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*µL⁻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/μL		•	ed for conf p-values	ounders	Adjusted for confounders p-values
	CN (n = 93)	naïve-iPD (n = 7)	iPD (n = 103)	AD (n = 28)	naïve-iPD vs iPD	naïve-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	6.20E-05	0.002
3-HK	0.04 (0.02)	0.05 (0.06)	0.05 (0.04)	0.03 (0.01)	0.22	0.98	0	1.05E-03
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	4.46E-04	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
β-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)		, ,	191.13 (22.99)	0.84	0.23	0	9.83E-04
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		729.43 (140.56)	690.75 (80.77)		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	7.40E-05	1.76E-04
Gly	274.57 (67.96)	, ,	, ,	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
lle	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)	,	165.33 (34.58)		0.31	0.18	1.76E-04	0.01
Lys	229.23 (33.62)	, ,	, ,	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	, ,	0.02(0)	0.03 (0.01)	0.02 (0.01)	0.75	0.71	2.30E-05	0.0016
Orn	63.82 (16.44)	66.93 (26.17)	74.95 (16.14)	61.41 (12.1)	0.32	0.88	7.30E-05	3.03E-04
Phe	79.92 (9.29)	80.7 (10.2)	83.44 (11.08)	75.63 (8.83)	0.48	0.85	1.75E-04	0.002
Pro	, ,	274.65 (98.72)	, ,	259.25 (83.25)		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)	, ,	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)	, ,	0.01	0.28	0	8.40E-05
Val	'	292.45 (31.63)	, ,	, ,	0.20	0.13	1.40E-03	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	p-value	Interaction CN/iPD*Age	Interaction CN/iPD*Sex
	Males	Females	p-value	coefficient with age		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		-1.01 (0.4)		-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		-3.46 (0.57)		-0.116	0.080	0.078	0.659
lle	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		-4.06 (0.49)		-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		z			Mean (SD	(SD)		nnad	justed for co	unadjusted for coundounders p-values	-values		Adjusted for confounders p-values	onfounde	s p-values
	CN	naive-PD iPD	IPD AD	CN	naive-PD	iPD	AD	naive-PD vs iPD naïve-PD vs CN iPD vs CN AD vs CN iPD vs AD	naive-PD vs C	N iPD vs CN	AD vs CN	IPD vs AD	iPD vs CN	AD vs CN	AD vs CN iPD vs AD
Homoserine*Orn	93	7	103 28	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	1.30E-05	0.239	1.74E-02
β-ala*Orn	93	7	103 28	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	1.50E-05	0.783	8.30E-05
Asp*Tyr	93	7	103 28	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
Gln*Tyr	93	7	103 28	4001.77 (2008.08)	4756.41 (1511.22)	5695.77 (2774.62)	3026.21 (1297.06)	0.430	0.109	1.00E-06	0.013	0.00E+00	2.10E-05	0.038	6.00E-06
Asp*Orn	93	7	103 28	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
Asp/L-KYN	93	7	103 28	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	4.58E-02	4.30E-05	0.151	2.22E-02
GIn*Orn	93	7	103 28	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
Homoserine*Asp	93	7	103 28	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
Homoserine*Gln	93	7	103 28	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
Asp*β-ala	93	7	103 28	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
Homoserine*β-ala	93	7	103 28	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
Gln*β-ala	93	7	103 28	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
Arg/Asp	93	7	103 28	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
Asp/Cys	93	7	103 28	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
Asp/2-Ambut	93	7	103 28	0.48 (0.28)	0.48 (0.3)	0.64 (0.32)	0.56 (0.29)	0.228	0.907	6.30E-05	0.00	2.32E-01	3.16E-04	0.182	1.16E-01
Asp*GIn	93	7	103 28	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
Asp/Lys	93	7	103 28	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
Asp*Thr	93	7	103 28	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
Orn*3-HK	93	7	103 28	2.28 (1.29)	1.92 (1.18)	3.46 (2.14)	1.58 (0.69)	990.0	0.480	3.90E-05	0.005	0.00E+00	6.31E-04	0.017	4.29E-04
GIn/Asp	93	7	103 28		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
Gln*Thr	93	7	103 28	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*hydroxy.antranilic.acid	93	7	103 28	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
Asp*3-HK	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	0.158	1.00E-06	9.15E-04	0.174	3.70E-04
Tyr*3-HK	93	7		3.12 (1.81)	2.48 (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
Asp*Pro	93	7	103 28	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
Tyr*N-Acetyl-phenylalanine	93	7			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
Asp/Put	93	7	103 28	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*hydroxy.anthranilic.acid	93	7	103 28	0.35 (0.24)	0.38 (0.29)	0.52 (0.34)	0.26 (0.12)	0.258	0.942	4.90E-05	0.197	2.00E-06	1.29E-03	0.358	1.10E-04
GIn*3-HK	93	7			1.48 (0.74)	2.41 (1.41)	1.04 (0.7)	0.113	996.0	8.60E-05	0.005	0.00E+00	1.45E-03	0.010	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)	0.584	0.052	3.90E-05	0.113	1.00E-06	1.63E-03	0.297	3.41E-04
Asp*N-Acetyl-phenylalanine	93	7	103 28	.=	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
L-KYN/3-HK	93	7	103 28	6	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
Asp/Cad	93	7	103 28	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	103 28	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	CN na	N aïve-PD	iPD AD		Mear naïve-PD	iPD	AD	naïve-PD vs	ınadjusted for cou PD naïve-PD vs Cl	N iPD vs CN	AD vs CN	iPD vs AD	Adjusted for a iPD vs CN		
Gln*Tyr	93	7	103 28			5695.77 (2774.62)	3026.21 (1297.06)	0.429841	0.109172	1.00E-06		0	2.10E-05	0.038469	6.00E
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	0.078795	0.057181	
Phe*3-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	0.031236	0.008569	
Asn*3-HK Gly/3-HK	93	7 7	103 28	1.5 (0.87)	1.17 (0.58)	1.91 (1.06)	0.99 (0.4)	0.05412 0.053147	0.319379 0.344501	0.006118 0.003957	0.000479	0	0.040923	0.006113	
Trp*3-HK	93	7	103 28	2.69 (1.54)	2.15 (0.92)	21150.56 (13713.42) 3.38 (1.92)	1.69 (0.79)	0.033147	0.391153		0.00322	0	0.023636	0.000913	
Tyr*3-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		0.000946	ō	0.001027	0.004979	
Val*3-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	0.0010
Leu*3-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		0.000537	0	0.055787	0.005586	
β-ala*3-HK Orn*3-HK	93 93	7 7	103 28 103 28	0.17 (0.13)	0.13 (0.07)	0.23 (0.15)	0.11 (0.06)	0.06062 0.065596	0.472436 0.480323	0.000287 3.90E-05	0.006723	0	0.001676 0.000631	0.037271 0.017262	
Cys/3-HK	93	7	103 28	2.28 (1.29) 6398.49 (3682.97)	1.92 (1.18) 6700.56 (2925.6)	3.46 (2.14) 4887.63 (3341.8)	1.58 (0.69) 8426.02 (2839.71)	0.065596	0.498573	0.000114		0	0.000631	0.017262	
Tyr*N-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	ŏ	0.001083	0.021083	
Cys/3-AA	93	7	103 28	6186.13 (5265.12)	5311.31 (2034.6)	4643.32 (2416.73)	7930.6 (3203.45)	0.320297	0.685893		0.000782	0	0.044868	0.018668	
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	
GIn*3-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		0.004892	0	0.001452		
Orn/Cad 3-HK*N-Acetyl-phenylalanine	93 93	7 7	103 28	423.33 (376.29)	588.37 (285.68)	549.44 (297.14) 0.001391 (0.000991)	319.84 (107.77)	0.583538 0.006541	0.051845 0.141354		0.112686 0.002334		0.001633 0.035667	0.297439 0.011182	
Thr*3-HK	93	7	103 28	4.5 (2.7)	3.36 (1.62)	6.31 (3.95)	3.18 (1.67)	0.00341	0.24121	0.004538	0.002334	1.00E-06	0.008525	0.011182	
Met*3-HK	93	7	103 28	1.08 (0.62)	0.82 (0.31)	1.38 (0.8)	0.72 (0.32)	0.039126	0.272283		0.001225		0.061353	0.007175	
Arg/3-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		1.00E-06	0.01425	0.013294	
3-HK*3-AA	93	7	103 28			0.00201 (0.00161)			0.336242		0.001668	1.00E-06	0.037652	0.015578	
Cad/3-HK	93	7	103 28	7.26 (5.4)	5.08 (2.25)	5.48 (4.98)	10.3 (8.43)	0.392329	0.339559		0.005529		0.026388	0.019806	
IIe*3-HK	93	7	103 28	2.92 (1.91)	2.22 (0.85)	3.83 (2.31)	1.94 (0.99)	0.042327 0.055771	0.367257 0.390078		0.003237		0.029495 0.083061	0.015047	
3-HK*Tryptamine GIn*3-AA	93	7 7	103 28	1.68 (1.19)	1.86 (1.12)	0.00103 (0.000743) 2.38 (1.6)	1.1 (0.66)	0.035771	0.413988		0.000359		0.003654	0.002841	4.80E
Citrulline/3-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		0.002422		0.084543		
Put/3-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		1.00E-06	0.013834	0.07132	
Aspartic acid*3-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		0.157868	1.00E-06	0.000915	0.174031	
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	0.006758	1.00E-06	0.037353	0.050129	0.000
Citrulline/N-Acetyl-phenylalanine	93	7	103 28	1671.7 (912.62)	1564.02 (558.53)	1328.1 (615.28)	2079.3 (826.09)	0.225429	0.907522		0.002205		0.280638		
Tyr*3-AA Orn*3-AA	93 93	7 7	103 28 103 28	3.18 (1.52) 2.27 (0.99)	3.05 (1.46) 2.18 (0.99)	4.28 (2.26) 3.16 (1.59)	2.23 (1.03) 1.71 (0.73)	0.116261 0.087234	0.931885 0.96763		0.003653 0.010214		0.002551 0.000894	0.027848 0.061088	
GIn/Cad	93	7	103 28	303.64 (252.81)	485.92 (228.02)	394.57 (227.23)	207.4 (131.79)	0.087234	0.022835		0.010214		0.000894	0.090504	
GIn*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	6.40
Gln*β-ala	93	7	103 28	217.91 (145.68)	253.6 (126.92)	292.63 (173.49)	159.33 (73.78)	0.589508	0.324185	4.50E-05	0.062006	2.00E-06	0.000167	0.234291	3.40
Orn*N-Acetyl-phenylalanine	93	7	103 28	1.66 (0.9)	1.43 (0.64)	2.21 (1.03)	1.22 (0.48)	0.031697	0.652049		0.020873		0.001138	0.080293	
Aspartic acid*3-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	0.00
Pro/3-HK	93 93	7	103 28 103 28			7613.87 (5203.18)		0.024345 0.097368	0.076968 0.591552		3.05E-04 0.002194		0.158969 0.067929	0.001566 0.019164	
N-Acetyl-phenylalanine*3-AA Leu*N-Acetyl-phenylalanine	93	7 7	103 28	0.001 (0.000754) 4.14 (2.35)	3.7 (1.3)	0.00128 (0.000878) 4.86 (2.31)	2.79 (1.21)	0.097368	0.591552		0.002194		0.067929	0.019164	
L-KYN/3-HK	93	7	103 28	104.79 (62.17)	98.49 (35.21)	76.58 (47.88)	115.67 (44.81)	0.034168	0.977929		0.134862		0.001779	0.020441	
Lys/3-HK	93	7	103 28		9354.34 (3955.75)	6796.95 (4315.02)	9405.52 (3190.14)	0.04445	0.334256		0.019449		0.02383	0.042697	
Gln*N-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		0.010359		0.004118	0.031017	4.60
Trp*N-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		0.000579		0.417407	0.009936	
Sarco*3-HK	93	7	103 28	0.06 (0.04)	0.06 (0.04)	0.08 (0.06)	0.04 (0.02)	0.196575	0.713436	0.014357	0.003344	5.00E-06	0.138804	0.018732	
Cad/Tyr Gin*Orn	93 93	7	103 28 103 28	0.00238 (0.00107) 3036.22 (1674.92)	3564.5 (1613.55)	0.00175 (0.000936) 4207.2 (2027.61)	0.0029 (0.00151) 2423.13 (1117.07)	0.492203 0.463051	0.051878 0.276786		0.048372		0.004528 4.90E-05	0.133011 0.194467	
His*3-HK	93	7	103 28	2.54 (1.42)	2.01 (0.72)	3.21 (1.85)	1.79 (0.8)	0.050759	0.40129		0.005963		0.074948	0.027765	
Gln*Leu	93	7	103 28	7404.65 (4171.7)	9156.52 (3621.55)	9235.58 (4493.86)	5500.41 (2688.68)	0.871337	0.140731		0.015704		0.011445		
Gly/3-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		0.000654		0.396266	0.004143	
Thr*3-AA	93	7	103 28	4.55 (2.02)	3.93 (0.81)	5.7 (2.71)	3.4 (1.47)	0.010941	0.601224		0.009227		0.020891	0.071985	
GIn/Put	93 93	7	103 28 103 28	301.94 (732.56)	257.28 (115.06)	430.48 (565.57)	160.08 (86.8)	0.47898 0.045942	0.217347	0.00037 0.004096	0.110822 0.014253		0.003408 0.020226	0.246435 0.03448	
Ser*3-HK Ala*3-HK	93	7 7	103 28	3.18 (1.78) 15.12 (9.49)	2.39 (1.09) 12.54 (6.88)	4.14 (2.24) 19.22 (10.64)	2.35 (1.05) 10.68 (5.1)	0.126161	0.263255 0.504828		0.014253		0.020226	0.03448	
Put/3-AA	93	7	103 28	9.73 (8.04)	7.82 (4.04)	7.63 (9.78)	12.05 (9)	0.183037	0.807811		0.028937		0.017505	0.136241	
Val*N-Acetyl-phenylalanine	93	7	103 28	7.28 (4)	6.38 (1.8)	8.37 (3.85)	4.95 (2.12)	0.149701	0.839714		0.001921		0.229127	0.019485	
Cys*Cad	93	7	103 28	36.02 (19.34)	21.59 (13.45)	26.8 (13.7)	41.96 (20.68)	0.32083	0.054959		0.049001		0.092863	0.157606	
β-ala*N-Acetyl-phenylalanine	93	7	103 28	0.12 (0.09)	0.11 (0.06)	0.15 (0.08)	0.08 (0.04)	0.129448	0.777164		0.023818		0.003528	0.147281	
Phe*N-Acetyl-phenylalanine	93	7	103 28	2.12 (1.18)	1.76 (0.52)	2.46 (1.09)	1.51 (0.58)	0.05781	0.528188		0.005886		0.101376	0.045162	
Tau*3-HK His/3-HK	93 93	7 7	103 28 103 28	4.05 (2.57) 2540.01 (1491.91)	3.43 (1.51) 3264.3 (1559.73)	5.64 (3.33) 2157.99 (1472.52)	3.05 (1.12)	0.110302 0.036043	0.681413 0.168984		0.093492 0.008256		0.006079 0.035078	0.110813 0.011359	
Thr*N-Acetyl-phenylalanine	93	7	103 28	3.26 (1.7)	2.59 (0.48)	4.08 (1.92)	2.42 (1)	0.001279	0.216968		0.014635		0.027611	0.074218	
Lys*3-HK	93	7	103 28	8.27 (4.86)	5.94 (2.25)	10.02 (5.69)	5.62 (2.55)	0.033567	0.167842		0.002277		0.092889	0.005932	
Asn*3-AA	93	7	103 28	1.51 (0.62)	1.36 (0.24)	1.76 (0.79)	1.08 (0.44)	0.060623	0.90475	0.03164	0.002676	1.30E-05	0.133535	0.036305	0.00
Leu*3-AA	93	7	103 28	5.78 (2.93)	5.79 (2.83)	7.09 (3.94)	3.99 (1.96)	0.462332	0.796057		0.002536		0.185994	0.026081	
Ser/3-HK	93 93	7	103 28		3615.51 (1518.01)		4098.81 (1714.24)	0.065587 0.035091	0.301325 0.178775		0.004076 0.006014		0.133817 0.078563	0.010791 0.021655	
Gly*3-HK Ala/3-HK	93	7 7	103 28 103 28	25.32 (13.7) 14898 76 (9211 42)	18.62 (7.33) 17544.18 (5029.36)	31.2 (17.53) 13457.52 (9520.16)	18.38 (7.88) 17748.22 (5994.8)	0.035091 0.014448	0.178775 0.095577		0.006014		0.078563 0.140332	0.021655 0.016582	
2-Ambut*3-HK	93	7	103 28	0.77 (0.47)	0.69 (0.46)	0.93 (0.58)	0.5 (0.24)	0.269419	0.610942		0.001282		0.243591	0.002118	
β-ala*3-AA	93	7	103 28	0.16 (0.09)	0.16 (0.08)	0.22 (0.12)	0.12 (0.06)	0.189766	0.998428	0.001046	0.018999	2.20E-05	0.003219	0.096979	0.00
Phe*3-AA	93	7	103 28	2.93 (1.33)	2.78 (1.36)	3.57 (1.86)	2.14 (0.98)	0.270832	0.912099		0.005257		0.109671	0.042357	
-Acetyl-phenylalanine*Tryptamine	93	7		0.000549 (0.000357) 845.07 (479.13)		0.000683 (0.000513) 1278.56 (593.25)			0.791392		0.001534		0.160935 1.90E-05	0.005783	
Aspartic acid*Tyr	93	7	103 28		974.6 (531.85) 7.24 (3.23)		772.85 (346.92) 7.55 (3.16)	0.295165	0.770235		0.946736 0.061154			0.85482	
Gly*3-HK Gln*Val	93 93	7 7	103 28 103 28	9.81 (5.73) 13050.45 (7106.07)	15783.17 (5522.65)	13.62 (8.75) 15977.96 (7789.44)	9827.11 (4812.04)	0.023418 0.769513	0.234005 0.107234		0.011154		0.005688 0.017195	0.083401 0.047302	
Aspartic acid/Cad	93	7	103 28	69.69 (84.73)	97.8 (71.97)	90.49 (58.89)	50.45 (24.12)	0.992424	0.195539		0.768588		0.002372	0.74455	
Arg/3-AA	93	7	103 28	2750.64 (2027.48)	2525.16 (1080.16)	2208.56 (1326.77)	3677.37 (2054.34)	0.325034	0.839025	0.001654		3.30E-05	0.038193	0.04057	0.00
Aspartic acid/Cys	93	7	103 28	0.06 (0.03)	0.07 (0.03)	0.08 (0.04)	0.05 (0.02)	0.361129	0.58866	1.00E-06	0.97942	3.40E-05	0.000259	0.929784	0.00
GABA/3-HK	93	7	103 28	11.35 (8.85)	12.98 (5.59)	9.47 (7.39)	15.88 (9.26)	0.020993	0.137992		0.004536		0.309533	0.02193	
Trp*3-AA	93	7	103 28	2.77 (1.35)	2.66 (1.22)	3.15 (1.59)	1.87 (0.86)	0.496499	0.896058	0.097389	0.001422	3.60E-05	0.422417	0.012592	0.00
Val*3-AA	93 93	7	103 28 103 28	10.16 (4.92)	10.11 (4.96)	12.26 (6.78)	7.1 (3.41)	0.495571 0.626654	0.828068 0.133771	0.050429	0.00263	3.70E-05	0.245297 0.003826	0.019078 0.34022	
β-ala/Cad Met*N-Acetyl-phenylalanine	93	7 7	103 28	30.21 (32.66) 0.79 (0.43)	44.57 (29.08) 0.65 (0.16)	37.28 (20.28) 0.9 (0.41)	22.31 (10.77) 0.56 (0.23)	0.026634	0.133771	0.000198	0.10445	4.00E-05 4.50E-05	0.003826	0.34022	
R-ala*Orn	93	7	103 28	297.95 (156.41)	336.65 (251.12)	398.66 (181.81)	259.8 (103.45)	0.324087	0.845322		0.335546		1.50E-05	0.037409	
4-OH-Pro/3-HK	93	7	103 28	415.34 (307.73)	562.19 (229.71)	357.87 (226.98)	528.65 (252.25)	0.039745	0.099694		0.002561		0.27719	0.004513	
IIe*3-AA	93	7	103 28	2.93 (1.44)	2.77 (1.15)	3.62 (2.02)	2.11 (1.04)	0.290957	0.919057	0.023551	0.008098	4.70E-05	0.103393	0.058277	
Ile*N-Acetyl-phenylalanine	93	7	103 28	2.1 (1.21)	1.78 (0.5)	2.48 (1.2)	1.52 (0.81)	0.075219	0.715886	0.013073			0.0901	0.064255	0.00
Put/Tyr	93	7	103 28		0.00263 (0.000857)		0.00388 (0.00243)	0.09805	0.404442		0.192363		0.002587	0.384697	
Gin*ile	93 93	7	103 28 103 28		4445.18 (1615.1)	4697.72 (2273.05)	2936.21 (1469.98)	0.952654 0.200855	0.173054		0.054998		0.004456 0.209935	0.129784	
Met*3-AA Cad/3-AA	93	7 7	103 28 103 28	1.1 (0.5) 7.14 (7.59)	1 (0.3) 4.88 (4.18)	1.28 (0.63) 5.1 (5.11)	0.79 (0.36) 9.98 (7.93)	0.200855 0.784315	0.910281 0.253878		0.004675 0.021202		0.209935	0.040596 0.068951	
Tyr*Tryptamine	93	7	103 28	7.14 (7.59) 1.83 (0.88)	4.88 (4.18) 1.91 (0.84)	5.1 (5.11) 2.35 (1.36)	1.35 (0.73)	0.784315	0.253878 0.641202		0.021202		0.064686	0.068951	
Cad/Leu	93	7	103 28	0.0013 (0.000571)	0.000838 (0.000558)	0.00108 (0.000573)	0.00163 (0.000863)	0.450734	0.07632	0.009118	0.00645	6.20E-05	0.222823	0.134688	
Ala*3-AA	93	7	103 28		14.32 (5.14)	18.24 (9.72)	11.38 (5.01)	0.269676	0.901188		0.013254		0.067935	0.06525	
Citrulline/3-AA	93	7	103 28	1212.4 (1024.35)	1079.73 (462.3)	971.76 (523.91)	1573.69 (821.84)	0.547544	0.838396	0.024221	0.009028	6.90E-05	0.29929	0.054399	0.00
Ala*N-Acetyl-phenylalanine	93	7	103 28	11.02 (6.39)	9.34 (2.9)	12.74 (5.96)	8.15 (3.77)	0.081225	0.714903	0.017487	0.02154	7.50E-05	0.070426	0.082104	0.00
Sarco*N-Acetyl-phenylalanine	93	7	103 28	0.05 (0.03)	0.04 (0.02)	0.05 (0.03)	0.03 (0.02)	0.468696	0.83369		0.00978		0.400022	0.08241	0.00
GIn*Thr	93	7	103 28		6358.46 (1537.65)	7709.95 (3964.18)	4873.56 (2521.66)	0.351404	0.138419		0.113124		0.000756	0.175657	
Met/3-HK	93	7	103 28		1286.32 (536.28)	923.11 (581.93)	1225.98 (460.06)	0.045689	0.232402		0.034418		0.037489	0.032448	
spartic acid*N-Acetyl-phenylalanine	93	7	103 28	0.26 (0.21)	0.24 (0.15)	0.37 (0.21)	0.2 (0.12)	0.175386	0.910972		0.324849		0.001756	0.394334	
Phe/3-HK	93	7	103 28	2870.14 (1670.86)	3400.74 (1382.76)	2505.74 (1508.61)	3369.97 (1263.59)	0.048549	0.215443	0.030136	0.017662	8.40F-05	0.068892	0.024016	0.02