

Electronic Supplementary Information (ESI)

Supplemental Data Table 1 (S1) Results from a parallelism of dilution experiment, to examine for matrix effects.

	Area	Internal Standard Area	Response	Measured Concentration (ng/mL)	Dilution	Dilution Factor	Concentration x Dilution Factor	% Difference from Initial Measurement
PAG^a	1337449.5	22343.4	59.859	1869.1	100	1	1869.1	0
	699290.688	24403.832	28.655	894.7	200	2	1789.4	-4.3
	289319.375	25737.021	11.241	350.9	500	5	1754.5	-6.1
	142214.109	25094.975	5.667	176.8	1000	10	1768	-5.4
	74930.68	24695.07	3.034	94.6	2000	20	1892	1.2
	29042.109	24325.092	1.194	37.2	5000	50	1860	-0.5
4-CS^b	503931.094	26133.35	19.283	803.1	100	1	803.1	0
	268851.188	26852.371	10.012	416.8	200	2	833.6	3.8
	108786.727	26994.072	4.03	167.5	500	5	837.5	4.3
	55185.492	26038.357	2.119	87.9	1000	10	879	9.5
	27329.834	27650.893	0.988	40.8	2000	20	816	1.6
	11128.986	27797.057	0.4	16.3	5000	50	815	1.5
HIPP^c	35935.645	753.622	47.684	3255.9	100	1	3255.9	0
	23753.045	992.613	23.93	1247.2	200	2	2494.4	-23.4
	13269.215	917.636	14.46	709	500	5	3545	8.9
	7905.832	1095.212	7.219	340.5	1000	10	3405	4.6
	4317.613	1216.13	3.55	164.9	2000	20	3298	1.3
	1872.566	1255.652	1.491	69.1	5000	50	3455	6.1

^a PAG = Phenylacetylglutamine

^b 4-CS = 4-Cresyl Sulphate

^c HIPP = Hippurate

Supplemental Data Table 2 (S2) Imprecision and Inaccuracy for 2000 Human Urine Samples.

	Target Concentration (ng/mL)	Mean concentration measured (ng/mL) (Mean SD)	Imprecision, CV (%)	Inaccuracy (%)
PAG	3	3.0 (0.2)	6.7	0
	30	30.9 (2.1)	6.8	3.0
	300	304.6 (12.8)	4.2	1.5
4-CS	3	2.9 (0.3)	10.3	-3.3
	30	30.7 (1.9)	6.2	2.3
	300	303.6 (15.4)	5.1	1.2
HIPP	10	9.7 (1.5)	15.5	-3.0
	100	103.3 (8.4)	8.1	3.3
	1000	1016.6 (77.7)	7.6	1.7

^a PAG = Phenylacetylglutamine

^b 4-CS = 4-Cresyl Sulphate

^c HIPP = Hippurate

Supplemental Data Table 3 (S3) Reference ranges for human urinary concentrations of phenylacetylglutamine, 4-cresyl sulphate and hippurate, according to ethnic group.

Metabolite, units		PAG, ng/mL	PAG, $\mu\text{mol/m mol Cr}$	PAG, $\mu\text{mol/24-hr}$	4-CS, ng/mL	4-CS, $\mu\text{mol/m mol Cr}$	4-CS, $\mu\text{mol/24-hr}$	HIPP, ng/mL	HIPP, $\mu\text{mol/mm ol Cr}$	HIPP, $\mu\text{mol/24-hr}$
White, Non Hispanic (n=1,065)	Mean	195.04	101.41	1285.64	122.02	89.75	1115.82	654.43	517.79	6637.62
	SD	128.81	60.00	728.08	93.84	66.06	746.12	432.53	337.68	4033.12
	Median	163.85	88.31	1122.54	100.30	76.39	988.89	567.35	446.36	5778.13
	2.5%	48.40	27.69	392.08	10.90	8.52	127.40	116.40	103.06	1292.53
	97.5%	547.50	250.27	3075.45	368.50	255.88	3188.86	1802.20	1372.39	16908.96
African American (n=339)	Mean	226.00	88.60	1219.01	140.96	77.19	1043.75	568.43	335.22	4689.59
	SD	129.02	49.29	624.37	99.65	50.32	637.39	357.61	213.57	2858.46
	Median	193.85	78.61	1111.66	117.80	64.77	938.37	502.75	301.48	4169.74
	2.5%	68.55	27.20	387.83	12.55	5.17	92.55	104.75	64.45	813.68
	97.5%	541.30	195.00	2826.29	394.85	199.07	2630.68	1414.90	960.17	11303.48
Japanese (n=259)	Mean	133.02	78.47	896.31	74.33	63.61	702.56	370.30	317.31	3656.63
	SD	80.43	45.69	494.44	64.92	55.21	566.27	312.94	256.80	2919.80
	Median	115.60	68.68	779.41	58.20	50.38	613.30	291.65	249.44	3116.05
	2.5%	35.75	22.50	277.86	3.85	2.40	35.68	48.70	41.56	610.75
	97.5%	382.65	190.26	2143.13	222.85	220.87	2231.52	1233.10	914.24	10433.55
Hispanic, Non White (n=165)	Mean	231.25	120.77	1362.81	116.94	90.95	1004.76	501.37	390.83	4566.79
	SD	150.22	72.78	806.27	81.12	70.65	717.51	321.62	237.27	3123.72
	Median	191.20	105.46	1235.75	99.10	70.30	802.59	429.80	337.96	3633.77
	2.5%	52.00	37.60	373.79	12.95	14.83	123.32	92.80	108.05	1021.34
	97.5%	606.95	303.52	3528.30	314.15	255.44	2595.78	1398.15	953.04	12845.00
Hispanic, White (n=107)	Mean	214.81	104.82	1276.27	112.87	78.32	934.73	508.09	374.62	4701.62
	SD	139.67	67.71	689.41	88.19	66.91	658.86	313.83	234.94	2961.77
	Median	202.75	87.03	1159.14	98.70	61.89	801.63	415.90	322.54	3959.74
	2.5%	40.65	29.31	399.42	6.30	10.04	92.43	111.65	97.39	1028.79
	97.5%	606.60	294.98	3116.60	368.10	279.81	2557.63	1282.05	1085.37	11274.68
Other (n=65)	Mean	146.13	73.32	854.53	85.21	58.37	674.24	436.44	329.32	3745.41
	SD	99.24	57.29	565.63	92.08	64.97	683.74	351.44	237.44	2528.34
	Median	118.85	59.07	690.62	45.50	30.02	356.33	331.50	284.58	3130.14
	2.5%	23.15	17.76	191.12	0.55	0.82	5.67	50.70	39.58	450.52
	97.5%	369.20	260.95	2626.24	364.80	236.06	2347.09	1277.40	1059.76	9705.17

^a PAG = Phenylacetylglutamine

^b 4-CS = 4-Cresyl Sulphate

^a HIPP = Hippurate