

Supplementary Table 2 - Inter day variability

SD1	compound	parent	SD1 Day 1	SD1 Day 2	SD1 Day 3	MEDIAN	STDEV	CV
L-2-Aminoadipate	C00956	162.076	7.63E+07	8.04E+07	8.67E+07	8.04E+07	5249282.349	6.53%
Alanine	C01401	90.0556	1.98E+07	2.48E+07	3.31E+07	2.48E+07	6711105.334	27.07%
L-Arginine	C00062	175.1189	3.78E+07	3.95E+07	3.99E+07	3.95E+07	1122125.817	2.84%
L-Aspartate	C00049	134.0448	2581076	2919057	3985464	2.92E+06	733003.0355	25.11%
L-3-Amino-isobutanoate	C03284	104.0711	5.50E+07	6.06E+07	6.88E+07	6.06E+07	6965526.844	11.50%
L-Cysteine	C00097	122.0273	102480.2	65430.21	117390.7	1.02E+05	26754.80421	26.11%
L-Cystine	C00491	241.0309	1123994	1651520	2000486	1.65E+06	441266.9592	26.72%
L-Citrulline	C00327	176.103	6702750	4892360	9851456	6.70E+06	2509465.234	37.44%
L-Glutamate	C00025	148.0604	7035512	7642614	9880888	7.64E+06	1498588.665	19.61%
Glycine	C00037	76.04011	1.49E+07	1.63E+07	1.51E+07	1.51E+07	766244.0092	5.09%
L-Histidine	C00135	156.0768	1.31E+07	1.47E+07	1.63E+07	1.47E+07	1572440.481	10.70%
trans-L-3-Hydroxyproline	C05147	132.0656	1.11E+07	1.59E+07	2.16E+07	1.59E+07	5245590.639	32.98%
L-Isoleucine	C00407	132.1019	1.48E+09	1.56E+09	1.58E+09	1.56E+09	55761484.45	3.57%
L-Leucine	C00123	132.1019	1.79E+09	1.56E+09	2.04E+09	1.79E+09	240081784.1	13.38%
L-Lysine	C00047	147.1128	2.41E+07	2.30E+07	2.65E+07	2.41E+07	1822698.082	7.55%
L-Methionine	C00073	150.0582	6.13E+08	6.66E+08	6.89E+08	6.66E+08	38851467.54	5.83%
N(pi)-Methyl-L-histidine	C01152	170.0923	3.33E+07	3.40E+07	4.37E+07	3.40E+07	5823935.992	17.13%
L-Ornithine	C00077	133.0972	1.09E+07	1.18E+07	1.40E+07	1.18E+07	1577120.7	13.34%
L-Phenylalanine	C00079	166.0861	1.75E+09	1.87E+09	1.86E+09	1.86E+09	63816426.52	3.43%
L-Proline	C00148	116.0709	1.14E+08	1.16E+08	1.58E+08	1.16E+08	24872708.74	21.37%
Sarcosine	C00213	90.05558	1.98E+07	2.48E+07	3.31E+07	2.48E+07	6711105.334	27.07%
L-Serine	C00065	106.0503	1577800	1968771	2380614	1.97E+06	401452.2176	20.39%
L-Threonine	C00188	120.0658	3870674	4893380	7370326	4.89E+06	1799479.238	36.77%
L-Tyrosine	C00082	182.081	1.12E+09	1.28E+09	1.47E+09	1.28E+09	175932662.8	13.72%
L-Valine	C00183	118.0865	1.88E+08	1.94E+08	2.15E+08	1.94E+08	14162591.02	7.28%
							MEDIAN CV	13.72%
							STDEV CV	10.76%