Supplementary Table S1. Concentration of Standards at Different Ca						
Analyte	**Concentration in µM**					
	Cal1	**Cal2**	**Cal3**	**Cal4**	**Cal5**	**Cal6**
Creatinine	10	20	100	200	400	600
Glycine	25	50	250	500	1000	1500
Alanine	20	40	200	400	800	1200
Serine	5	10	50	100	200	300
Histamine	1	2	10	20	40	60
Proline	10	20	100	200	400	600
Valine	10	20	100	200	400	600
Threonine	5	10	50	100	200	300
Phenylethylamine	0.1	0.2	1	2	4	6
Taurine	2.5	5	25	50	100	150
Putrescine	0.1	0.2	1	2	4	6
trans-Hydroxyproline	1	2	10	20	40	60
Leucine	5	10	50	100	200	300
Isoleucine	5	10	50	100	200	300
Asparagine	5	10	50	100	200	300
Aspartic acid	5	10	50	100	200	300
Glutamine	20	40	200	400	800	1200
Glutamic acid	10	20	100	200	400	600
Methionine	5	10	50	100	200	300
Dopamine	1	2	10	20	40	60
Histidine	5	10	50	100	200	300
Phenylalanine	5	10	50	100	200	300
Arginine	5	10	50	100	200	300
Citrulline	5	10	50	100	200	300
Serotonin	0.1	0.2	1	2	4	6
Tyrosine	5	10	50	100	200	300
DOPA	0.5	1	5	10	20	30
Asymmetric dimethylarginine	0.25	0.5	2.5	5	10	15
Total dimethylarginine	0.25	0.5	2.5	5	10	15
Tryptophan	5	10	50	100	200	300
Kynurenine	1	2	10	20	40	60
Carnosine	0.5	1	5	10	20	30
Nitro-Tyrosine	1	2	10	20	40	60
Ornithine	5	10	50	100	200	300
Lysine	10	20	100	200	400	600
Spermidine	0.25	0.5	2.5	5	10	15
Spermine	0.25	0.5	2.5	5	10	15

Sarcosine	1	2	10	20	40	60
Diacetylspermine	0.25	0.5	2.5	5	10	15
Tyramine	0.5	1	5	10	20	30
Creatine	2.5	5	25	50	100	150
Betaine	5	10	50	100	200	300
Choline	2.5	5	25	50	100	150
Trimethylamine N-oxide	10	20	100	200	400	600
Methylhistidine	1	2	10	20	40	60
Proline-Betaine	20	40	200	400	800	1200
Zeatin	1.25	2.5	12.5	25	50	75
Homoserine	2.5	5	25	50	100	150
Shikimic acid	1.25	2.5	5	10	20	40
Glyceric acid	2.5	5	10	20	40	80
beta-Hydroxybutyric acid	5	10	20	40	80	160
Lactic acid	50	100	200	400	800	1600
HPHPA	0.1	0.2	0.4	0.8	1.6	3.2
Propionic acid	0.55	1.1	2.2	4.4	8.8	17.6
5-Hydroxyindoleacetic acid	0.02	0.04	0.08	0.16	0.32	0.64
para-Hydroxyphenylacetic acid	0.2	0.4	0.8	1.6	3.2	6.4
Malic acid	1.25	2.5	5	10	20	40
Butyric acid	0.2	0.4	0.8	1.6	3.2	6.4
Hippuric acid	0.5	1	2	4	8	16
Succinic acid	1	2	4	8	16	32
Glutaric acid	2.5	5	10	20	40	80
Methylmalonic acid	0.05	0.1	0.2	0.4	0.8	1.6
Fumaric acid	0.5	1	2	4	8	16
Valeric acid	0.2	0.4	0.8	1.6	3.2	6.4
Benzoic acid	0.5	1	2	4	8	16
Oxalic acid	1.25	2.5	5	10	20	40
Indole acetic acid	0.1	0.2	0.4	0.8	1.6	3.2
Oxaloacetic acid	1.25	2.5	5	10	20	40
Salicylic acid	1.25	2.5	5	10	20	40
Citric acid	5	10	20	40	80	160
Abscisic acid	0.125	0.25	0.5	1	2	4
Aconitic acid	0.125	0.25	0.5	1	2	4
Jasmonic acid	0.125	0.25	0.5	1	2	4
Pyruvic acid	2.5	5	10	20	40	80
alpha-Ketoglutaric acid	0.5	1	2	4	8	16

alibration Levels	
Cal7	Solvents
800	Water
2000	
1600	
400	
80	
800	
800	
400	
8	
200	
8	
80	
400	
400	
400	
400	
1600	
800	
400	
80	
400	
400	
400	
400	
8	
400	
40	
20	
20	
400	
80	
40	
80	
400	
800	
20	
20	

80	
20	
40	
200	
400	
200	
800	
80	
1600	
100	
200	
100	75% aqueous methanol
200	
400	
4000	
8	
44	
1.6	
16	
100	
16	
40	
80	
200	
4	
40	
16	
40	
100	
8	
100	
100	
400	
10	
10	
10	
200	
40	