

Table S3: Analysis of the Blank, related to “Systems performance check” section.

Compound Name	Blank	Average 3 replicates	SD
2-Aminobutyric acid			
2-Ketoglutaric acid			
3-Hydroxy-D, L-Kynurenine			
4-Aminobutyric acid			
4-Hydroxyproline			
5-Glutamylcysteine			
Acetylcarnitine			
Acetylcholine			
Aconitic acid			
Adenine			
Adenosine 3':5'-cyclic monophosphate			
Adenosine monophosphate			
Adenosine			
Adenylysuccinic acid			
Alanine			
Allantoin			
Anthranoilic Acid			
Arginine			
Argininosuccinic acid			
Asparagine			
Aspartic acid	0.005	0.001	
Asymmetric dimethylarginine			
Carnitine			
Carnosine			
Cholic Acid (CA)			
Choline	0.528	0.042	
Citicoline			
Citrin Acid			
Citrulline			
Creatine			
Creatinine			
Cystathione			
Cysteamine			
Cysteine			
Cystine			
Cytidine 3',5'-cyclic monophosphate			
Cytidine monophosphate			
Cytidine			
Cytosine			
Dimethylglycine			
Dopa			
Dopamine			
FAD			
Epinephrine			
FMN			
Fumaric Acid			
Glutamic acid			
Glutamine			
Glutathione oxidized			
Glutathione reduced			
Glycine	0.030	0.001	
Guanine			
Guanosine 3',5'-cyclic monophosphate			
Guanosine monophosphate			
Guanosine	0.007	0.001	
Histamine			
Histidine			
Homocysteine			
Homocystine			
Hypoxanthine			
Inosine			
Isocitric Acid			
Isoleucine			
Kynurenic Acid			
Kynurenone			
Lactic Acid	0.028	0.001	
Leucine			
L-Hydroxyprootic Acid			
Lysine			
Malic Acid			
Methionine sulfone			
Methionine sulfoxide			
Methionine			
NAD			
Niacinamide			
Nicotinic acid			
Norepinephrine			
Ophthalmic acid			
Omitine			
Orotic Acid Pos			
Pantothenic acid			
Phenylalanine			
Picolinic Acid			
Proline			
Putrescine	5.165	0.720	
Pyruvic acid			
Ribitol			
S-Adenosylhomocysteine			
S-Adenosylmethionine			
Sarcosine			
Serine			
Serotonin			
Spermidine			
Spermine			
Succinic acid	0.007	0.001	
Symmetric dimethylarginine			
Taurine			
Taurocholic acid			
Threonine	0.003	0.001	
Thymidine monophosphate			
Thymidine	0.001	0.000	
Thymine			
Tryptophan			
Tyrosine			
Uracil			
Uric acid			
Uridine			
Valine			
Xanthine			

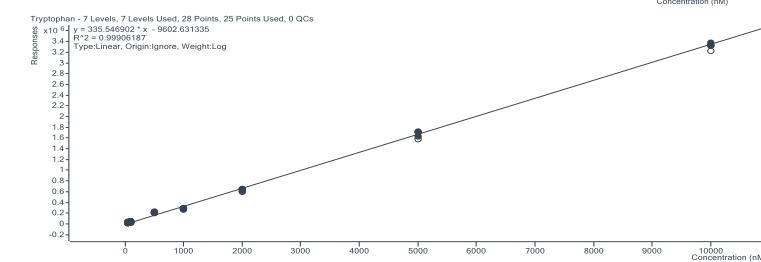
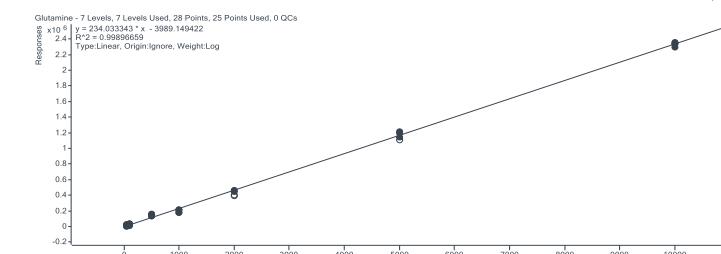
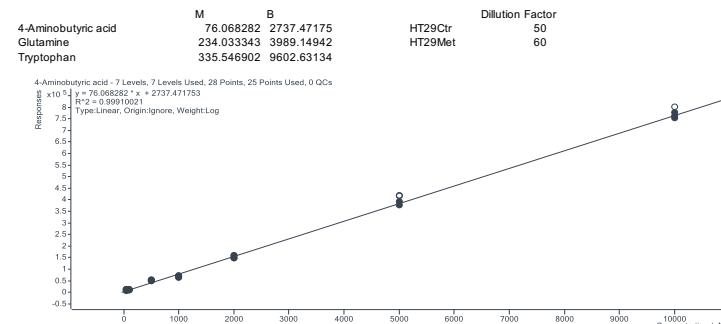
Table S6: Absolute quantification, related to “Basic data analysis” section.

Uncorrected	HT29 Ctrl 1	HT29 Ctrl 2	HT29 Ctrl 3	HT29 Ctrl 4	HT29 Ctrl 5	Met 10mM 1	Met 10mM 2	Met 10mM 3	Met 10mM 4	Met 10mM 5	Met 10mM 6
Compound Name	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area
2-Morpholinioethansulfonic Acid	295073.12	248122.62	209222.36	302957.98	211807.71	466792.9	452862.37	400524.53	458171.03	443308.52	521175.5825
4-Aminobutyric acid	860262.423	93547.79	841638.645	952086.577	959341.184	62467.5009	5582.099	4883.699	59977.223	59245.9859	54019.8729
Glutamine	51937.7803	46106.4544	44745.9871	45507.01	43488.9601	102278.494	46516.7256	65590.3006	79145.6457	75659.4364	41280.31657
Tryptophan	554144.172	570531.451	501869.129	608669.808	64947.587	467055.267	577361.316	502435.63	462233.088	439092.52	604016.4963

Correction 1 1.18917506 1.41026521 0.97397377 1.39311793 0.63212856 0.65157351 0.73671674 0.64402397 0.66561573 0.566168358

Corrected	HT29 Ctrl 1	HT29 Ctrl 2	HT29 Ctrl 3	HT29 Ctrl 4	HT29 Ctrl 5	Met 10mM 1	Met 10mM 2	Met 10mM 3	Met 10mM 4	Met 10mM 5	Met 10mM 6
Compound Name	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area
2-Morpholinioethansulfonic Acid	295073.12	295073.12	295073.12	295073.12	295073.12	295073.12	295073.12	295073.12	295073.12	295073.12	295073.1241
4-Aminobutyric acid	860262.42	1110151.7	1186933.7	927307.35	1336475.4	39487.491	36215.823	36012.976	38626.769	39435.06	30584.35086
Glutamine	51937.78	54828.646	63103.709	44322.634	60585.25	64653.157	30309.066	48321.472	50971.693	50360.111	23371.60903
Tryptophan	554144.17	678461.77	707768.57	592828.43	898488.05	295238.97	376193.34	370152.74	297689.19	292266.89	341975.0276

Corrected	HT29 Ctrl 1	HT29 Ctrl 2	HT29 Ctrl 3	HT29 Ctrl 4	HT29 Ctrl 5	Met 10mM 1	Met 10mM 2	Met 10mM 3	Met 10mM 4	Met 10mM 5	Met 10mM 6
Compound Name	Conc. (nM)	Conc. (nM)	Conc. (nM)	Conc. (nM)	Conc. (nM)	Conc. (nM)	Conc. (nM)				
4-Aminobutyric acid	567253.44	731506.74	781975.84	611322.35	880270.22	33305.574	30724.996	30564.998	32626.666	33264.218	26283.08809
Glutamine	11948.496	12566.114	14334.038	10321.56	13795.983	17598.084	8793.1613	13411.069	14090.516	13933.722	7014.579574
Tryptophan	84004.173	102528.8	106895.82	89768.532	135315.01	54509.507	68985.164	67905.029	54947.636	53978.061	62866.50067



Corrected	HT29 Ctrl		HT29 Met	
Compound Name	Average	SD	Average	SD
4-Aminobutyric acid	714465.72	127130.991	31128.257	2664.72553
Glutamine	12593.238	1585.39664	12473.522	3878.97126
Tryptophan	103702.47	19956.8624	60531.983	6952.36786

