2.28 (1.29)	1.92 (1.18)	3.46 (2.14)	1.58 (0.69)	0.065596	0.480323	3.90E-05	0.004936	0	0.000631	0.017262	0.000429	
Cys <sup>3</sup> -HK	93	7	103	28	6398.49 (382.97)	6700.56 (239.6)	487.63 (341.8)	8428.02 (283.71)	0.027059	0.397943	0.000114	0.000137	0	0.003464	0.000729	0.003464	
Tyr <sup>n</sup> -Acetyl-phenylalanine	93	7	103	28	2.27 (1.24)	1.92 (0.43)	2.93 (1.29)	1.55 (0.61)	0.005488	0.645799	6.90E-05	0.00193	0	0.001083	0.021083	1.20E-05	
Cys <sup>3</sup> -AA	93	7	103	28	6186.13 (5265.12)	5311.31 (2034.6)	4643.32 (2416.73)	7930.6 (3203.45)	0.320297	0.685993	0.004027	0.000782	0	0.044668	0.018668	0.000118	
Cys/n-Acetyl-phenylalanine	93	7	103	28	8623.12 (4711.73)	7829.53 (2482.68)	6474.26 (3256.57)	11065.7 (4615.72)	0.107346	0.949113	0.000313	0.00107	0	0.046458	0.018842	0.000139	
Gln <sup>3</sup> -HK	93	7	103	28	1.82 (1.94)	1.48 (0.74)	2.41 (1.41)	1.04 (0.7)	0.112678	0.966084	8.60E-05	0.004892	0	0.001452	0.010409	4.30E-05	
Orn/Cad	93	7	103	28	423.33 (376.29)	588.37 (285.68)	549.44 (297.14)	319.84 (107.77)	0.583538	0.051845	3.90E-05	0.12686	1.00E-06	0.001633	0.297439	0.000341	
3-HK <sup>n</sup> -Acetyl-phenylalanine	93	7	103	28	0.001069 (0.001035)	0.000583 (0.000245)	0.001391 (0.000991)	0.000548 (0.000365)	0.006541	0.141354	0.004538	0.002334	1.00E-06	0.035867	0.11132	0.006999	
Thr <sup>3</sup> -HK	93	7	103	28	4.5 (2.7)	3.36 (1.62)	6.31 (3.95)	3.18 (1.67)	0.023122	0.21421	0.000992	0.004898	1.00E-06	0.008525	0.016323	0.001826	
Met <sup>3</sup> -HK	93	7	103	28	1.08 (0.62)	0.82 (0.31)	1.38 (0.8)	0.72 (0.32)	0.039126	0.272823	0.008666	0.001225	1.00E-06	0.061353	0.007175	0.001166	
Arg <sup>3</sup> -HK	93	7	103	28	2931.38 (1651.62)	3064.42 (992.07)	2288.53 (1570.57)	3913.32 (2138.55)	0.010803	0.317445	0.000544	0.004038	1.00E-06	0.01425	0.013294	0.002674	
3-HK <sup>3</sup> -AA	93	7	103	28	0.00143 (0.00119)	0.000956 (0.000668)	0.00201 (0.00161)	0.000762 (0.000515)	0.037884	0.336242	0.005973	0.001668	1.00E-06	0.037652	0.015578	0.000491	
Cad <sup>3</sup> -HK	93	7	103	28	7.26 (5.4)	5.08 (2.25)	5.48 (4.98)	10.3 (8.43)	0.393239	0.339559	0.001312	0.005299	1.00E-06	0.026388	0.019806	0.000806	
lle <sup>3</sup> -HK	93	7	103	28	2.92 (1.91)	2.22 (0.85)	3.83 (2.31)	1.94 (0.99)	0.042327	0.67257	0.003028	0.00237	1.00E-06	0.029495	0.015047	0.001511	
3-HK <sup>n</sup> Tryptamine	93	7	103	28	0.000801 (0.000651)	0.000563 (0.000281)	0.00103 (0.000743)	0.000423 (0.000244)	0.055771	0.390078	0.19616	0.00359	1.00E-06	0.083061	0.002841	0.000792	
Gln <sup>3</sup> -AA	93	7	103	28	1.68 (1.19)	1.86 (1.12)	2.08 (1.6)	1.1 (0.66)	0.437945	0.413988	0.00308	0.004406	1.00E-06	0.003654	0.01639	4.80E-05	
Citrulline <sup>3</sup> -HK	93	7	103	28	1246.18 (727.42)	1348.03 (617.07)	997.43 (622.64)	1669.81 (820.34)	0.074145	0.469849	0.003778	0.002422	1.00E-06	0.084543	0.0113	0.004335	
Pu <sup>3</sup> -HK	93	7	103	28	10.58 (7.67)	9.99 (5.73)	8.4 (10.06)	12.7 (7.6)	0.033521	0.583456	0.001762	0.019651	1.00E-06	0.0013834	0.01732	0.00281	
Aspartic acid <sup>3</sup> -HK	93	7	103	28	0.37 (0.37)	0.32 (0.21)	0.57 (0.37)	0.24 (0.12)	0.154509	0.712281	3.00E-05	0.157868	1.00E-06	0.000915	0.174031	0.00037	
Arg/n-Acetyl-phenylalanine	93	7	103	28	3926.17 (2159.37)	3715.33 (1335.45)	3003.72 (1547.55)	4906.1 (2164.19)	0.122444	0.877465	0.001112	0.00758	1.00E-06	0.037353	0.050129	0.000546	
Citrulline/n-Acetyl-phenylalanine	93	7	103	28	1671.7 (912.62)	1564.02 (553.4)	1328.21 (615.28)	2079.3 (826.09)	0.225429	0.907522	0.01352	0.002205	1.00E-06	0.280638	0.03978	0.002344	
Tyr <sup>3</sup> -AA	93	7	103	28	3.18 (1.52)	3.05 (1.46)	4.28 (2.26)	2.23 (1.03)	0.116261	0.931885	0.000274	0.003653	1.00E-06	0.002551	0.027848	5.10E-05	
Orn <sup>3</sup> -AA	93	7	103	28	2.27 (0.99)	2.18 (0.99)	2.61 (1.59)	1.73 (0.9)	0.087234	0.96763	8.70E-05	0.10214	1.00E-06	0.000894	0.061088	0.000133	
Gln/Cad	93	7	103	28	303.64 (252.81)	485.92 (228.02)	394.57 (220.27)	207.4 (131.79)	0.274427	0.022835	0.000101	0.031859	2.00E-06	0.004261	0.090504	6.20E-05	
Gln/tryptamine	93	7	103	28	0.99 (0.73)	1.06 (0.27)	1.26 (0.81)	0.62 (0.36)	0.871071	0.052914	0.004258	0.001814	2.00E-06	0.018255	0.008659	6.40E-05	
Gln/β-ala	93	7	103	28	1.67 (1.45)	2.33 (0.68)	292.53 (173.49)	150.33 (73.78)	0.463051	0.277866	4.50E-05	0.062066	2.00E-06	0.000167	0.234291	3.40E-05	
Orn <sup>n</sup> -Acetyl-phenylalanine	93	7	103	28	2.16 (0.91)	1.43 (0.64)	2.21 (1.03)	1.22 (0.48)	0.031697	0.652049	8.90E-05	0.020873	2.00E-06	0.001138	0.080293	0.000133	
Aspartic acid <sup>3</sup> -AA	93	7	103	28	0.35 (0.24)	0.38 (0.29)	0.52 (0.34)	0.26 (0.12)	0.257562	0.941777	4.90E-05	0.19695	2.00E-06	0.001286	0.35838	0.00111	
Pro <sup>3</sup> -HK	93	7	103	28	8238.42 (5364.92)	11311.22 (4990.47)	7613.87 (5203.18)	10877.88 (4732.36)	0.024345	0.076968	0.101548	0.305E-04	3.00E-06	0.158969	0.001566	0.00847	
N-Acetyl-phenylalanine <sup>3</sup> -AA	93	7	103	28	0.001 (0.000754)	0.000759 (0.00038)	0.00128 (0.00078)	0.000578 (0.000381)	0.097368	0.951552	0.010025	0.02194	3.00E-06	0.067929	0.019164	0.000294	
Leu <sup>n</sup> -Acetyl-phenylalanine	93	7	103	28	4.14 (2.35)	3.7 (1.3)	4.86 (3.21)	2.79 (1.21)	0.183035	0.914658	0.01471	0.001912	3.00E-06	0.176846	0.026441	0.000448	
L <sup>3</sup> -HK <sup>n</sup> -HK	93	7	103	28	104.78 (62.77)	98.49 (35.21)	76.58 (47.88)	115.67 (44.81)	0.034166	0.977929	4.00E-06	0.134862	3.00E-06	0.001779	0.156997	0.006533	
lle <sup>n</sup> -Acetyl-phenylalanine	93	7	103	28	8300.6 (4861.08)	9354.34 (3955.75)	6796.95 (4315.02)	9405.52 (3190.14)	0.04445	0.334255	0.003307	0.019449	4.00E-06	0.02383	0.046287	0.006848	
Gln <sup>n</sup> -Acetyl-phenylalanine	93	7	103	28	1.24 (0.97)	1.16 (0.44)	1.63 (0.92)	0.8 (0.48)	0.196697	0.527486	0.000326	0.010359	4.00E-06	0.004118	0.031017	4.60E-05	
Trp <sup>n</sup> -Acetyl-phenylalanine	93	7	103	28	1.97 (1.08)	1.67 (0.34)	2.19 (0.97)	1.29 (0.5)	0.084184	0.669714	0.068393	0.000579	4.00E-06	0.0417407	0.009036	0.008314	
Sarco <sup>3</sup> -HK	93	7	103	28	0.06 (0.04)	0.06 (0.04)	0.08 (0.06)	0.04 (0.02)	0.195675	0.713436	0.014357	0.003344	5.00E-06	0.138804	0.018732	0.008118	
Cad/Tyr	93	7	103	28	0.00238 (0.00107)	0.00149 (0.000808)	0.00175 (0.000936)	0.0029 (0.00151)	0.492203	0.051878	0.000104	0.048372	6.00E-06	0.004528	0.133011	0.000215	
Gln/Orn	93	7	103	28	3036.22 (1674.92)	3564.5 (1613.55)	4207.2 (2022.61)	2423.13 (1117.07)	0.045942	0.263255	0.004096	0.14253	6.00E-06	0.490E-05	0.194467	2.70E-05	
His <sup>3</sup> -HK	93	7	103	28	2.54 (1.42)	2.01 (0.72)	3.21 (1.88)	1.73 (0.8)	0.050759	0.40129	0.012175	0.005863	6.00E-06	0.074948	0.027765	0.004739	
Gln <sup>3</sup> -Leu	93	7	103	28	7404.65 (4171.7)	9156.52 (3621.55)	9235.58 (4943.86)	5500.41 (2688.68)	0.077107	0.314073	0.000675	0.015704	7.00E-06	0.011445	0.06131	0.001102	
Gly <sup>3</sup> -HK	93	7	103	28	9881.47 (5522.65)	11454.21 (5059.55)	8971.94 (5991.74)	13150.68 (5491.54)	0.154258	0.377303	0.110062	0.000654	7.00E-06	0.396266	0.00413	0.018546	
Thr <sup>3</sup> -AA	93	7	103	28	4.55 (2.02)	3.93 (0.81)	5.7 (2.71)	3.4 (1.47)	0.001224	0.002681	0.009227						