

**Table S1 The expression level of 130 metabolites in samples**

label	Baicalein	Baicalein	Baicalein	Baicalein	Baicalein	Baicalein	Control	Control	Control	Control
Palmitic Acid	117451355	1192428286	912179668.5	1406119117	131730838	65662388.73	762591521.7	2354156462	1524702476	891344200
Adenosine	206993227.8	911982158.7	777790969.5	330113550.4	1937354834	1150144064	514981613	965400664.9	411371436.8	1.216E+09
Isoleucine	837096216.8	1551970951	1182347334	900865746.9	1474045588	872528005.3	316201306.7	1089161669	280831942.9	1.068E+09
Olanzapine-1	767077.9611	2896706.825	1669766.671	622945.9657	503317.5757	1240462.657	4545497.165	3883607.334	2382296.897	2064684.8
Formononetin	639554.7117	534691.2522	760963.4559	679253.3589	735983.4547	508965.0129	961995.7373	545682.7033	574826.1959	1761042.3
CLOFAZIMINE	324778.0439	276108.5616	336035.5981	415180.5669	334827.782	232790.9754	2578428.757	6234311.761	29070164.36	1082351.2
Olanzapine	370127.433	2459120.256	1364511.324	275950.0959	362017.3424	880711.9341	3891602.14	3959692.954	1364929.782	1375074
Genistein-1	433885.0136	206594.4617	108524.7808	518819.5742	274482.2924	88162.19666	51442.09209	327301.5128	47473.57644	480757.88
L-(+)-Lactic acid	17487717.55	335454208.4	186451291.5	23618974.18	209287309.7	97868882.47	35145453.85	134922398.7	29853744.56	216288864
L-Glutamic acid-1	283038441.5	364011330	474455084.3	201474406.1	487978903.8	428098889.6	202287360.4	330873597.7	318386156.9	368966784
D-(+)-Proline	114017961.2	262593480.7	221043778.1	116441341.2	278361333.4	241006686	29144649.73	215485253.4	53262545.08	254019892
Choline monomethyl phosphate	141845411.9	251796197.3	136604672	174468118.5	264163213.8	155954912.9	108525397	206845041.7	80304153.71	120703365
	152343017.4	614732151.8	400230811.7	179069649.8	779625203.3	536748948.1	206675958.6	536285926.1	125377150.8	529962667

N-Undecanoylglycerine	88832867.13	77868320.28	203865557	70492489.89	84874373.04	71142265.56	228108091.5	277110337.1	125869271.1	122789967
DL-Citrulline-1	83338207.6	127416538.2	99383184.82	81760368.87	100122957.6	86004709.19	25267026.04	101621995.2	15794018.22	127163893
Chlorpromazine	202255.2315	171270.6989	473735.7899	186380.032	207133.1401	208989.3085	302421.4665	166043.8567	1340600.91	190780.11
sphinganine	66619031.99	30390498.39	51856759.88	65330509.22	48967373.42	2224725.753	3564259.148	18594538.11	11433257.56	8742534.7
DL-Malic acid	200335536.5	273839053.9	313411758.8	248508205.3	197045481.8	122933892.7	167280966.7	249322915.7	217607770.6	187199596
Hypoxanthine	85672619.12	254845265.7	47620928.54	210603292.5	246569600.6	115736628.2	209429257	103667626.7	41628096.06	79670152
Creatine	231051694.1	369427177.7	318946575.9	242441938.5	283902039.4	273658457.5	145810798.2	372429872.3	189836275.4	329655341
Trifluoroacetic acid	402959008.4	427833116.4	434809371.8	418166993.8	427010252.5	397791466.7	445480309.8	428934238.2	394036074.8	409356993
L-Glutamic acid-2	115002233.9	230483293.1	259496381.6	154039406.5	263217038.6	147028724.8	113352255.2	129004825.3	156788232.3	171760791
methadone-d9	380413129.8	372316806.1	369793746.4	388148190.6	353154405.9	323763371.3	397018411	364264002.1	349951522.3	329021034
Amide C18	301459435.4	114616973.1	120271092.4	72156990.89	112717690.3	29760227.3	25515692.52	71788177.51	51128735.61	41096024
Spermidine-1	63142775.71	109939814.2	110175242.9	71651621.72	65423079.38	200929899.2	117643249.3	182107962.3	89815848.14	68264171
Genistein	387229.9684	59530.76699	41746.05861	502302.4884	42412.50294	42537.37962	37312.94766	33387.09097	30689.42208	82240.835
Diisobutylphthalate	210241216.5	382575065.9	300284661.7	272227154.6	338879167.7	212043889.2	135228156.5	225879893	141671134.4	212266219

DL- Carnitine	95248035.66	150731210.9	319422249.1	116935612	114687606.1	114678632.1	69071966.32	134880426.1	47542618.48	112512135
spermidine	55202679.5	95929916.48	95064158.07	61429855.78	56916387.22	164731104.9	101998043.4	152197851.5	78400773.17	60566120
D- Sphingosine	132002204.1	146091224.5	320210033.7	198720694.5	186860868.8	9699909.621	3993696.928	17514606.78	12542846.93	15474834
D-(-)- Glutamine	106562565.1	70048334.75	80401820.75	73350053.84	73649434.08	102256646.8	56087930.65	38814647.66	78639796.79	42173643
L- Phenylalanine	297642098.5	217446926.6	207466943.2	260608785.5	204465137.6	118457533.5	83321469.05	143799564.1	79552647.15	123273937
L- Pyroglutamic acid	78225678.15	47208106.79	57234264.13	48421750.21	55536900.38	85514398.64	45497705.67	35941904.41	60989588.92	40722744
S-Allyl- L- cysteine	13884798.21	89173589.7	43237403.69	26904998.77	72205328.62	25293557.69	2964409.488	65173576.19	2710218.83	66462648
Cinnamyl alcohol	17579474.6	26503684.41	21357313.26	16088145.3	12546789.2	11840180.51	14783919.29	97831845.6	6819605.073	67979136
Taurine- l	97344070.01	69696739.52	89174461.84	44903041.15	62557486.28	81208001.13	48501217.24	85515540.55	74210057.69	105919638
Thiamine	82259554.26	75597589.95	88828865.19	64230874.62	95665952.68	57298086.7	49023739.51	105555704.6	46050752.19	103425369
Erythrose-4- phosphate	25847055.99	34575265.63	82170303.31	11191810.32	40228975.05	24824998.98	23858926.42	46565968.3	68917731.38	55431779
L- Glutamic acid	96668225.22	107337243.6	135033203.8	77508121.74	157752265.5	133653365	68826839.29	101114720.9	75184397.46	99507193

Pantothe nic acid	14935889.19	47857233.31	33121966.82	14777674.77	26113108.92	17166806.47	23175369.71	32247894.63	30730287.84	27437624
Misopros tol	2080017.271	1961457.009	2026426.813	2237547.839	1849569.068	1750698.737	3814583.805	2778097.782	2454682.855	2742634.4
Ac-Ala- OH	26216669.7	51863416.37	39885711.83	47519248.53	92077736	47076315.13	17865618.5	69267992.35	45333557.97	77776212
Hexitol	15575842.08	17702922.75	14604827.21	15847393.23	12441408.81	15864043.1	14097134.12	119561595.9	12766185.96	63331579
Taurine	61298926.73	108300869.9	79247359.79	60162387.43	102760448.1	53334134.97	30609949.77	74950793.78	50569178.57	79775596
L- Glutamin e	51555609.54	36710959.23	36043801.21	36068951.96	25208677.89	32513694.68	31076315.5	10312774.03	41965061.29	10594631
DL- Citruilli ne-2	24048646.28	42518869.66	23902361.03	13138745.58	30285590.19	16571589.94	6085939.282	28498295.94	4673686.514	34644656
Creatini ne	27011470.29	61092371.02	50644652.01	33846013.94	65236860.48	37851022.99	29472755.94	41475947.84	22498853.12	67628109
6- Oxohexan oic acid	1301309.017	18515610.78	12236173.13	3181722.151	9332767.044	5569767.871	1016676.57	21424966.51	812303.9047	16458987
Estazola m	1177187.382	2524440.092	506199.0556	1021676.859	354652.9421	18554558.31	15715737.98	15459307.09	7187533.536	9104246.3
Indole- 3- acrylic acid	109031534	71501408.47	66269189.47	120691108.8	64518870.53	37957496.95	21767015.52	22752124.22	21341851.71	11938447
Pyrophos phoric Acid	89789064.93	67412005.24	58566451.66	107522464.6	88440546.27	118512081.8	78504083.81	107195043	76850563.04	96302082
Caprolac tam-1	43914819.57	55954598.34	65688523.49	48966276.65	66949499.29	49094117.83	29204557.71	54965022.58	41246897.85	43350464
L-(+)- Aspartic acid	21396611.1	47313504.59	35941303.83	17595545.31	20597988.64	22560656.88	16825170.06	30189663.93	21137599.34	40869030

Ketotifen	819474.6546	733484.2477	760490.6518	633549.6504	722125.291	618325.8363	1123464.958	815352.1117	644268.138	684267.51
D-Mannose	17866621.18	48758966.25	14650684.02	33696523.19	38112502.67	73010308.6	79797219.09	91942819.64	38335120.76	104735081
6-phosphate	77642202.98	71702375.32	60979906.3	76035361.43	59620327.56	49550034.02	27659688.73	45746462.15	24458933.39	41472016
L-(-)-Methionine-1	20355027.91	32267775.25	17056481.77	13049343.04	15949447	22891616.24	8031944.623	19229200.3	13152401.41	30877891
L-(-)-Asparagine-1	66073321.99	59633888.87	51074365.6	62374802.35	50016465	42034928.36	23500093.25	37141107.02	21323378.51	32923459
L-(-)-methionine-2	988572.5131	921736.9838	1136000.821	1001991.672	1077473.17	869862.9501	1439549.2	861680.4554	899306.3013	870035.56
Mycophenolic acid	22164993.41	54858619.68	29909354.69	18891650.22	51538820.23	53248067.53	45816971.16	76862072.02	19673191.58	84173567
ribulose 5-phosphate	32501924.37	47572654.53	55337622.41	37377106.44	70021322.09	45675943.67	18485419.24	54776071.89	21214988.23	52393928
g-Butyrobetaine (9Z)-9-Octadecanamide	30996352.6	34656177.2	54975244.49	48987278.22	41637082.6	2962722.905	2899983.925	6871267.003	4701022.141	5364802.4
Hypotaaurine	18653751.57	26253791.26	17344383.55	13956663.44	12008560.46	17208805.09	8988553.042	33679383.91	10731415.33	29935076

Arabinosylhypoxanthine gamma-Aminobutyric acid	3057928.583	13543942.82	7084908.635	6763500.832	17214316.61	14250635.64	13098322.06	14083516.28	2111200.77	12693600
DL-Citrulline Sulfamic acid	20292870.71	12811757.01	15750639.55	9084263.011	22434886.62	14901377.6	6753071.287	18009753.11	7614427.245	17625901
Methionine sulfoxide	11585344.96	16909955.8	13907889.35	8618253.717	13268334.32	10940620.76	2366113.507	13384444.52	1554689.242	15745498
DL-Arginine	1771040.943	8623760.918	4129784.373	1368418.286	3931670.799	22159029.9	12137448.1	19794874.41	12601993.07	22108985
Methylmalonic acid	12428160.54	18753456.9	16093069.4	10832325.62	17045228.7	17364303.74	8394529.868	22139818.5	11500453.57	30395642
Adenosine 5'-monophosphate-1	2050498.254	1518133.098	1043368.986	13675916.81	1382883.328	2482812.838	5859159.588	2498625.194	31485119.12	4141284.3
N-Acetylaspartic acid	1064321.825	4561189.786	3895171.02	4418071.512	3880957.813	1113954.67	7345586.908	1606659.252	6891008.151	1530277.2
Hippuric acid	8650327.519	8328056.168	9047587.091	7258774.659	7263030.298	32695858.93	7212949.228	10664368.71	13484862.3	13161136
Nicotinamide	15896585.8	42324420.44	44734064.8	12733804.99	43411766.78	31045114.22	11666477.35	47818455.52	13396614.52	40707006
	454583.4355	7201278.847	2603345.689	660153.8093	1614120.056	1420661.837	790419.5507	2584386.292	416699.2153	2484770.7
	8850858.602	21570214.5	21740830.35	6820896.61	24879379.08	23124624.41	8437012.323	24560422.62	11044379.69	27368217

Glycerol 3- phosphat e	10468639.36	24524883.69	20750767.76	6069211.227	30228532.91	39847373.16	12195375.96	30201715.64	10492585.18	30010665
noradren aline	1415289.711	10265524.55	8422717.685	1855325.056	6969046.552	4054555.466	1258890.203	6129689.704	1327599.287	3229447.5
Dihydr ot hymine (E)-p-	4706644.694	11674678.34	10848958.18	3040862.228	11615776.22	10482953.63	3606045.922	16793608.72	3981712.526	19321946
coumaric acid	21223622.72	21782933.48	19093715.57	17697142.11	18503482.45	12364438.39	4115244.816	23738466.5	8755078.835	24485177
propiony lcarniti ne	7909611.993	19174566.81	17251423.81	8891924.151	25681885.48	12348678.88	2546932.973	17497326.27	2793328.909	16120172
Fomepizo le	5499302.677	5481818.189	5189799.922	5500420.038	6024054.63	5449505.221	4049697.234	4077652.018	6173260.87	4806843.4
Flavin mononucl eotide	4593647.559	10486259.2	6123254.741	5445679.953	5549670.702	8204623.458	4964094.425	10574765.47	6646660.268	15471850
N- Acetyl- L- aspartic acid	6900960.717	19116977.95	22561855.1	6910527.145	29666927.33	11346844.9	4404339.53	22831738.14	5133491.876	21318400
L- Hydroxyp roline	16130097.51	21073142.38	18518304.7	9490544.833	18333434.02	15036498.56	4452418.214	17993809.43	4472092.606	24984238
L-(-)- Threonin e	11444828.96	6291840.094	7394506.57	8104664.84	5541038.198	7990324.994	5668339.394	7614064.257	6963337.506	10630180

6- methylte trahydro pterin	5824135.459	8069264.089	2015990.444	13134381.14	9675389.358	6829450.119	13680063.52	4688125.722	3034441.188	4133427.2
L-(-)- Asparagi ne	14825025	11230555.87	11510631.21	11286441.31	19206657.83	2175540.326	2797619.05	11595972.93	4237534.926	12838800
DL- Glutamin e	20199562.7	12374230.97	11565776.98	15989055.7	11354801.17	11219911.3	6519673.077	2915230.976	9930480.902	2739838.1
DL- Histidin e	2447020.224	15073406.12	12427473.67	3772170.277	10810652.27	9147755.841	830018.2555	6692882.018	995645.8412	5354641.5
g- Glutamyl cysteine l-	5033713.362	5169389.354	5470703.817	6136991.898	5579745.095	4094420.112	1926732.497	4273431.76	2948459.414	3908145.6
Histidin al	14053166.61	14050149.95	17688428.95	10537872.69	16126865.78	9174645.665	8009872.786	10803677.39	6756903.238	13677830
TROLEAND OMYCIN Cyclo(le ucylprol yl)	3653818.387	6195926.983	3382031.606	8484049.302	7043852.177	1596459.395	9010086.204	3757349.469	2626796.657	2799643.1
putresci ne	1255581.592	25502277.26	795264.542	982899.0899	942348.0917	3116895.339	1262658.966	774778.7019	609600.1354	671859.76
N- methylpr oline	6415225.146	16077316.3	13327800.43	8421043.966	15027022.78	16203351.76	13416433.72	17336251.78	15128156.72	19454160
N- Tridecan oylglyci ne	5312969.457	18128178.19	6946417.272	9208315.811	24187141.77	13325454.58	3083274.409	8317023.413	6893821.246	7742883.2
	3553294.719	2039880.541	6475391.981	1898107.565	2986926.64	2810540.499	7018470.774	10394897.48	4354158.667	2720613.3



Adenine	4306415.819	12741883.84	4717009.339	5584212.906	8624092.619	8092760.937	2542125.223	8749104.225	1107665.064	9961700.8
L-(-)- Methioni ne	10683425.18	10356746.93	8127340.294	10690128.24	8746031.563	8172073.503	4936509.126	8308019.933	4012369.534	6153611.1
Pregabal in	8005906.764	13016610.11	12590258.02	6165175.664	11551673.66	9536464.717	5815936.599	13812177.54	5105768.706	15106116
3- (Sulfoox y)-L- tyrosine	10648257.43	12861689.73	12696752.54	9391742.497	12887892.72	10660374.51	4051090.327	11361158.67	4312325.952	11289908
Nitrazep am	358922.6688	418213.3494	475455.1393	17138225.24	403363.2709	513881.5939	2253496.758	2800889.917	857868.5684	1326462.3
.alpha.- Aminoadi pic acid	3589779.857	5553068.72	5176548.741	3558012.283	5466368.233	5120757.093	2660591.349	4834319.686	1968839.55	6436861.6
DL- Ceruleni n	10207703.91	9755505.116	9765760.808	8619791.391	9722046.651	11487655.59	12153573.28	8750786.961	10609143.42	10084700
Pyridoxa l	2622630.762	1953007.307	2893768.188	2762168.574	2936854.144	1655009.3	468922.2717	2155108.087	443250.0037	2404157.2
Adenosin e 5'- monophos phate	1300610.48	1624881.209	1643510.073	936818.4423	1454529.38	2288809.064	1193977.784	1940087.231	2748535.531	2212905
Caprolac tam	9700493.9	5891718.368	8889843.262	6572264.671	9169695.359	7154830.008	6829914.001	9114699.603	7829512.389	10684625
Hispidul in	120248.94	98569.05313	111205.8364	112069.72	130924.1343	98755.74836	52245.53817	55284.71046	51320.38662	54921.243
8- hydroxy- deoxygua nosine	1410727.118	9987806.914	4944571.209	1931268.591	11637885.98	11230759.23	11419668.8	9762965.934	1792122.816	8552287.3

2S- Amino- tridecan oic acid	708717.7681	589256.5209	362386.2621	676913.7474	792210.9079	861165.2699	9111444.806	12770427.04	3211701.208	3123205.9
N- Acetylne uraminic acid	1069327.784	896844.6295	1314191.264	848831.4239	1848713.571	3548251.732	1533807.323	1731347.142	1935893.968	2781720.5
Fumaric acid	3000083.414	13099938.72	7346135.263	3074452.614	9394541.608	5223513.462	3902257.219	8342021.503	4629274.307	7935135.8
acetylsp ermine alpha-	410285.6568	1606384.158	1723320.978	421191.8475	1129983.693	1483305.679	408602.9323	3323472.051	452510.9893	1090944.4
Ketogluc aric acid	1029095.751	485237.8417	2925271.399	795459.629	1474057.808	894188.4755	708307.6589	3519017.311	817115.0621	3392100.1
meglumin e	4236394.926	3376337.972	5802006.678	4406769.392	4171704.846	5213533.401	8796383.396	2996972.68	1921905.335	2893339.7
N- Acetyl- L- histidin e	161867.1247	2820612.415	1381680.074	174084.526	901921.7884	706824.089	356123.3918	1695908.418	233890.5536	1128672.1
beta-L- fucose 1- phosphat e	364778.7335	1561707.971	1410718.88	346723.1542	5143159.056	2558740.274	296978.0305	2764345.068	286834.8467	2784866.4
Guanine	722750.5934	3765930.138	1118467.728	1623853.179	4106603.777	1748928.512	6306999.032	1274728.524	540138.1303	1198635.3
L- Cysteiny lglycine	3412056.501	6839102.46	7937879.13	3656038.342	7655492.621	5020745.295	3414318.993	6257201.601	4775130.681	6100196

D-a-											
Hydroxyglutaric acid	1523992.864	2483835.679	2221804.747	1553403.676	2810306.019	3045861.712	2355900.309	2184632.941	2801476.769	2494039.8	
Adipic acid	2629810.658	2145261.32	1984409.116	2802949.775	922540.554	2486662.079	5148729.744	5351731.846	3806855.175	2323296.5	
Luteolin	73738.82609	77355.83211	79239.80253	75432.35822	79932.89203	73270.17416	46940.29154	46893.81196	45823.99158	46929.417	
Ecgonine	2175610.167	1211658.423	852357.7903	2131016.179	3178886.682	2403324.097	1995575.288	964514.4663	745226.7414	985159.94	
Metirosine	1815983.934	5395222.672	5590144.052	2278699.736	5442746.675	3371907.555	1951894.729	4642779.013	3030911.488	3566253.7	
16-Hydroxyhexadecanoic acid	733684.1396	2674963.744	1175986.947	653664.7894	1731702.242	803143.7109	577772.3464	689828.8707	300350.961	976118.31	
g-Guanidinobutyrate	1349677.576	4798989.338	6503509.185	1779698.527	7876339.857	5575486.579	834819.7768	2581450.068	656554.3584	2489783.6	
trimethadione	2339253.842	2946658.92	2081724.223	3228614.545	2020444.525	2296466.917	1039452.851	1722271.167	3224235.364	2428007.8	
acetyltaurine	952473.8453	3194619.892	2640299.205	1081640.685	3014374.239	1982156.209	711174.8018	5191092.914	671008.5413	4286420.4	
2-Mercaptobenzothiazole	87056.84989	158031.5196	4394526.408	1374743.197	453333.3307	184586.0276	41924.09243	136929.0764	64405.63627	169102.07	
Chrysin	775000.7666	7790401.698	3862745.392	1071608.207	3188360.328	2261688.755	41037.92634	38406.03753	33966.91352	37113.999	
Orotic acid	1357033.235	1288999.51	1264655.729	1213033.783	3928868.695	3044701.066	821487.6609	5988647.939	95090.7466	4310886.6	
Dibutylphthalate	737726.0829	634855.5193	854731.7923	407332.1902	689214.8338	670713.8194	416856.1337	564906.288	811771.9979	720904.4	
label	Control	Control	Control	QC	QC	QC	QC	QC	QC		

Palmitic Acid	77898794.46	1869303771	1370193176	145663049.6	156598532.5	144524001.5	172996555.3	157434433.3	215861100.2
Adenosine	31893130.07	2028422605	378496699.4	615324397.7	470820676.1	612720657.3	679854177.4	541062431.4	572148839.7
Isoleucine	145218653.3	1600192647	523835631.9	889171954.4	886981015.9	870616911	448251685.5	723345707.8	787506163
Olanzapine-1	2768647.205	961300.9856	1621784596	35494043.47	32279015.93	32546649.16	26686669.42	28169208.24	30183738.23
Formononetin	622872.1379	649728.9191	1054464.809	16771641.61	17879081.94	17721049.96	13400609.89	15656060.4	16833236.58
CLOFAZIMINE	216653.5922	289775.4446	10064351.47	1335098862	1482572383	1507384258	1368973875	1182798898	1518254232
Olanzapine	1889228.169	198707.5894	1555986390	35391834.17	31831643.09	31559923.54	25967391.69	27557092.19	29314241.28
Genistein-1	97175.86343	1287170.176	59978.14886	89831254.4	86902818.1	113221445.9	77722856.18	77281555.07	82752499.01
L-(+)-Lactic acid	32352072.21	394550519.7	45962601.83	95405786.28	89859710.4	107635403.4	67946486.62	87137944.41	118545279.1
L-Glutamic acid-1	139319653.1	240653686.8	268603058.1	320443293.6	311373946.3	317146661.1	284138627	288413004.4	277553567.7
D-(+)-Proline	99754138.82	306622108.5	45135381.17	184541876.7	222262450.8	160195210.1	160584769.9	187521812	195981212.1
Choline monomethyl phosphate	42137870.95	194541295.6	166451711.9	171413358.6	192491605.6	209875458.2	199073251.8	194810947.3	169784306.4
N-Undecanoylglycine	52559121.12	730806455.8	315471053.1	260466080.9	262916356.9	263925220.6	234662962.6	239096792.8	257719120.2
	61581510.71	62278870.08	62785737.06	211890348.3	212364861.3	213587347.4	152808130.2	169598918.2	160041916.5

DL- Citrulline-1	48219376.21	130737048.8	35437823.61	67129003.55	82474842.86	91627974.1	68863861.2	69276899.76	75582463.16
Chlorpromazine sphinganine	164528.8475	540501.9544	196587.5364	3268049.568	3385011.648	3821483.193	3285831.686	3001680.112	3985487.797
DL-Malic acid	8435895.857	271943342.4	355560259.9	192273944.8	206375670	224521898.8	152096846.2	156312608.3	180537695.2
Hypoxanthine	1525065.33	218849625.4	514527141.8	85982391.69	95969882.3	105167045.5	85980714.32	91367459.85	102077356.4
Creatine Trifluoroacetic acid	20606661.97	411037688.7	196569400	245220197.1	256177802	320980284.8	256862042.2	290212723.2	303517022.6
L- Glutamic acid-2 methadone-d9 Amide C18	285871532	430653292.1	490533282.7	411731294.7	401421927.3	421896816.2	409042586.1	426447479.5	416763940.5
Spermidine-1 Genistein	39222183.19	234110540.9	147444597	143786049.7	191234894.5	230864008.4	93265963.84	119631990.2	159455397.8
Diisobutylphthalate	208528500.3	385590040.8	432323829.6	360986530.5	366272477.3	374561632.2	344415540.2	358666488.5	343638309
DL- Carnitine	15951335.23	156947117.6	48702047.47	104440180.1	109186763.9	64619417.79	96921897.06	86235023.73	90106243.22
	45231124.98	53037701.87	191122611.4	103394148.7	101645976.3	104015392	61958077.97	71066527.32	97970674.88
	32011.49375	161631.6977	33148.71773	31026235.13	32924922.22	32930741.2	22181567.84	25552209.76	28469162.69
	93466575.07	378520050.9	336336457.8	218983679.4	237343141.3	221838298.6	139066473.9	155977096.9	174373509
	25165633.13	202050045.5	86844816.93	120288984.1	84964948.53	115946073.4	65011991.58	84826000.09	107338527.3

spermidine	35985581.47	47561965.29	164501252.2	88635598.9	87670401.9	90227457.51	54947428.72	62485760.61	85713658.95
D-Sphingosine	6558247.998	247450074	76995197.86	57433275.68	61062699.35	63996274.61	50443461.94	65606990.37	75058103.75
D-(-)-Glutamine	25714785.52	24476292.79	51152161.35	62283287.56	62565064.64	77198639.69	64979882.87	64356132.8	59963396.49
L-Phenylalanine	17805243.09	176139272.9	149600917.7	190324779.4	199075216.9	197683343.5	151969176.1	167716271.5	179164781.3
L-Pyroglutamic acid	23917681.1	30188841.43	40082884.46	48167013.2	48296799.02	54297088.86	49322285.32	46591186.18	44962239.37
S-Allyl-L-cysteine	5681229.951	99987895.21	7578398.829	37417699.44	39252342.78	39763875.52	27454533.54	25689841.33	26553919.68
Cinnamyl alcohol	94784329.86	125336010.6	11762658.96	47326807.96	49607922.45	45059243.3	38076883.96	31440110.49	29108940.98
Taurine-1	58532905.18	74003614.68	51521089.6	72031510.28	66725482.76	67826706.5	82285018.84	65492311.94	76817280.81
Thiamine	36432374.42	121626640.5	82814519.7	93106885.54	89547363.43	114825918.6	66658980.83	67561123.13	72487140.61
Erythrose-4-phosphate	4697367.928	55056922.6	32579883.35	39738170.33	37967384.94	39709092.81	33225392.69	34438961.91	35820090.02
L-Glutamic acid	13746989.8	90223108.2	82348437.29	108171686.5	84694627.38	85521813.4	100559346.3	91815159.49	86585748.16
Pantothenic acid	3077108.173	47451339.74	38010332.29	39340307.71	39419988.86	37999651.62	27630567.16	29345709.94	32094613.21

Misopros tol	1818444.933	2620695.101	3184038.664	5377189.938	6550855.936	6134487.109	6310587.003	4917685.121	6431492.84
Ac-Ala- OH	32082027.03	51990923.72	27180921.89	31133577.69	33591061.97	38522584.44	30826236.61	32022380.46	33389310.13
Hexitol	41709665.2	35514558.42	13703309.32	29138630.36	30170139.12	22758789.18	29005049.97	21221583.48	33726615.85
Taurine	9525171.021	74125747.89	52417214.04	62124841.32	65434332.98	66403812.28	33172276.27	55614496.33	64780204.6
L- Glutamin e	11820019.59	8560095.211	19155162.76	28064832.04	28211009.41	34423504.9	33410061.98	28886581.52	24864911.76
DL- Citrulli ne-2	8054078.413	28252170.68	9000224.357	19148205.94	15710245.22	20609572.44	13595684.97	16031091.67	17222752.92
Creatini ne 6-	12074240.78	49854777.49	31548862.57	26985921.29	30414037.14	37658317.99	29464095.85	48489600.81	37888270.08
Oxohexan oic acid	1033314.158	35241598.07	2872220.507	10757946.55	12087019.95	13284191.23	7044232.347	9618671.286	10234944.55
Estazola m	9119235.875	1943449.76	1659967.512	8058462.194	8077650.094	7223186.944	9136426.249	8900560.558	8762694.069
Indole- 3- acrylic acid	2390733.4	48427141.45	45383916.18	65486313.27	63159664.06	67239227	46252478.85	52003596.54	56463045.87
Pyrophos phoric Acid	32334431.25	4836540.215	54589365.66	85770096.94	73382394.64	88650237.84	76002857	78160125.75	88159282.45
Caprolac tam-1	32392778.1	69572712.82	44870827.04	57653507.98	57953130.65	66177441.17	59453719.93	60453410.9	69497763.2
L-(+)- Aspartic acid	17076875.03	44356508.19	17117977.79	26207982.25	27396367.46	28560473.35	28533095.03	25724671.24	30476775.02
Ketotife n	607962.4383	727193.667	894888.3511	2514685.927	1961051.76	1980395.585	1919314.976	2065793.439	3013184.909

D- Mannose 6- phosphat e	14064593.7	76098245.52	25149169.56	44112203.49	36801386.48	45319478.88	40979245.34	30323763.11	41273989.1
L-(-)- Methioni ne-1	6799319.622	74040101.41	39928006.27	58741950.03	51421406.07	63130086.97	49761240.25	52352302.43	51360795.15
L-(-)- Asparagi ne-1	23007831.44	21748818.91	8179722.441	20269101.55	15427675.22	20510123.09	21552457.16	20258514.21	17885290.46
L-(-)- methioni ne-2	5898472.839	62300879.75	32567887.82	48919094.77	42353469.08	53172792.57	43569204.28	45057553.07	42428182.4
Mycophen olic acid ribulose 5- phosphat e	829525.2957	1000554.481	1015092.48	3869220.599	3999358.339	3934374.28	2707369.194	2889741.491	2900429.668
g- Butyrobe taine (9Z)-9-	9030009.337	56015333.62	19584320.07	40538173.69	36712963.38	33878977.02	32740773.9	29565851.09	36730646.97
Octadec namide	2690788.971	63525066.97	18939745.3	14085843.64	14527713.62	17244391.41	14063296.52	17851265.43	18906230.86
Hypotaur ine	10847259.79	30881291.62	4398323.065	18457527.36	24355366.82	18165740.23	16428107.95	18252124.15	12567879.4
Arabinos ylhypoxa nthine	640107.2344	21756045.51	15791193.42	9231249.034	7142324.909	7764724.959	7357516.235	7177188.36	7123806.41



gamma- Aminobutyric acid	5590167.691	12626045.61	5999123.688	17474666.59	14367772.91	16565019.27	13146359.82	13477033.81	13659799.54
DL- Citruilline	1322284.427	18825303.4	4421515.398	8220992.542	9102797.914	9967204.385	7625230.768	8684907.337	10079501.33
Sulfamic acid	11786618.59	3652419.281	2520324.44	11708463.25	10445810.5	10134279.75	10703815.85	10963036.6	13753964.57
Methionine sulfoxide	11772954.84	26469873.88	6677597.956	15456458.88	17642571.89	15663085.43	17394972.55	15436233.5	15645875.2
DL- Arginine	10255238.56	2603386.994	3770080.181	10626564.91	12176173.9	11892941.45	8388147.863	8914224.118	9008238.95
Methylmalonic acid	1176198.984	7742981.247	1162138.202	3251119.48	1795188.569	3482046.137	3907281.285	3364388.531	3995458.759
Adenosine 5'- monophosphate-1	6430053.884	4391513.592	5956420.344	14830225.53	14718321.91	16202504.61	12557907.86	11437009.02	12987857.43
N- Acetylaspartic acid	3427419.446	49687388.28	26964969.23	22034931.98	26105039.17	29524378.23	18165935.19	23434144.09	23085084.01
Hippuric acid	421533.4541	5181176.172	2183351.14	2607772.785	2536322.439	2610952.133	3510396.898	3939973.423	3713600.648
Nicotinamide	4095267.31	17993475.33	5777390.6	20522307.31	22767188.07	16328240.32	14435265.04	16381466.58	21521140.58

Glycerol 3- phosphat e	4965837.565	29995160.86	15456773.09	17215017.67	17054038.15	18832028.23	16500155.2	19335035.39	18060364.27
noradren aline	904553.171	8367933.539	5086257.778	3445502.913	4165466.126	5569777.039	3317458.424	3258847.859	4039798.725
Dihydr ot hymine (E)-p-	7002058.717	19366851.82	3758524.682	9924222.071	9236079.933	8083913.393	8110177.244	6711988.687	9155800.235
coumaric acid	7974198.082	23085665.71	4902007.412	15955489.87	20167795.6	18894445.63	13117096.84	17695499.16	18137535.76
propiony lcarniti ne	746974.3531	17197712.33	5043444.496	8829667.79	7505311.063	9995172.282	8140077.079	10971335.97	6643353.677
Fomepizo le	4342832.896	6735623.786	6014084.321	4730608.138	4098621.95	7067090.437	5778223.885	5120248.542	5425582.498
Flavin mononucl eotide	4606347.508	7084013.108	5015116.153	8585483.313	9162086.667	10420925.18	7768919.29	9605251.861	8263737.164
N- Acetyl- L- aspartic acid	282402.8558	32632285.7	11797795.4	12125138.06	12305738.31	12732388.39	7429686.29	8102349.86	9375333.037
L- Hydroxyp roline	3582727.399	26942622.57	5573433.038	12297272.44	14557285.71	12748654.05	10681591.02	14396866.61	12836623.13
L-(-)- Threonin e	4502034.836	5370863.517	3298753.46	6989155.385	9013481.528	8904162.992	8774175.751	8614919.472	8538728.161

6- methylte trahydro pterin	81556.73678	12089932.16	29112335.77	4465269.895	5779382.484	6185323.502	5197658.55	5409980.612	6526392.752
L-(-)- Asparagi ne	6729335.842	15419459	2949058.948	9974416.543	9699112.209	10368174.18	6049916.749	8511331.091	7087207.567
DL- Glutamin e	639477.9813	2169520.455	11075713.6	10387748.32	12533527.01	12360605.14	8947067.674	12029331.07	13184877.26
DL- Histidin e	849449.6335	16953754.93	1907000.924	2791009.849	2666433.908	3538514.612	2038800.146	2727283.566	2715238.724
g- Glutamyl cysteine l-	260061.0734	4072533.974	2963149.718	6774245.271	6419947.844	6526819.256	4367810.335	5030044.231	5984918.382
Histidin al	4138015.209	15245203.73	13782134.15	12969975.6	11306111.4	12775949.3	9332582.277	9885047.541	9926797.187
TROLEAND OMYCIN	2741679.279	3040313.414	3419378.949	3262485.135	2843143.347	4974313.481	940146.5338	944076.7601	1050484.781
Cyclo(le ucylprol yl)	736183.205	804253.3089	936627.9489	1138871.988	1143881.441	1179401.871	1778878.459	1987191.027	1772788.769
putresci ne	5160226.422	12482593.61	12515949.91	10011559.27	10207158.88	10814091.76	12307504.17	12901638.63	15578575.42
N- methylpr oline	3117316.825	16394116.85	4909440.498	6648611.358	7392602.222	6802099.828	6306422.54	7629751.504	9248840.444
N- Tridecan oylglyci ne	2380520.904	2428116.036	1591268.923	6678606.776	6101313.82	6713248.022	6593112.192	6191330.142	6629916.236

Adenine	2451833.958	10613476.38	6360664.077	3556610.097	3677079.092	3973640.29	2844442.913	5438391.36	3269202.129
L-(-)- Methioni ne	3086053.834	9410864.61	5900677.382	8159715.65	4857857.2	8450616.548	7862909.897	6817156.905	7594106.37
Pregabal in	6218934.142	13536894.7	5944005.733	11385478.7	10389934.66	10428232.8	11517560.86	12712340.89	11162448.56
3- (Sulfoox y)-L- tyrosine	2846009.257	11933183.91	4473292.943	9007406.002	13326513.53	10984606.64	8425586.965	9161646.25	9250634.836
Nitrazep am	1652713.124	392647.2326	984194.3897	1094301.992	1445464.91	1272612.072	1587314.708	1374424.839	1240760.333
.alpha.- Aminoadi pic acid	4161807.325	4220859.568	2078516.358	4456720.648	5074078.394	3711727.106	3329559.15	3980458.508	4131268.329
DL- Ceruleni n	16127292.82	8378158.127	10740996.83	11167607.82	9671710.11	9568220.547	12238347.71	12287612.62	10641376.14
Pyridoxa l	583392.696	2823876.935	1266543.65	1485043.022	1864797.126	2712258.893	2257979.617	2281765.18	2202180.363
Adenosin e 5'- monophos phate	2085736.924	769667.4391	884419.5673	3331663.673	2326768.047	2938538.996	2549663.034	2153661.488	2238978.468
Caprolac tam	4370703.537	6838515.216	11055539.34	7448994.329	6275075.724	7735692.997	8099587.5	8128834.515	6565710.07
Hispidul in	52266.07658	85599.69124	77105.23046	556396.7084	617239.1092	625627.3733	465109.8206	537784.7433	673601.7273
8- hydroxy- deoxygua nosine	968939.4643	8013561.657	6329331.52	5537146.939	3642416.022	4242574.658	3565937.651	3647234.656	4188607.627

2S- Amino- tridecan oic acid	2581329.421	336651.1421	340887.5274	1703828.683	1883516.638	1797489.19	1635015.463	1776599.752	2101551.449
N- Acetylne uraminic acid	1193286.94	800372.6443	1446599.315	2273550.509	1850586.554	3376057.181	3345518.864	3049870.928	2772112.65
Fumaric acid	1025132.934	15074272.87	10203510.37	5333032.87	4893485.163	5102208.336	3382321.277	4013261.209	3926650.51
acetylsp ermine alpha-	591133.7011	957889.5044	470777.6704	1641172.025	2188037.287	2046048.565	1192833.817	1634987.714	1620956.676
Ketoglut aric acid	85484.54756	1172487.611	685253.7448	2684320.492	2273058.167	1869875.702	1879866.608	2266298.811	2244647.011
meglumin e	3293299.044	4821224.926	5637800.238	1385688.416	2132366.267	2083022.666	1591636.642	1198380.882	1448030.7
N- Acetyl- L- histidin e	190415.3696	3568829.227	1242173.119	711955.8708	923174.1679	1140263.347	923967.0293	873432.4907	866408.8857
beta-L- fucose 1- phosphat e	1575690.828	3119132.632	385638.9331	905532.0214	1063382.062	1195661.731	997345.5619	996553.9651	1229535.657
Guanine L-	41024.56351	4239885.297	12562361.92	1782814.371	1275833.539	974358.1799	1212188.748	1183784.008	1321761.825
Cysteiny lglycine	429140.5446	5464918.546	4893019.363	6652257.77	6624614.795	6824599.414	4640003.613	5242240.659	5712339.679

D-a-										
Hydroxyglutaric acid	294695.8509	1773367.229	4420123.735	2111045.414	2402300.283	2841177.774	1650548.199	2069577.433	1982783.271	
Adipic acid	2263267.45	1565791.177	3681426.257	2728629.763	2693095.137	3390624.41	3583344.149	2465289.674	4531102.958	
Luteolin	46144.22862	50030.89877	53383.17639	383185.1696	399280.7155	462022.1352	213800.6368	403724.9601	439249.4707	
Ecgonine	642023.3437	1119320.384	1441181.772	753887.1939	548986.036	792496.9373	630527.7319	826224.7446	755790.1656	
Metirosine	995578.0736	4006624.698	2394610.632	4336828.613	4694037.361	4419251.856	4812134.445	3401708.726	4914801.894	
16-Hydroxyhexadecanoic acid	316761.5137	1353289.439	563804.6033	1255499.549	1522951.75	2177232.263	1401441.887	1173506.202	1460136.093	
g-Guanidinobutyrate	379489.6035	1970242.485	538725.5413	2133975.55	1939354.435	1900098.215	2362816.51	1919909.622	2326720.7	
trimethadione	3292549.909	1246011.804	1402843.429	2546356.503	2377577.584	2148626.164	1819401.69	2421264.155	3020765.508	
acetyltaurine	505925.7778	4390447.775	643047.4356	2003283.695	2244612.145	2557582.355	2029688.659	2063872.754	2632244.632	
2-Mercaptobenzothiazole	114726.4179	617182.234	480452.2465	308671.6815	288836.8021	315296.3986	259823.0527	174210.5147	186059.2169	
Chrysin	35871.95945	36797.44713	37564.32459	188645.5675	149602.6837	213649.8399	120313.658	132654.81	180035.1857	
Orotic acid	598149.1016	2629371.168	798616.0254	1292820.416	1301422.836	1276461.77	1112813.392	970397.3054	1045292.301	
Dibutylphthalate	566968.6393	734903.3847	579810.2965	953725.5771	789179.1237	576475.8083	631631.5388	554266.7652	612693.8276	
label	QC	QC	QC							

Palmitic Acid	169916328.2	156591297.2	140548478.7
Adenosin e	516305572.7	627328467.6	580428341.3
Isoleuci ne	933480869.7	822369004.2	756095997.4
Olanzapi ne-1	36930138.54	31913544.9	30700781.99
Formnon etin	17269671.15	18560335.92	15191721.47
CLOFAZIM INE	1400183540	1504489248	1349035497
Olanzapi ne	35776379.16	31439214.58	30409399.5
Genistei n-1	104646208.5	106446543.1	79637811.75
L-(+)- Lactic acid	129074822	75675197.28	84433008.05
L- Glutamic acid-1	316514490.4	302231438.5	323568629.9
D-(+)- Proline	180761021.9	217257617.4	160563885.9
Choline monometh yl phosphat e	232856413.3	204694031.5	168596270.2
N- Undecano ylglycin e	277116457.1	249041447.9	255315409.2
	245617501.6	171976640.5	213685615.2

DL- Citrulline-1	88148851.24	81957448.13	71009007.37
Chlorpromazine	3125869.699	3508528.92	3433605.352
sphinganine	30022329.99	23262468.59	24665963.21
DL-Malic acid	232536344.8	197715853.8	182581181.7
Hypoxanthine	92219119.01	99086885.3	89400164.89
Creatine	309941770.4	265161752.5	254385304.5
Trifluoroacetic acid	424678518.5	401832985.4	411307100.6
L- Glutamic acid-2	129281610.8	153255469.3	146623914.1
methadone-d9	359666346.6	363114895.4	370456095.3
Amide C18	110039601.8	93839977.31	86656316.4
Spermidine-1	111614346.7	94184448.21	90317499.04
Genistein	29034746.03	31532814.67	32238291.08
Diisobutylphthalate	267043731.9	207067110.6	201172309.9
DL- Carnitine	122754347.3	86878021.05	96754474.1



spermidine	99008235.84	81015984.78	76894383.63
D-Sphingosine	64479101.86	61612884.96	53867413.47
D-(-)-Glutamine	68800675.58	73956135.39	61892793.81
L-Phenylalanine	211199680.3	186206662.4	181001128.9
L-Pyroglutamic acid	48299495.91	56656063.9	46988044.74
S-Allyl-L-cysteine	44466082.82	37415966.21	32533010.68
Cinnamyl alcohol	42094052.54	47300109.65	54955874.09
Taurine-1	71249178.94	68917887.72	68526482.27
Thiamine	106299074.5	92654950.39	89956479.19
Erythrose-4-phosphate	41124892.33	37391782.17	38119331.77
L-Glutamic acid	97582038.61	93475297.05	94389858.21
Pantothenic acid	38986191.24	37843238.02	36375070.42

Misopros tol	4594017.182	6559327.803	6098436.554
Ac-Ala- OH	34951828.33	35587362.97	31888421.57
Hexitol	27295267.38	24622010.74	28425954.16
Taurine	61748557.89	54878662.24	62323087.67
L- Glutamin e	31584083.64	33161836.01	29297959.42
DL- Citrulli ne-2	21220165.75	11112144.24	17309429.92
Creatini ne 6-	42909155.71	26551544.77	29574406.25
Oxohexan oic acid	14916676.96	8654625.85	11503440.53
Estazola m	7301758.784	7640338.808	8448662.722
Indole- 3- acrylic acid	72298446.08	60891528.7	59110609.87
Pyrophos phoric Acid	70292123.16	77760425.57	90268904.57
Caprolac tam-1 L-(+)-	71899927.72	57382944.4	56045109.02
Aspartic acid	25043795.11	28595271.05	27189844.02
Ketotife n	2417888.415	1925349.117	1919179.747

D- Mannose 6- phosphat e	39509979.72	41647237.15	42748165.16
L-(-)- Methioni ne-1	59091462.88	56647097.17	55491908.77
L-(-)- Asparagi ne-1	20169631.36	21802533.3	16813072.83
L-(-)- methioni ne-2	50902792.29	47226771.55	46464482.7
Mycophen olic acid ribulose 5- phosphat e	3695257.536	3446397.013	4066345.587
g- Butyrobe taine (9Z)-9-	37392418.45	35199441.67	36494786.4
Octadece namide	17233997.64	18410883.82	12103772.59
Hypotaur ine	24691833.72	18848626.08	19358210.75
Arabinos ylhypoxa nthine	7266575.648	8047561.551	8159573.07

gamma- Aminobut yric acid	14348948.32	21422275.06	12408517.46
DL- Citrulli ne	9907591.1	10076089.94	7854568.525
Sulfamic acid	10532348.44	10053075.27	10604552.02
Methioni ne sulfoxid e	19961486.42	16283721.14	14831131.75
DL- Arginine	10829152.08	10869942.01	10829185.81
Methylma lonic acid	3479253.138	2793373.54	2930579.81
Adenosin e 5'- monophos phate-1	14144061.32	17679552.39	13284984.99
N- Acetylas partic acid	27538770.91	25310295.33	23078158.47
Hippuric acid	3295630.93	2318362.257	2742121.228
Nicotina mide	26135848.12	14190203.21	18664864.23

Glycerol 3- phosphat e	15841582.26	15894535.77	19687857.49
noradren aline	4976494.307	4365836.824	3687435.874
Dihydrot hymine (E)-p-	9398224.196	9837787.792	7869973.693
coumaric acid propiony lcarniti ne	17997119.89	18882636.65	16172987.31
Fomepizo le	7261340.635	10570268.89	8415286.646
Flavin mononucl eotide	6220118.059	4539433.99	5465498.043
N- Acetyl- L- aspartic acid	10766793.76	9261803.79	8491068.793
L- Hydroxyp roline	15354499.14	11507397.01	11386616.46
L-(-)- Threonin e	12279277.35	12391496.55	13464845.3
	8041714.139	8194338.019	8561720.225

6- methylte trahydro pterin L-(-)-	5533889.661	4760398.935	5485887.977
Asparagi ne DL-	10914440.48	7553417.667	9974366.298
Glutamin e DL-	12672925.32	12352186.12	9678230.644
Histidin e g-	3404589.162	2826530.305	2597376.886
Glutamyl cysteine l-	6741581.514	5985825.714	6150763.545
Histidin al TROLEAND OMYCIN	12597328.32	11946443.85	11901488.76
Cyclo(le ucylprol yl) putresci ne N-	8541249.534	3972919.429	3412404.124
methylpr oline N-	1559750.48	1559619.518	1113925.984
Tridecan oylglyci ne	11717783.29	10297519.95	9334805.242
	6885975.704	6134229.411	6979214.61
	7201224.444	6471682.604	6178414.321

Adenine	3248924.167	4329664.29	3418046.921
L-(-)-			
Methionine	8871128.148	8194494.74	5664498.229
Pregabalin	11996656.06	10652751.24	10611764.29
3-			
(Sulfoox-			
y)-L-	10988462.36	10449051.31	10964339.46
tyrosine			
Nitrazepam	1413287.969	1534839.764	1127574.661
.alpha.-			
Aminoadi-	4952139.581	4117073.018	4025256.314
pic acid			
DL-			
Ceruleni-	9678583.069	10317828.73	11001879.18
n			
Pyridoxal	2441037.648	2183003.554	1835361.071
Adenosine			
5'-			
monophosphate	2594293.091	3407625.627	2475713.178
Caprolactam	6753445.66	7382323.363	7693514.906
Hispidulin	482034.6834	501918.2086	670338.2871
8-			
hydroxy-			
deoxyguanosine	4593424.816	5163572.551	3574899.5

2S- Amino- tridecan oic acid	1672943.153	1595393.386	1883996.846
N- Acetylne uraminic acid	2490107.147	1862509.524	2345586.071
Fumaric acid	6017402.142	4366061.744	4799538.694
acetylsp ermine alpha-	2227941.277	1968819.376	1585219.037
Ketoglut aric acid	2633005.127	2269463.629	1995361.697
meglumin e	2569430.422	1697403.053	1663719.587
N- Acetyl- L- histidin e	1057761.54	657101.8143	1055874.578
beta-L- fucose 1- phosphat e	1079579.832	1094441.869	930935.3653
Guanine	1218560.528	1321698.383	1397043.018
L- Cysteiny lglycine	6225030.901	6793853.415	6241247.972



D-a- Hydroxyg lutaric acid	2594592.737	2235110.459	2304535.832
Adipic acid	3462545.981	2789543.643	2699085.378
Luteolin	393301.5363	313285.7715	430920.7086
Ecgonine	772632.5381	670561.2029	660462.5295
Metirosi ne	4436781.666	4544287.074	4398130.6
16- Hydroxyh exadecan oic acid	1688178.847	1269739.335	1860334.372
g- Guanidin obutyra te	2371031.691	2199629.277	1750287.676
trimetha dione	2044018.833	2193121.677	2597599
acetylt urine	2280515.755	2215042.669	2119669.535
2- Mercapto benzothi azole	322816.2708	316557.1901	318182.4291
Chrysin	189562.7303	137371.7344	206076.6059
Orotic acid	1453932.948	1385772.896	1074653.428
Dibutyl phthalat e	815595.3471	702280.8343	801477.5957

Table S 2. Targeted-proteins of baicalein

names	names	names	names	names	names
ABO	FHIT	PCK1	CCL24	IMPDH2	SRC
ACE	FKBP1A	PCMT1	CCL5	INSR	SRR
ACPP	FKBP1B	PCP4	CCNA2	ISG20	STAT1
ADAM33	FKBP3	PDE3B	CCNT1	ITK	SULT1A1
ADAMTS17	FNTA	PDE4B	CD1A	ITPKA	SULT1E1
ADH1C	FOLH1	PDE4D	CD209	IVD	SULT2A1
ADH5	GALE	PDE5A	CDC42	JAK2	SULT2B1
ADK	GALK1	PDPK1	CDK2	JAK3	SYK
AGXT	GART	PGF	CDK5R1	KAT2B	TAP1
AHCY	GBA	PGR	CDK6	KDR	TEK
AK1	GLO1	PITPNA	CDK7	KIF11	TGFB2
AKR1B1	GM2A	PKIA	CES1	KIT	TGFBR1
AKR1C1	GMPR	PLA2G2A	CHEK1	LGALS2	TGFBR2
AKR1C3	GMPR2	PLAU	CHIT1	LGALS3	TGM3
AKT1	GNPDA2	PNMT	CLEC4M	LSS	THRA
AKT2	GP1BA	PNP	CLK1	LTA4H	THRB
ALB	GPI	PPARA	CMA1	LYZ	TK1
ALDH2	GSK3B	PPARG	CRABP2	MAN1B1	TNK2
ALDOA	GSR	PPCDC	CRAT	MAOA	TPH1
AMD1	GSTA1	PPIA	CSNK1G2	MAOB	TPSB2
AMY1B	GSTA3	PRKCQ	CTNNA1	MAP2K1	TREM1
AMY1B	GSTM1	PTPN1	CTSB	MAPK10	TTPA
AMY2A	GSTM2	PYGL	CTSF	MAPK14	TTR
ANG	GSTO1	RAB11A	CTSG	MAPKAPK2	TYMS
APAF1	GSTP1	RAB5A	CTSK	ME2	UAP1
APRT	GSTT2B	RAC1	CTSS	MET	UCK2
AR	GSTZ1	RAN	CYP2C9	METAP1	UMPS
ARG1	HADH	RAP2A	DAPK1	METAP2	VDR
ARG2	HAGH	REG1A	DCK	MIF	XIAP
ARHGAP1	HCK	REN	DCPS	MME	ZAP70
ARL5A	HDAC8	RFK	DCXR	MMP1	PARP1
ARL5B	HEXB	RHOA	DHFR	MMP12	IGF2
ARSA	HINT1	RNASE2	DHODH	MMP13	CYCS
ATIC	HK1	RNASE3	DPEP1	MMP16	ALOX12
AURKA	HMGCR	RNASEL	DPP4	MMP3	PTGS1
BACE1	HMOX1	RND3	DTYMK	MMP7	TDRD7
BAG1	HNMT	RORA	DUT	MMP8	PTGS2
BCAT2	HPGDS	RXRA	EEA1	MMP9	CDK1
BHMT	HPRT1	RXRB	EGFR	MTAP	CCNB1
BIRC7	HRAS	SEC14L2	EIF4E	MTHFD1	MPO
BST1	HSD11B1	SELE	ELANE	NME1-NME2	PDE3A
BTK	HSD17B1	SELP	ENSG00000259288	NMNAT1	PRSS1

CA1	HSP90AA1	SERPINA1	ERBB4	NMNAT3	NCOA2
CA12	HSP90AB1	SHBG	ERI1	NOS2	NCOA1
CA2	HSPA8	SHMT1	ESR1	NQO1	CALM2
CASP1	IGF1R	SOD2	ESR2	NR1H2	RELA
CASP3	IL2	SORD	ESRRG	NR1H4	AHR
CBR1	IMPA2	SPARC	F10	NR1I2	BCL2
CCBL1	IMPDH1	SPR	F11	NR3C1	FOS
FABP6	NUDT9	TP53	F2	NR3C2	BAX
FECH	OAT	HIF1A	F7	NSUN2	NFATC1
FGFR1	OTC	FOSL1	FABP3	NT5M	EGLN1
FGG	PAH	FOSL2	NOX5	FABP5	APOD

Table S 3. Glycolysis-related genes

names	names	names	names	names	names
GSME	ME1	LDHC	DSC2	STMN1	ACOT12
ABCB6	ME2	PGAM4	ECD	TFF3	ACSS1
ADORA2B	MED24	PGK2	EFNA3	TGFA	ACSS2
AGL	MERTK	PGM1	EGFR	TGFBI	BRP44
AGRN	MET	ENO3	EGLN3	TKTL1	BRP44L
AK3	MIF	GAPDHS	ELF3	TPBG	DLAT
AK4	MIOX	GPI	ERO1L	TPST1	DLD
ALG1	MXI1	LOC642969	EXT1	TSTA3	DLST
ANG	NANP	PFKFB1	EXT2	TXN	FASN
ANGPTL4	NASP	PFKFB2	FAM162A	UGP2	KYNU
ANKZF1	NDST3	PFKFB3	FKBP4	VCAN	MLYCD
ARPP19	NDUFV3	PFKFB4	FUT8	VEGFA	MVD
ARTN	NOL3	PFKL	GAL3ST1	VLDLR	MVK
AURKA	NSDHL	PGAM2	GALE	XYLT2	NUDT7
B3GALT6	NT5E	PKLR	GALK1	ZNF292	PDHA1
B3GAT1	P4HA1	PPP2CA	GALK2	BID	PDHA2
B3GAT3	P4HA2	PPP2CB	GCLC	CD4	PDHB
B3GNT3	PAM	PPP2R1A	GFPT1	LCT	PDHX
B4GALT1	PAXIP1	PPP2R1B	GLCE	MPI	PIPOX
B4GALT2	PC	PPP2R5D	GLRX	PYGL	PMVK
B4GALT4	PDK3	TPI1P1	GMPPA	PYGM	TDO2
B4GALT7	PHKA2	ACO1	GMPPB	TREH	ALDH1A1
BIK	PKP2	ACO2	GNE	ADH1A	ALDOB
BPNT1	PLOD1	ALDOA	GNPDA1	ADH1B	DAK
CACNA1H	PLOD2	ALDOC	GOT1	ADH1C	DERA
CAPN5	PMM2	ENO1	GOT2	ADH4	G6PD
CASP6	POLR3K	ENO2	GPC1	ADH5	GLYCTK
CD44	PPFIA4	FH	GPC3	ADH6	H6PD
CDK1	PPIA	GAPDH	GPC4	ADH7	KHK
CENPA	PRPS1	IDH1	GPR87	AKR1A1	LOC729020

CHPF	PSMC4	IDH2	GUSB	ALDH1A3	PGD
CHPF2	PYGB	IDH3B	GYS1	ALDH1B1	PGLS
CHST1	QSOX1	IDH3G	GYS2	ALDH2	PGM2
CHST12	RARS	LDHA	HAX1	ALDH3A1	RPE
CHST2	RBCK1	MDH1	HDLBP	ALDH3A2	RPIA
CHST4	RRAGD	PCK1	HMMR	ALDH3B1	SHPK
CHST6	SAP30	PCK2	HOMER1	ALDH3B2	TALDO1
CITED2	SDC1	PFKM	HS2ST1	ALDH7A1	TKT
CLDN3	SDC2	PFKP	HS6ST2	ALDH9A1	TPI1
CLDN9	SDC3	PGAM1	HSPA5	BPGM	EMB
CLN6	SDHC	PGK1	IDUA	FBP1	SLC16A1
COG2	SLC25A10	PKM2	IER3	FBP2	SLC16A11
COL5A1	SLC25A13	SDHA	IGFBP3	G6PC	SLC16A12
COPB2	SLC35A3	SDHB	IL13RA1	G6PC2	SLC16A13
CTH	SLC37A4	SDHD	IRS2	GALM	SLC16A3
CXCR4	SOD1	SUCLG1	ISG20	GCK	SLC16A4
CYB5A	SOX9	AADAT	KDEL3	HK1	SLC16A5
DCN	SPAG4	AASS	KIF20A	HK2	SLC16A6
DDIT4	SRD5A3	ACACA	KIF2A	HK3	SLC16A7
DEPDC1	STC1	ACACB	LHPP	LDHAL6A	SLC16A8
DPYSL4	STC2	ACLY	LHX9	LDHAL6B	SLC5A12
MDH2	LDHB				

---