

Table S1 All differential metabolites in ketamine treated rat urine samples compared to control group

MS2 name	Type	VIP	P value	Fold change
p-Chlorophenylalanine	MS2 reverse	1.482664661	0.022581683	2.088403489
Myristoleic acid	MS2 reverse	2.09799238	0.000179994	1.726790289
Salicylic acid	MS2 forward	1.824331269	0.010147158	1.591570624
L-homoserine	MS2 reverse	1.746636855	0.010277906	1.548048138
3-Methoxy-4-hydroxyphenylethyleneglycol	MS2 reverse	1.370359686	0.034436936	0.829686969
Sulfaphenazole	MS2 reverse	1.029843202	0.03273948	0.795389004
1,2-Benzenedicarboxylic acid	MS2 forward	1.5430191	0.045110528	0.777020585
Quinolinate	MS2 forward	2.082448204	0.00236724	0.775982736
D-glucosamine 1-phosphate	MS2 forward	1.833854214	0.008842721	0.771064659
Phosphorylcholine	MS2 forward	1.117232921	0.028263596	0.769568172
D-ribose 5-phosphate	MS2 forward	1.780321548	0.018475696	0.768976317
Allantoin	MS2 forward	2.046300074	0.010595984	0.762709318
Glyceric acid	MS2 reverse	2.121688111	0.01057002	0.761944433
Galactonic acid	MS2 forward	1.951851055	0.0313966	0.758280251
Picrotoxinin	MS2 reverse	2.079133994	0.018233279	0.755109009
Thiamine monophosphate	MS2 reverse	2.063228119	0.006774628	0.75347008
N-Acetylaspartylglutamate (NAAG)	MS2 reverse	2.291827297	0.003445462	0.749532403
Methylthiouracil	MS2 reverse	2.160625989	0.005118714	0.746049357
Glutaric acid	MS2 reverse	1.557278238	0.047708268	0.745016803
L-Cysteic acid	MS2 reverse	1.623170822	0.04716071	0.741823206
3',5'-Cyclic guanosine monophosphate	MS2 forward	1.710857486	0.020098057	0.730690388
N-Acetylneuraminic acid	MS2 forward	1.749960452	0.033525987	0.728765601
Biopterin	MS2 forward	1.227077427	0.044781799	0.722976261
Hydroxyproline	MS2 reverse	1.901941039	0.031785026	0.719187455
(S)-2-Hydroxyglutarate	MS2 forward	1.610349719	0.034992987	0.710700459
D-Glucose 6-phosphate	MS2 reverse	2.086381705	0.004901267	0.685505863
3-Hydroxy-3-methylglutaric acid	MS2 forward	1.501667044	0.046499813	0.67649715
Xanthine	MS2 forward	2.091674633	0.011043818	0.674563903
Gallic acid	MS2 forward	1.468370852	0.01298651	0.669149235
Succinate	MS2 forward	1.649946217	0.021349092	0.665581289
Uracil	MS2 forward	1.52020403	0.022438883	0.659230513
3-Hydroxyisovaleric acid	MS2 reverse	1.667482832	0.021694764	0.647310844
Allocystathionine	MS2 reverse	1.883617934	0.038591377	0.646847067
2'-Deoxyuridine	MS2 reverse	1.230308737	0.040283808	0.620371895
Hydroxyhydroquinone	MS2 reverse	1.662096942	0.007088873	0.618218772
Deoxyuridine monophosphate	MS2 reverse	1.649252621	0.025565738	0.614569781
Jasmonic acid	MS2 reverse	1.514285312	0.036044238	0.610840674
Pantetheine	MS2 forward	1.675574703	0.022016291	0.600185386
Apigenin 7-glucoside	MS2 reverse	1.580735469	0.021473258	0.574226734
Prephenate	MS2 reverse	1.358369196	0.014242113	0.567506361
2-Amino-3-methoxy-benzoic acid	MS2 reverse	1.787397399	0.017242521	0.561417149
5-Hydroxymethylcytidine	MS2 reverse	1.396897031	0.019620982	0.556911219
L-Ascorbic acid	MS2 forward	1.413277202	0.048514968	0.5558384
D-Ribulose 1,5-bisphosphate	MS2 reverse	2.031981268	0.015979171	0.550204342
Oxazepam	MS2 reverse	1.860735515	0.039675759	0.54668473
L-Histidinol	MS2 reverse	1.613477995	0.021146814	0.53101848
D-Threitol	MS2 forward	1.902102624	0.016490356	0.530728427
Uric acid	MS2 forward	1.720076229	0.045187868	0.517918642
Glafenine	MS2 reverse	2.137081115	0.005373777	0.5110753
Clozapine	MS2 reverse	1.939712787	0.025412069	0.499340036
2-Deoxy-D-glucose 6-phosphate	MS2 reverse	1.656468689	0.039200661	0.495137978
Estrone-3-glucuronide	MS2 reverse	2.097005256	0.006118495	0.487421812
2-Methyl-3-hydroxybutyric acid	MS2 reverse	1.72070876	0.037063118	0.486247008
N-Acetyl-L-aspartic acid	MS2 reverse	2.398347827	0.002969733	0.436451439
Anthranilic acid (Vitamin L1)	MS2 reverse	1.858261397	0.030461366	0.355221406
Hydroxyphenyllactic acid	MS2 reverse	2.633650228	0.019664464	17.03006355
Epsilon-caprolactone	MS2 reverse	2.477916359	0.038380883	9.592274572
Allocystathionine	MS2 reverse	2.172458016	0.0480407	7.017815453

Table S1 (continued)

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MS2 name	Type	VIP	P value	Fold change
(+)-Methamphetamine	MS2 forward	2.347313599	0.001415391	6.949027624
Dimethylformamide	MS2 reverse	1.940048907	0.006059808	4.206489916
Meso-2,6-diaminoheptanedioate	MS2 reverse	1.257826352	0.023069712	2.675236496
Uridine	MS2 reverse	2.020893568	0.003712476	1.699312722
Verapamil	MS2 reverse	2.16242187	0.002288484	1.683733074
Lys-Gly	MS2 reverse	1.473315216	0.0448077	1.520242251
Arg-Ala	MS2 reverse	1.377219343	0.0099348	1.301056568
Val-Glu	MS2 reverse	1.718494154	0.025726621	1.2977372
DL-alpha-phenylglycine	MS2 reverse	1.694713395	0.014759062	1.183587801
4-acetamidobutanoate	MS2 forward	1.624612075	0.008246869	0.843757376
O-Desmethylnaproxen	MS2 reverse	1.520776335	0.005264959	0.769378923
5-Methylcytosine	MS2 forward	1.64652063	0.013511683	0.76512237
Thymidine	MS2 reverse	1.496465311	0.017604915	0.761783666
Acetylglycine	MS2 reverse	1.255082407	0.020875357	0.759055512
Pro-Glu	MS2 forward	1.476630987	0.033605868	0.75816417
Thr-His	MS2 reverse	1.220499196	0.036751716	0.751130341
5-Methylcytidine	MS2 forward	1.658484074	0.014583692	0.745343053
Nitrobenzene	MS2 reverse	1.209341788	0.03705139	0.744022402
3,3-Dimethylacrylic acid	MS2 forward	1.589224968	0.02691495	0.740013662
Ser-Val	MS2 reverse	1.555183809	0.024983138	0.738083133
N-(omega)-Hydroxyarginine	MS2 reverse	1.333257353	0.009896441	0.730639649
Glycerophosphocholine	MS2 forward	1.078812605	0.018463782	0.729971001
Sanguinarine	MS2 reverse	1.494057237	0.043342222	0.723800293
Anthranilic acid (vitamin L1)	MS2 reverse	1.163473953	0.02848806	0.717913533
Atropine	MS2 reverse	1.679877549	0.004653833	0.712118058
N2,N2-Dimethylguanosine	MS2 reverse	1.755659554	0.01585386	0.7087619
N-Acetyl-D-glucosamine	MS2 forward	1.629226838	0.01782848	0.707239534
Biopterin	MS2 forward	1.000834999	0.042091843	0.705518001
Pro-Trp	MS2 reverse	1.793857835	0.014064219	0.704400066
Cytidine	MS2 reverse	1.574311055	0.018826082	0.703354023
Flumequine	MS2 reverse	1.813932221	0.010658893	0.703252572
Pyruvaldehyde	MS2 reverse	1.142383824	0.049498601	0.700527032
Met-Thr	MS2 reverse	1.249302443	0.021575958	0.694715977
Leu-Trp	MS2 reverse	1.745869501	0.00711319	0.682205215
Xanomeline	MS2 reverse	1.923823003	0.008476593	0.674795605
Ala-Pro	MS2 reverse	1.579299618	0.005411376	0.661127047
N-Glycolylneuraminic acid	MS2 reverse	1.57156514	0.030426096	0.659859161
Acetyl-DL-Valine	MS2 reverse	1.734203519	0.011445194	0.655074708
Ethisterone	MS2 reverse	1.755203974	0.032942997	0.649340674
1-Deoxy-D-xylulose 5-phosphate	MS2 reverse	1.893722005	0.004923546	0.643672651
Clofibrate	MS2 reverse	1.778152384	0.019533896	0.639236238
N-Acetylneuraminic acid	MS2 forward	1.893214103	0.011852953	0.637754926
Procaine	MS2 reverse	1.267212456	0.021033961	0.634484755
Methoxyacetic acid	MS2 reverse	1.613501592	0.017177443	0.62354792
N,N-Dimethylaniline	MS2 reverse	1.38670469	0.047154221	0.622392371
Lys-Leu	MS2 reverse	1.226355959	0.026133676	0.621554911
Lys-Ser	MS2 reverse	1.248923791	0.027392882	0.619395745
Ala-Ala	MS2 reverse	1.563839603	0.00849707	0.606806261
7-Methylguanosine	MS2 reverse	1.712194102	0.009144798	0.603191597
Equol	MS2 forward	1.255913117	0.030707226	0.588731875
Malonic acid	MS2 reverse	1.965097321	0.004436536	0.583918122
Ajmalicine	MS2 reverse	1.687588952	0.007489708	0.582624244
D-Mannose	MS2 forward	1.286248655	0.033116293	0.563901819
Quinate	MS2 reverse	1.422653095	0.039765564	0.559847402
Arg-Phe	MS2 forward	1.665346043	0.010164035	0.493562524
1-Aminocyclopropanecarboxylic acid	MS2 reverse	1.78917087	0.017018907	0.458740484
7,8-Dihydrobiopterin	MS2 forward	1.424846621	0.010708745	0.430668925
Tyr-Glu	MS2 reverse	2.119367582	0.00081498	0.428884596