Fig. S1 Grouping.

Fig. S2 Points selection for acupuncture group (**A**) and sham acupuncture group (**B**).

Fig. S3 PCA score plot of in positive (**A**) and negative (**B**) ion mode respectively.

Fig. S4 Protein-metabolite interaction based on Stitch, IntAct, and Reactome databases.

Table S1 Significant differences in amplitude of low-frequency fluctuation (ALFF) between groups.

Table S2 Significant differences in regional homogeneity (ReHo) between groups.

Table S3 Detailed information about the differentially expressed metabolites between groups.

Table S4 Detailed information about the differentially expressed proteins between groups.

Table S5 Migraine related targets collected from databases.

Table S6 Detailed information about the protein-metabolite interaction network.

Table S7 Detailed information about the enriched pathways in acupuncture group.

Table S8 Detailed information about the enriched pathways in sham acupuncture group.

Table S9 Correlation analysis and mediation analysis of clinical, fMRI and omics data

Fig. S1

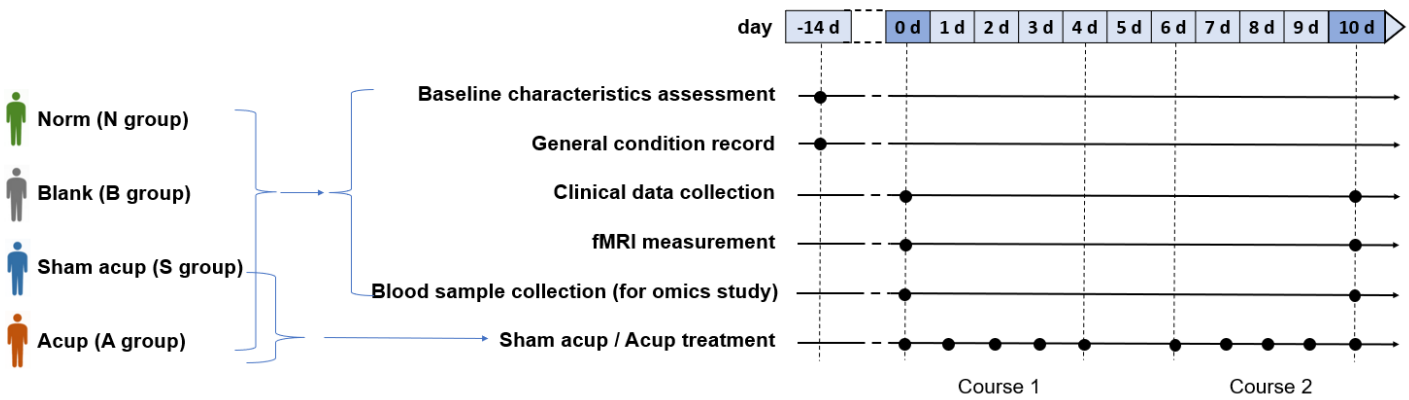
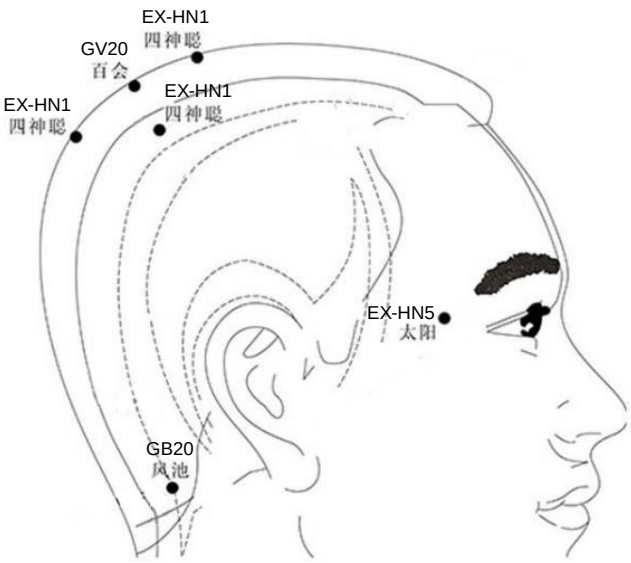
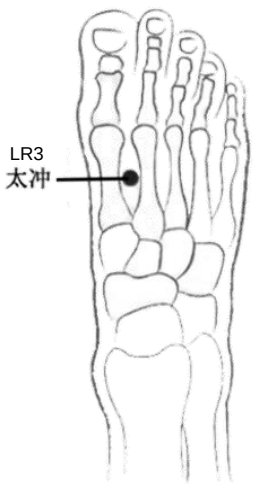

day
-14 d
0 d
1 d
2 d
3 d
4 d
5 d
6 d
7 d
8 d
9 d
10 d
Norm (N group)
Blank (B group)
Sham acup (S group)
Acup (A group)
Baseline characteristics assessment
General condition record
Clinical data collection
fMRI measurement
Blood sample collection (for omics study)
Sham acup / Acup treatment
Course 1
Course 2

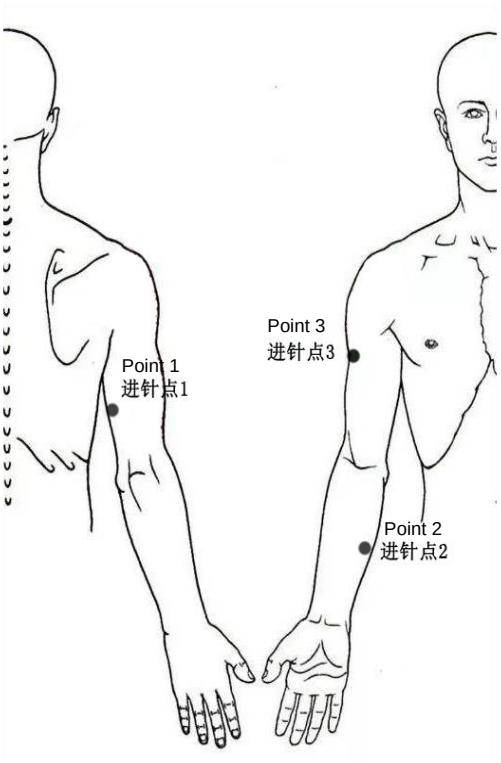
Fig. S2

A


EX-HN1
四神聪
GV20
百会
EX-HN1
四神聪
EX-HN1
四神聪
EX-HN5
太阳
GB20
风池


LR3
太冲

B


Point 1
进针点1
Point 3
进针点3
Point 2
进针点2

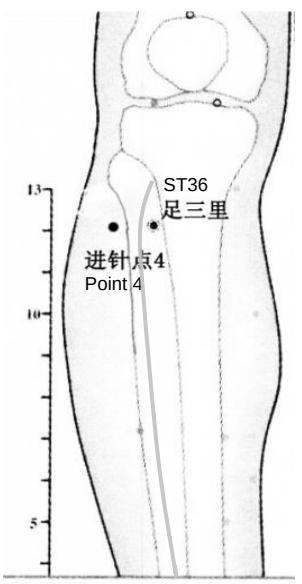

ST36
足三里
进针点4
Point 4

Fig. S3

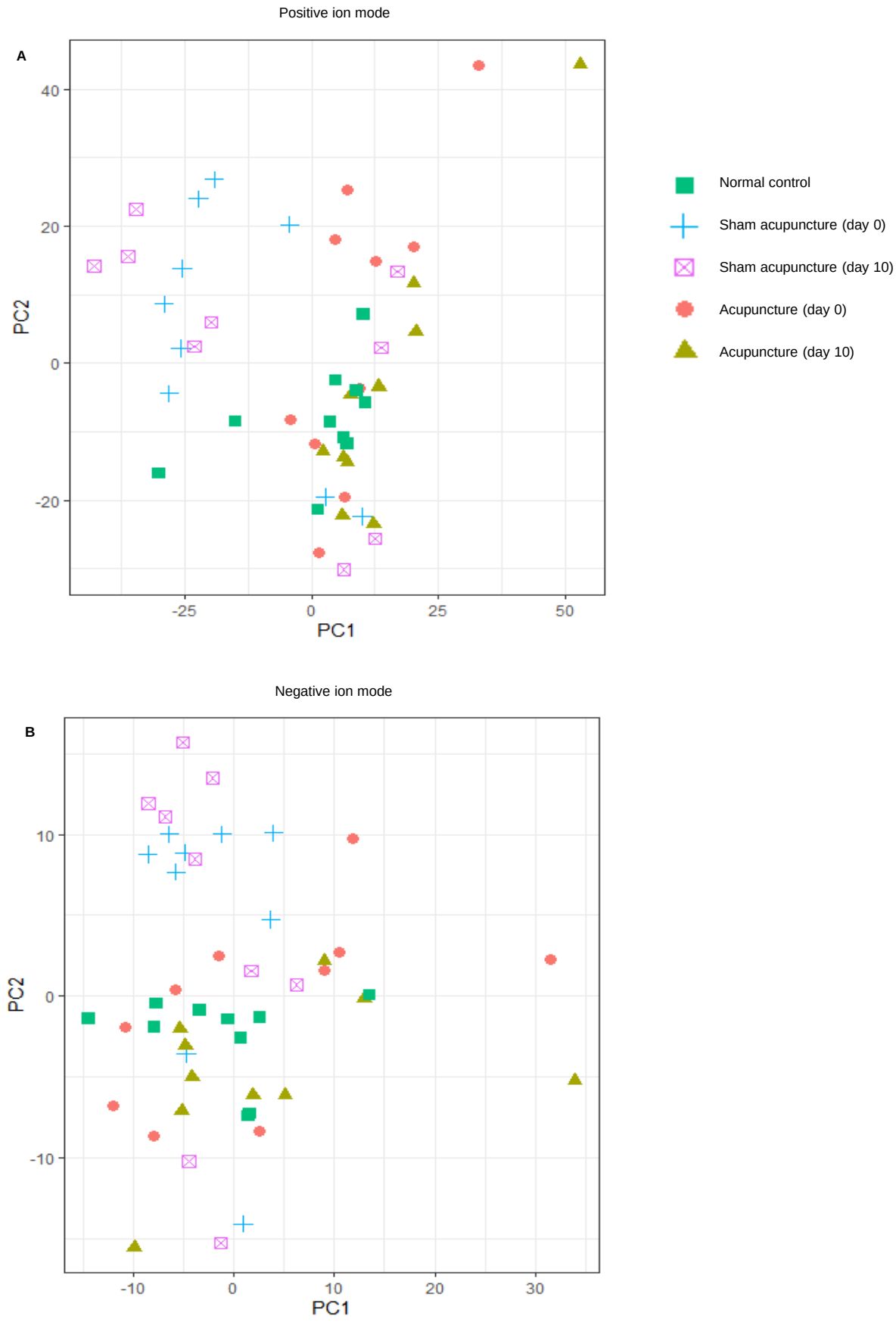

Positive ion mode
A
40
20
0
-20
PC2
-25
0
25
50
PC1
Normal control
Sham acupuncture (day 0)
Sham acupuncture (day 10)
Acupuncture (day 0)
Acupuncture (day 10)
Negative ion mode
B
10
0
-10
PC2
-10
0
10
20
30
PC1

Fig. S4

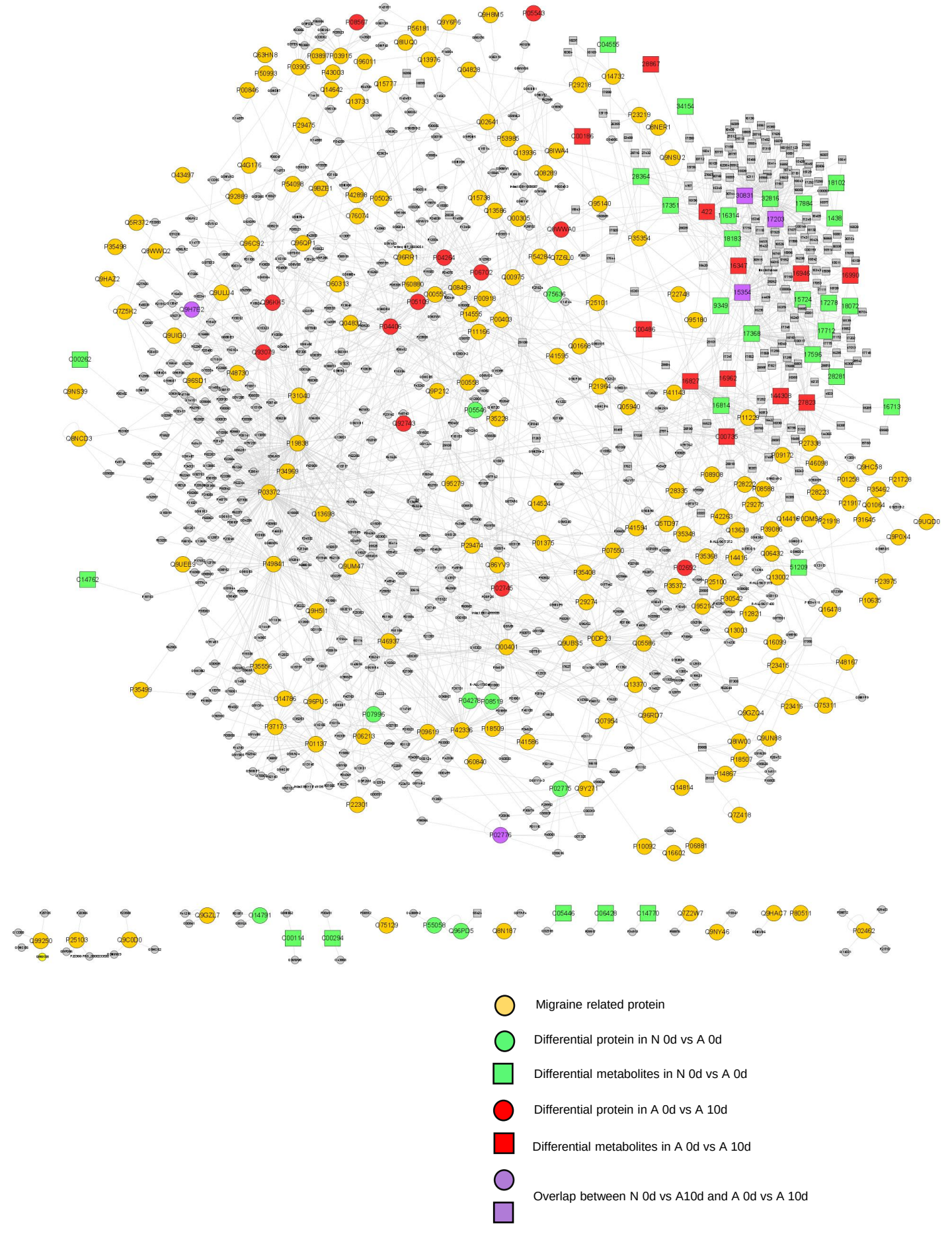

Migraine related protein
Differential protein in N 0d vs A 0d
Differential metabolites in N 0d vs A 0d
Differential protein in A 0d vs A 10d
Differential metabolites in A 0d vs A 10d
Overlap between N 0d vs A10d and A 0d vs A 10d

Table S1

Table S1 Significant differences in amplitude of low-frequency fluctuation (ALFF) between groups

Regions with differential ALFF values in migraineurs compared with normal controls

Region	Cluster size	Peak T value	MNI coordinates		
			x	y	z
Temporal_Mid_R	18	4.63	54	-9	-15

Note：*P<0.05* (AlphaSim corrected)

Regions with differential ALFF values after acupuncture treatment compared with before

Region	Cluster size	Peak T value	MNI coordinates		
			x	y	z
Lingual Gyrus_R	63	6.76	12	-99	-12
Temporal Lobe_L	19	-6.25	-48	-45	-6
Precuneus_L	19	4.88	0	-69	51
Cerebelum_6_L	17	-7.03	-18	-72	-21

Note：*P<0.05* (AlphaSim corrected)

Table S2

Table S2 Significant differences in regional homogeneity (ReHo) between groups

Regions with differential ReHo values in migraineurs compared with normal controls

Region	Cluster size	Peak T value	MNI coordinates		
			x	y	z
Temporal_Mid_L	85	4.49	-60	-3	-15
ACC_sup_R	16	-3.88	6	30	9

Note：*P<0.05* (AlphaSim corrected)

Regions with differential ReHo values in blank control group before and after treatment

Region	Cluster size	Peak T value	MNI coordinates		
			x	y	z
Frontal_Mid_Orb_L	21	-5.92	-36	57	-12
Frontal Lobe_L	18	6.17	-21	24	21

Note：*P<0.05* (AlphaSim corrected)

Regions with differential ReHo values after acupuncture treatment compared with before

Region	Cluster size	Peak T value	MNI coordinates		
			x	y	z
Cerebelum_6_L	22	-5.2	-18	-75	-21

Note：*P<0.05* (AlphaSim corrected)

Table S3

Table S3 Detailed information about the differentially expressed metabolites between groups

Differential metabolites identified in positive mode (N 0d vs A 0d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.709_75.0684	Trimethylamine n-oxide	C01104	HMDB0000925	up
0.715_98.0367	2491	C20441	HMDB0013742	up
0.719_177.0458	Fmet	NA	NA	up
0.736_338.0837	Ascorbyl glucoside	NA	NA	down
0.742_94.0088	Methylsulfonylmethane	C11142	HMDB0004983	up
0.749_103.0997	Choline	C00114	HMDB0000097	up
0.764_129.0425	L-pyroglutamic acid	C01879	HMDB0000267	up
0.767_122.0367	Benzoic acid	C00539	HMDB0001870	up
0.768_162.1083	(s)-1-methoxy-3-heptanethiol	null	HMDB0032380	up
0.769_115.0632	L-proline	C16435	NA	up
0.777_75.0684	Trimethylamine n-oxide	C01104	HMDB0000925	up
0.783_352.0283	Mfcd00060109	NA	NA	up
0.791_155.0348	N-methylethanolamine phosphate	C01210	HMDB0060173	up
0.904_184.0233	5-hydroxyisouric acid	C11821	HMDB0030097	down
0.937_94.0089	Methylsulfonylmethane	C11142	HMDB0004983	up
0.946_181.0962	6-methyltetrahydropterin	null	HMDB0002249	down
0.957_253.1174	Penciclovir	C07417	HMDB0014444	down
0.989_109.064	3,4-diaminopyridine	NA	NA	up
1.02_152.0333	Xanthine	C00385	HMDB0000292	down
1.516_176.0949	Cotinine	null	HMDB0001046	down
10.006_309.3028	1-hexadecanoylpyrrolidine	null	HMDB0032740	down
10.076_335.3183	(2e,4z)-n-isobutyl-2,4-octadecadienamide	null	HMDB0031678	down
10.12_269.2716	Capsi-amide	C17515	HMDB0040940	down
10.139_323.3185	1-(14-methylhexadecanoyl)pyrrolidine	null	HMDB0034373	down
10.218_398.3394	Dilauroyl peroxide	NA	NA	down
10.262_436.3549	5b-cholestane-3a,7a,12a,26-tetrol	C05446	HMDB0001231	down
11.458_757.5612	Pc	null	HMDB0007973	down
2.272_104.0296	Methional	null	HMDB0031857	up
2.571_99.1048	Cyclohexylamine	C00571	HMDB0031404	up
2.586_120.0245	4-thiapentanoic acid	C08276	HMDB0001527	up
2.654_104.0296	Methional	null	HMDB0031857	up
2.751_148.0523	Cinnamic acid	C10438	HMDB0000930	up
2.877_383.115	Acutumidine	NA	NA	up
3.007_127.0998	Lq1825000	NA	NA	up
3.221_133.0527	2-oxindole	C12312	HMDB0061918	up
3.222_264.0898	Diftalone	NA	NA	up
3.271_333.1324	Oglufanide	null	HMDB0028830	down
3.388_143.0734	6-methylquinoline	null	HMDB0033115	down
3.46_165.1152	Pseudoephedrine	D08449	NA	up
3.477_208.0735	(2e)-3-(3,4-dimethoxyphenyl)acrylic acid	null	HMDB0034315	up
3.798_129.1517	Octylamine	NA	NA	up
3.88_265.1313	Z-leu-oh	NA	NA	up
3.955_279.147	Metalaxyl	C10947	HMDB0031802	up
3.989_264.1108	N-phenylacetylglutamine	C04148	HMDB0006344	up

3.994_309.1687	2762577	NA	NA	up
4.091_257.1626	2-hexenoylcarnitine	null	HMDB0013161	down
4.667_183.0895	Normetanephrine	C05589	NA	up
4.727_244.1423	4-hydroxyprolylleucine	null	HMDB0028867	down
4.742_259.1783	Hexanoylcarnitine	null	HMDB0000705	down
4.912_185.1051	(2r,3s)-3-hydroxy-8-methyl-8-azabicyclo[3.2.	C10858	HMDB0006548	up
5.761_179.0438	181594	C03975	HMDB0000704	up
5.852_582.2476	Azelnidipine	NA	NA	up
5.854_129.0578	Leucoline	C06413	HMDB0033731	up
5.854_189.0787	Methyl indole-3-acetate	C20635	HMDB0029738	up
5.855_234.1366	Gy5875000	NA	NA	up
5.858_205.0737	5-methoxy-3-indoleaceate	C05660	HMDB0004096	up
5.863_219.0894	Aniracetam	NA	NA	up
5.871_446.0845	Baicalin	null	HMDB0041832	up
5.989_226.1206	Butopyronoxyl	NA	NA	down
6.182_164.0837	4-phenylbutyric acid	NA	NA	down
6.185_154.0993	Ri2735000	null	HMDB0031302	down
6.186_94.0782	1,3,5-heptatriene	null	HMDB0061889	down
6.189_108.0939	4-vinylcyclohexene	NA	NA	down
6.248_287.2094	5955761	C02838	HMDB0000791	down
6.319_228.1472	Leu-pro	null	HMDB0011175	down
6.33_446.0846	Baicalin	null	HMDB0041832	up
6.379_311.2095	(4s)-4-[(2e,4z)-2,4-decadienoyloxy]-4-(trimet	null	HMDB0013325	down
6.557_120.0575	Acetophenone	C07113	HMDB0033910	up
6.56_106.0418	Benzaldehyde	C00261	HMDB0006115	up
6.751_168.1149	Trans-geranic acid	NA	NA	down
6.756_185.1415	Atagabalin	NA	NA	down
6.756_200.1412	9-hydroxy-10-undecenoic acid	null	HMDB0032662	down
6.757_154.0993	Ri2735000	null	HMDB0031302	down
6.758_108.0939	4-vinylcyclohexene	NA	NA	down
6.758_186.1255	1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane-6,7	C17620	HMDB0041376	down
6.797_298.1415	Sesamex	NA	NA	down
6.803_320.1235	4-(2-carboxy-1-azetidinyl)-n-(3-carboxy-3-hy	null	HMDB0033555	down
6.875_313.225	9-decenoylcarnitine	null	HMDB0013205	down
7.19_331.2137	Megastachine	NA	NA	down
7.225_228.1361	Traumatic acid	C16308	HMDB0000933	down
7.226_164.1201	Fenipentol	NA	NA	down
7.228_242.1518	5-octyl-2-oxotetrahydro-3-furancarboxylic ac	null	HMDB0030987	down
7.264_200.1411	9-hydroxy-10-undecenoic acid	null	HMDB0032662	down
7.281_315.2407	Decanoylcarnitine	null	HMDB0000651	down
7.401_204.115	3688	null	HMDB0033379	down
7.575_242.1518	5-octyl-2-oxotetrahydro-3-furancarboxylic ac	null	HMDB0030987	down
7.576_256.1673	4-[(2-isopropyl-5-methylcyclohexyl)oxy]-4-o	null	HMDB0036143	down
7.65_341.2565	Trans-2-dodecenoylcarnitine	null	HMDB0013326	down
7.717_263.1882	(+)-tramadol	C07153	HMDB0014339	up
7.733_214.1568	3-oxolauric acid	C02367	HMDB0010727	down
7.741_245.1448	S-3-oxodecanoyl cysteamine	null	HMDB0059773	down
7.945_367.2721	3, 5-tetradecadiencarnitine	null	HMDB0013331	down

8.107_208.1826	2-decylfuran	null	HMDB0032215	down
8.146_214.1568	3-oxolauric acid	C02367	HMDB0010727	down
8.146_286.2141	1792831	C19615	HMDB0000672	down
8.17_190.1721	1,4-di-tert-butylbenzene	null	HMDB0094670	down
8.182_222.1982	(2e,6e)-farnesol	C06081	HMDB0004305	down
8.183_208.1826	2-decylfuran	null	HMDB0032215	down
8.206_354.2556	Bufa-20,22-dienolide	NA	NA	up
8.223_256.0759	Benfuresate	NA	NA	down
8.332_356.2712	Ethyl docosahexaenoate	NA	NA	up
8.403_395.3034	9,12-hexadecadienoylcarnitine	null	HMDB0013334	down
8.458_248.1774	3222	null	HMDB0037719	down
8.47_314.2455	Vs1150000	null	HMDB0041220	down
8.471_368.1648	Dehydroepiandrosterone sulfate	C04555	HMDB0001032	down
8.561_240.1722	(1s,2r,5s)-2-isopropyl-5-methylcyclohexyl 3-(	null	HMDB0032369	down
8.627_204.1877	(e,e)-alpha-farnesene	C09665	HMDB0036066	up
8.632_257.199	N-lauroylglycine	null	HMDB0013272	up
8.705_300.2298	1,3-dihydroxy-2-propanyl (9z)-9-tetradecenoa	null	HMDB0011531	down
8.705_314.2456	Vs1150000	null	HMDB0041220	down
8.707_286.2142	1792831	C19615	HMDB0000672	down
8.716_324.2301	6-decylubiquinol	NA	NA	down
8.734_316.261	9,10-dihydroxystearic acid	NA	NA	down
8.739_298.2505	Ricinoleic acid	null	HMDB0034297	down
8.809_296.2348	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
8.854_312.2299	(10e,12z)-9-hydroperoxy-10,12-octadecadien	null	HMDB0006940	down
8.863_182.167	4,8a-dimethyl-decahydronaphthalen-4a-ol	null	HMDB0036461	down
8.863_242.1881	3-oxotetradecanoic acid	null	HMDB0010730	down
8.863_94.0782	1,3,5-heptatriene	null	HMDB0061889	down
8.866_108.0939	4-vinylcyclohexene	NA	NA	down
8.884_310.2506	(+/-)-methoprene	NA	NA	down
8.941_310.2505	(+/-)-methoprene	NA	NA	down
8.944_296.2349	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
8.992_302.2244	Eicosapentanoic acid	C06428	HMDB0001999	down
9.027_298.2505	Ricinoleic acid	null	HMDB0034297	down
9.075_278.0968	Egualen	NA	NA	down
9.076_310.123	Porphine	NA	NA	down
9.079_296.235	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
9.081_397.2252	Drotaverine	null	HMDB0015669	up
9.292_316.24	Pregnane-3,20-dione	NA	NA	down
9.293_334.2506	Tetrahydrodeoxycorticosterone	C13713	HMDB0000879	down
9.479_279.2559	Linoleamide	null	HMDB0062656	down
9.48_262.2293	Sl3675000	NA	NA	down
9.597_332.1435	9-fluoro-17?-oxa-dextro-homoandrosta-1,4-di	NA	NA	down
9.598_330.1482	Gibberellin a7	NA	NA	down
9.611_299.282	Threo-sphingosine, (-)-	null	HMDB0000252	down
9.643_255.2559	Hexadecanamide	NA	NA	down
9.715_281.2714	Oleamide	C19670	HMDB0002117	down
9.779_516.3793	3,16-dihydroxy-13,28-epoxyoleanan-22-yl ac	null	HMDB0034645	down
9.784_332.1638	Gibberellin a4	NA	NA	down

9.784_336.1595	Plinabulin	NA	NA	down
9.785_514.3634	3,22-dihydroxy-28-oxoolean-12-en-16-yl acet	null	HMDB0034529	down
9.785_614.3993	Chaps	NA	NA	down
9.787_280.2399	2210856	null	HMDB0006270	down
9.791_356.2922	1-oleoyl-rac-glycerol	NA	NA	down
9.926_333.3028	(2e,4e,12z)-n-isobutyl-2,4,12-octadecatrienan	null	HMDB0032033	down
9.962_283.2871	Amide c18	C13846	HMDB0034146	down

Differential metabolites identified in negative mode (N 0d vs A 0d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.701_102.0317	2-oxobutyric acid	C00109	HMDB0000005	up
0.714_88.0161	Pyruvic acid	C00022	HMDB0000243	up
1.128_136.0383	Hypoxanthine	C00262	HMDB0000157	down
10.062_280.2399	Linoleic acid	C01595	HMDB0000673	down
10.284_256.24	Ethyl myristate	NA	NA	down
11.875_805.5826	O-{[(2r)-2-(docosanoyloxy)-3-(pentadecanoy	null	HMDB0112334	up
2.177_268.0806	Inosine	C00294	HMDB0000195	down
3.116_213.0094	3-indoxyl sulphate	NA	NA	up
3.416_264.1107	N-phenylacetylglutamine	C04148	HMDB0006344	up
3.814_204.0091	Guaiacol sulfate	null	HMDB0060013	up
4.186_188.0142	P-cresylsulfate	null	HMDB0011635	up
4.198_232.0039	4-formyl-2-methoxyphenyl hydrogen sulfate	null	HMDB0041789	down
4.423_189.0788	Methyl indole-3-acetate	C20635	HMDB0029738	up
4.437_346.1626	[3-(hydroxymethyl)-3-methyl-2-oxobicyclo[2	null	HMDB0033223	up
4.477_216.0091	2-hydroxy-5-vinylphenyl hydrogen sulfate	null	HMDB0124978	down
5.415_446.0845	Baicalin	null	HMDB0041832	up
5.586_228.1359	Traumatic acid	C16308	HMDB0000933	down
6.252_270.0851	4-imino-1-(beta-d-ribofuranosyl)-1,4-dihydro	NA	NA	down
7.902_367.9077	Triclosan sulfate	null	HMDB0061387	up
8.295_286.2142	Hexadecanedioic acid	C19615	HMDB0000672	down
8.619_257.199	N-lauroylglycine	null	HMDB0013272	up
8.627_331.2147	Megastachine	NA	NA	up
8.812_316.2611	9,10-dihydroxystearic acid	NA	NA	down
8.851_296.2349	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
8.952_296.235	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
8.963_314.2456	Vs1150000	null	HMDB0041220	down
9.021_296.2349	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
9.118_298.2505	Ricinoleic acid	null	HMDB0034297	down
9.121_320.2351	11,12-epoxy-(5z,8z,11z)-icosatrienoic acid	C14770	NA	down
9.226_298.2505	Ricinoleic acid	null	HMDB0034297	down
9.375_300.2662	12-hsa	null	HMDB0061706	down
9.438_296.2349	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
9.501_300.2662	12-hsa	null	HMDB0061706	down
9.817_278.2243	Elaidolinolenic acid	NA	NA	down

Differential metabolites identified in positive mode (N 0d vs S 0d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
2.085_268.0805	Inosine	C00294	HMDB0000195	down
5.81_188.1048	Azelaic acid	C08261	HMDB0000784	up

2.468_100.0524	5-valerolactone	C02240	NA	up
3.982_138.068	Veratrole	NA	NA	up
3.983_110.0731	Trans,trans-2,4-heptadienal	NA	NA	up
4.333_179.0944	Salsolinol	C09642	HMDB0042012	up
4.55_152.12	Pulegone	C09893	HMDB0035604	up
4.742_259.1783	Hexanoylcarnitine	null	HMDB0000705	down
5.632_208.0734	3,4-dimethoxycinnamic acid	NA	NA	up
6.068_144.0575	1-naphthol	C11714	HMDB0012138	up
7.281_315.2407	Decanoylcarnitine	null	HMDB0000651	down
8.006_343.2721	Lauroylcarnitine	NA	NA	down
8.047_318.2192	15-deoxy-δ12,14-prostaglandin a1	NA	NA	up
8.113_288.2087	Epitestosterone	null	HMDB0000628	up
9.551_378.2766	2-arachidonoyl glycerol	C13856	HMDB0004666	up
9.791_356.2922	1-oleoyl-rac-glycerol	NA	NA	up
3.076_185.105	Ecgonine	C10858	HMDB0006548	up
3.119_141.0789	Hypoglycin a	NA	NA	up
3.987_155.0945	Arecoline	C10129	HMDB0030353	up
5.235_181.1102	3,4-dimethoxyphenethylamine (dmpea)	NA	NA	up
5.81_202.1204	Sebacic acid	C08277	HMDB0000792	up
8.847_299.2822	D-sphingosine	C00319	NA	up
0.694_174.0503	(e)-2-[(2s)-2-amino-2-carboxyethoxy]-2-hydr	NA	NA	up
0.709_75.0684	Trimethylamine n-oxide	C01104	HMDB0000925	up
0.719_177.0458	Fmet	NA	NA	up
0.736_338.0837	Ascorbyl glucoside	NA	NA	down
0.957_253.1174	Penciclovir	C07417	HMDB0014444	down
10.195_344.2712	Cardanolide	NA	NA	down
10.244_434.243	1-linoleyl-sn-glycerol 3-phosphate	NA	NA	up
10.314_292.2375	Edetol	NA	NA	down
10.332_363.3133	Terminaline	NA	NA	down
10.334_346.2868	Cetyl benzoate	null	HMDB0094685	down
11.425_731.546	1-tetradecanoyl-2-[(9z)-octadecenoyl]-sn-gly	null	HMDB0007873	down
11.458_757.5612	Pc	null	HMDB0007973	down
2.272_104.0296	Methional	null	HMDB0031857	up
2.372_173.1416	Imagabalin	NA	NA	up
2.468_189.1	(+)-castanospermine	NA	NA	up
2.565_189.1	(+)-castanospermine	NA	NA	up
2.586_120.0245	4-thiapentanoic acid	C08276	HMDB0001527	up
2.654_104.0296	Methional	null	HMDB0031857	up
2.926_226.0953	Dl-carbidopa	NA	NA	up
3.14_159.0895	N-acetylvaline	null	HMDB0011757	up
3.141_124.0524	Guaiacol	C15572	HMDB0001398	up
3.343_412.2366	Ethyl (2r)-2-[(3s,5as,9ar,10as)-3-methyl-1,4-d	null	HMDB0061178	up
3.755_186.1367	Capuride	NA	NA	up
3.863_216.1473	Valylvaline	null	HMDB0029140	up
3.917_216.09	1,2,3,4-tetrahydro-beta-carboline-3-carboxyli	null	HMDB0035665	up
3.955_279.147	Metalaxyl	C10947	HMDB0031802	up
3.982_109.0892	3662332	NA	NA	up
3.983_187.1207	Pivagabine	NA	NA	up

3.984_127.0996	Lq1825000	NA	NA	up
3.985_94.0782	1,3,5-heptatriene	null	HMDB0061889	up
4.064_215.1155	O-propenoyl-d-carnitine	null	HMDB0013124	up
4.083_217.1312	Propionylcarnitine	C03017	HMDB0000824	up
4.272_285.1576	3-[2-(dimethylamino)ethyl]-5-(1h-1,2,4-triazc	null	HMDB0060847	up
4.33_260.1734	Carisoprodol	C07927	HMDB0014539	up
4.331_215.1156	O-propenoyl-d-carnitine	null	HMDB0013124	up
4.332_244.1787	Leu-leu	C11332	HMDB0028933	down
4.397_217.1313	Propionylcarnitine	C03017	HMDB0000824	up
4.432_171.1256	Gabapentin	C07018	HMDB0005015	up
4.5_211.1207	Isoprenaline	C07056	HMDB0015197	up
4.558_238.1204	2444643wxk	null	HMDB0034046	up
4.615_227.1157	Dimetofrine	NA	NA	up
4.688_170.0578	3,4-dihydroxyphenylglycol	C05576	HMDB0000318	down
4.738_198.0529	Vanillyl mandelic acid	C05584	HMDB0133489	down
4.742_166.0264	Phthalic acid	C01606	HMDB0002107	down
4.78_169.1101	Aceclidine	NA	NA	up
4.781_124.0888	3721	null	HMDB0031686	up
4.782_123.1048	6-[(1z)-1-propen-1-yl]-2,3,4,5-tetrahydropyri	null	HMDB0033365	up
4.782_141.1154	8-methyl-8-azabicyclo[3.2.1]octan-3-ol	NA	NA	up
4.782_187.1207	Pivagabine	NA	NA	up
4.782_78.0469	Benzene	C01407	HMDB0001505	up
4.783_151.0996	Hydroxyamphetamine	null	HMDB0060765	up
4.783_201.1364	Capryloylglycine	null	HMDB0000832	up
4.784_152.0836	2128	null	HMDB0041326	up
4.79_231.1469	N-(tert-butoxycarbonyl)-l-leucine	NA	NA	up
4.804_226.084	Genipin	null	HMDB0035830	up
5.052_187.1206	Pivagabine	NA	NA	up
5.076_229.1313	Butenylcarnitine	null	HMDB0013126	up
5.159_244.1211	Rac-etomidate	NA	NA	up
5.163_185.1414	Atagabalin	NA	NA	up
5.165_225.1363	2616	C07129	HMDB0015009	up
5.233_199.1207	Methyl (2r,3s)-3-hydroxy-8-methyl-8-azabicy	C12448	HMDB0006406	up
5.237_182.0918	(e)-dacarbazine	NA	NA	up
5.238_142.0993	2347	null	HMDB0031403	up
5.292_184.1099	5,5-dimethyl-4-(3-oxobutyl)dihydro-2(3h)-fu	NA	NA	up
5.314_243.1469	Tiglylcarnitine	null	HMDB0002366	up
5.412_180.0785	Propylparaben	null	HMDB0032574	down
5.412_220.0711	Carbamorph	NA	NA	down
5.514_155.1309	To0127900	null	HMDB0031179	up
5.514_183.1259	Methyprylon	null	HMDB0015239	up
5.514_201.1364	Capryloylglycine	null	HMDB0000832	up
5.76_201.1363	Capryloylglycine	null	HMDB0000832	up
5.789_106.0783	P-xylene	C06756	HMDB0059924	up
5.808_205.1315	Panthenol	null	HMDB0004231	up
5.81_124.0888	3721	null	HMDB0031686	up
5.811_152.0836	2128	null	HMDB0041326	up
5.811_216.1361	1780537	null	HMDB0000888	up

5.819_225.1365	2616	C07129	HMDB0015009	up
5.9_195.1259	4-(2-aminopropoxy)-3,5-dimethylphenol	null	HMDB0060954	up
5.9_307.1782	Buflomedil	NA	NA	up
5.901_167.1309	2-n-butyl-4-ethyl-5-methyloxazole	null	HMDB0037886	up
5.902_213.1363	C7-hsl	NA	NA	up
5.952_311.2094	(4s)-4-[(2e,4z)-2,4-decadienoyloxy]-4-(trimet	null	HMDB0013325	up
6.009_140.1201	2389	null	HMDB0031834	up
6.011_168.1149	Trans-geranic acid	NA	NA	up
6.039_592.3263	Urobilinogen	C05790	HMDB0001898	up
6.067_219.0895	Aniracetam	NA	NA	up
6.097_196.1098	Hexyl 2-furoate	null	HMDB0037725	up
6.103_213.1364	C7-hsl	NA	NA	up
6.133_310.1415	Lersivirine	NA	NA	up
6.147_311.2095	(4s)-4-[(2e,4z)-2,4-decadienoyloxy]-4-(trimet	null	HMDB0013325	up
6.157_215.152	11343172	NA	NA	up
6.248_287.2094	5955761	C02838	HMDB0000791	down
6.346_170.0941	2-(diethoxymethyl)furan	NA	NA	down
6.379_311.2095	(4s)-4-[(2e,4z)-2,4-decadienoyloxy]-4-(trimet	null	HMDB0013325	down
6.598_534.0282	Udp-beta-l-threo-pentopyranos-4-ulose	NA	NA	down
6.622_301.2251	3-[(2,6-dimethylheptanoyl)oxy]-4-(trimethyla	null	HMDB0006320	down
6.649_286.2296	Vitamin a	C17276	HMDB0000305	up
6.708_229.1677	1872050	null	HMDB0013267	up
6.797_212.1411	Mfcd18781916	null	HMDB0033601	up
6.875_313.225	9-decenoylcarnitine	null	HMDB0013205	down
6.88_329.2563	O-(4,8-dimethylnonanoyl)carnitine	null	HMDB0006202	up
7.016_279.1833	Moxisylyte	NA	NA	up
7.167_330.2557	Ethyl eicosapentaenoic acid	C16184	HMDB0039530	down
7.332_329.1502	Cypendazole	NA	NA	down
7.508_327.2407	Cxa-10	null	HMDB0062737	up
7.57_414.204	Inspra	C12512	HMDB0014838	down
7.623_270.2346	1-methyl-4-[(8e)-10-methyl-6-methylene-8-ur	null	HMDB0039155	up
7.636_327.2407	Cxa-10	null	HMDB0062737	up
7.65_341.2565	Trans-2-dodecenoylcarnitine	null	HMDB0013326	down
7.679_344.2098	Oxyphencyclimine	C07851	HMDB0014527	up
7.689_590.3103	Urobilin, (-)-	null	HMDB0004160	down
7.698_414.204	Inspra	C12512	HMDB0014838	down
7.717_263.1882	(+)-tramadol	C07153	HMDB0014339	up
7.76_329.2563	O-(4,8-dimethylnonanoyl)carnitine	null	HMDB0006202	up
7.781_263.1884	(+)-tramadol	C07153	HMDB0014339	up
7.785_286.0863	Ethofumesate	NA	NA	up
7.857_263.1883	(+)-tramadol	C07153	HMDB0014339	up
7.945_367.2721	3, 5-tetradecadiencarnitine	null	HMDB0013331	down
7.977_327.2406	Cxa-10	null	HMDB0062737	up
8.005_184.1462	10-undecenoic acid	C13910	HMDB0033724	down
8.111_408.2511	Asebotoxin ii	NA	NA	up
8.118_302.2244	Eicosapentanoic acid	C06428	HMDB0001999	up
8.146_286.2141	1792831	C19615	HMDB0000672	down
8.153_307.2145	Betaxolol	C06849	HMDB0014341	up

8.174_388.261	7alpha-hydroxy-3-oxochol-4-en-24-oic acid	null	HMDB0062744	down
8.182_313.2613	Palgly	null	HMDB0013034	up
8.223_256.0759	Benfuresate	NA	NA	down
8.246_315.277	(8e)-2-amino-8-octadecene-1,3,4-triol	null	HMDB0038057	up
8.252_236.1411	4-(heptyloxy)benzoic acid	NA	NA	up
8.258_369.2877	Cis-5-tetradecenoylcarnitine	null	HMDB0002014	down
8.304_414.204	Inspra	C12512	HMDB0014838	down
8.349_301.2978	Sphinganine	C00836	HMDB0000269	down
8.393_315.277	(8e)-2-amino-8-octadecene-1,3,4-triol	null	HMDB0038057	up
8.396_279.2557	Linoleamide	null	HMDB0062656	up
8.403_395.3034	9,12-hexadecadienoylcarnitine	null	HMDB0013334	down
8.406_297.2666	Unii:out5yhb7bo	NA	NA	up
8.454_162.1408	Hexylbenzene	null	HMDB0061815	down
8.455_240.1725	(1s,2r,5s)-2-isopropyl-5-methylcyclohexyl 3-(	null	HMDB0032369	down
8.536_371.3034	4149853	null	HMDB0005066	down
8.561_240.1722	(1s,2r,5s)-2-isopropyl-5-methylcyclohexyl 3-(	null	HMDB0032369	down
8.575_313.2613	Palgly	null	HMDB0013034	up
8.593_287.2457	N,n-bis(2-hydroxyethyl)dodecanamide	null	HMDB0032358	down
8.645_331.2145	Megastachine	NA	NA	down
8.658_397.3191	(2e)-hexadecenoylcarnitine	null	HMDB0006317	down
8.707_286.2142	1792831	C19615	HMDB0000672	down
8.786_330.2557	Ethyl eicosapentaenoic acid	C16184	HMDB0039530	down
8.859_415.3087	Myxalamid a	NA	NA	up
8.863_242.1881	3-oxotetradecanoic acid	null	HMDB0010730	down
8.924_430.3082	Hecogenin	NA	NA	down
8.969_252.1725	Cuauhtemone	NA	NA	down
8.992_302.2244	Eicosapentanoic acid	C06428	HMDB0001999	down
9.02_416.3288	Calcitriol	C01673	HMDB0001903	down
9.075_278.0968	Egualen	NA	NA	down
9.076_310.123	Porphine	NA	NA	down
9.081_397.2252	Drotaverine	null	HMDB0015669	down
9.094_338.2455	8,9-dihetre	C14773	HMDB0002311	down
9.292_316.24	Pregnane-3,20-dione	NA	NA	down
9.379_335.3185	(2e,4z)-n-isobutyl-2,4-octadecadienamide	null	HMDB0031678	up
9.382_352.2611	Glyceryl 2-linolenate	null	HMDB0011540	up
9.401_330.1281	Flurbiprofen axetil	NA	NA	down
9.458_268.24	Mfcd00133175	null	HMDB0060038	down
9.529_354.2765	1715064	null	HMDB0011538	up
9.537_402.2768	1,3-dihydroxy-2-propanyl (4z,7z,10z,13z,16z	null	HMDB0011557	up
9.551_395.3033	9,12-hexadecadienoylcarnitine	null	HMDB0013334	up
9.583_408.1959	(6beta,8xi,11beta,14xi,16alpha)-9-fluoro-6,11	null	HMDB0061022	up
9.588_262.2294	Sl3675000	NA	NA	up
9.589_354.2766	1715064	null	HMDB0011538	up
9.59_336.2661	Pregnanetriol	null	HMDB0006070	up
9.592_371.3034	4149853	null	HMDB0005066	up
9.636_421.3189	(4s)-4-[(9z,12z,15z)-9,12,15-octadecatrienoyl	null	HMDB0006319	up
9.686_386.3393	1,3-dihydroxy-2-propanyl icosanoate	null	HMDB0011542	down

Differential metabolites identified in negative mode (N 0d vs S 0d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
1.128_136.0383	Hypoxanthine	C00262	HMDB0000157	down
2.177_268.0806	Inosine	C00294	HMDB0000195	up
4.36_201.1364	Capryloylglycine	null	HMDB0000832	up
5.964_180.0786	Propylparaben	D01422	NA	up
8.244_216.1723	12-hydroxydodecanoic acid	C08317	HMDB0002059	down
8.295_286.2142	Hexadecanedioic acid	C19615	HMDB0000672	down
9.121_320.2351	11,12-epoxy-(5z,8z,11z)-icosatrienoic acid	C14770	NA	down
0.631_174.0162	Trans-aconitic acid	C02341	HMDB0000958	down
3.156_217.1311	Propionylcarnitine	C03017	HMDB0000824	up
3.326_187.1206	Pivagabine	NA	NA	up
3.373_187.1206	Pivagabine	NA	NA	up
3.814_204.0091	Guaiacol sulfate	null	HMDB0060013	up
5.057_246.0195	3-(3-sulfooxyphenyl)propanoic acid	null	HMDB0094710	up
5.523_212.0319	5-carboxyvanillic acid	NA	NA	up
5.53_184.1098	5,5-dimethyl-4-(3-oxobutyl)dihydro-2(3h)-fu	NA	NA	up
5.553_346.1626	[3-(hydroxymethyl)-3-methyl-2-oxobicyclo[2	null	HMDB0033223	up
5.65_184.1097	5,5-dimethyl-4-(3-oxobutyl)dihydro-2(3h)-fu	NA	NA	up
5.712_178.0628	(e)-4-methoxycinnamic acid	null	HMDB0002040	up
6.219_228.0456	(3e)-4-phenyl-3-buten-2-yl hydrogen sulfate	null	HMDB0133731	up
6.252_270.0851	4-imino-1-(beta-d-ribofuranosyl)-1,4-dihydro	NA	NA	down
6.807_408.2146	Cascarillin	null	HMDB0036836	down
7.758_214.1567	2-hexyltetrahydrofuran-4-yl acetate	null	HMDB0037398	down
7.787_396.1968	20-oxopregn-5-en-3-yl hydrogen sulfate	null	HMDB0000774	down
7.902_367.9077	Triclosan sulfate	null	HMDB0061387	up
8.092_454.2566	Rhodojaponin iv	NA	NA	up
8.308_240.1724	(1s,2r,5s)-2-isopropyl-5-methylcyclohexyl 3-	null	HMDB0032369	down
8.622_312.23	(10e,12z)-9-hydroperoxy-10,12-octadecadien	null	HMDB0006940	down
8.627_331.2147	Megastachine	NA	NA	down
8.727_242.1881	3-oxotetradecanoic acid	null	HMDB0010730	down
8.959_433.3192	B-d-glucopyranosiduronic acid, (3a,5b)-24-[(	C15557	HMDB0000698	up
9.034_244.2036	Mfcd00059633	null	HMDB0061656	down
9.068_430.3079	Hecogenin	NA	NA	down
9.068_476.3136	2,3,14,20-tetrahydroxy-22,23-epoxyergost-7-	null	HMDB0038497	down
9.438_296.2349	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
9.501_300.2662	12-hsa	null	HMDB0061706	down
9.645_434.2447	1-linoleyl-sn-glycerol 3-phosphate	NA	NA	up
9.731_298.2505	Ricinoleic acid	null	HMDB0034297	down
9.818_410.2433	1-palmitoyl lysophosphatidic acid	C04036	HMDB0007853	up

Differential metabolites identified in positive mode (N 0d vs B 0d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.66_215.9152	Mutagen x	NA	NA	down
0.715_98.0367	2491	C20441	HMDB0013742	up
0.719_177.0458	Fmet	NA	NA	up
0.736_338.0837	Ascorbyl glucoside	NA	NA	down
0.769_115.0632	L-proline	C16435	NA	up
0.791_155.0348	N-methylethanolamine phosphate	C01210	HMDB0060173	up
0.837_131.0583	N-acetyl-l-alanine	null	HMDB0000766	up

0.946_181.0962	6-methyltetrahydropterin	null	HMDB0002249	down
0.957_253.1174	Penciclovir	C07417	HMDB0014444	down
10.026_535.4004	Vitamin e nicotinate	NA	NA	up
10.218_398.3394	Dilauroyl peroxide	NA	NA	down
11.215_755.546	1-palmitoyl-2-[(9z,12z,15z)-octadecatrienoyl	null	HMDB0007975	down
2.085_268.0805	Inosine	C00294	HMDB0000195	down
2.586_120.0245	4-thiapentanoic acid	C08276	HMDB0001527	up
2.654_104.0296	Methional	null	HMDB0031857	up
2.926_226.0953	Dl-carbidopa	NA	NA	up
3.53_243.147	Tiglylcarnitine	null	HMDB0002366	up
3.706_245.1626	2-methylbutyrylcarnitine	null	HMDB0000378	up
3.76_224.0908	Etofylline	NA	NA	down
3.917_216.09	1,2,3,4-tetrahydro-beta-carboline-3-carboxyli	null	HMDB0035665	up
3.955_279.147	Metalaxyl	C10947	HMDB0031802	up
4.091_257.1626	2-hexenoylcarnitine	null	HMDB0013161	down
4.151_174.0714	4,4'-thiobis-2-butanone	null	HMDB0037155	down
4.154_191.0979	Trihomomethionine	NA	NA	down
4.272_285.1576	3-[2-(dimethylamino)ethyl]-5-(1h-1,2,4-triazc	null	HMDB0060847	up
4.307_209.0688	Qv1mvo1r	NA	NA	up
4.308_134.0367	Ortho-phthalaldehyde	NA	NA	up
4.508_200.1524	Hmba	null	HMDB0041901	down
4.688_170.0578	3,4-dihydroxyphenylglycol	C05576	HMDB0000318	down
4.853_283.1782	6571082	null	HMDB0060994	down
5.039_256.142	Pulcherriminic acid	NA	NA	down
5.159_244.1211	Rac-etomidate	NA	NA	up
5.352_279.1833	Moxisylyte	NA	NA	up
5.433_92.0626	Toluene	C01455	HMDB0034168	down
5.548_285.1938	(4s)-4-[(2e)-2-octenoyloxy]-4-(trimethylamm	null	HMDB0013324	down
5.612_302.0788	Hesperetin	C01709	HMDB0005782	up
5.871_309.1938	Metipranolol	C07915	HMDB0015345	down
5.9_307.1782	Buflomedil	NA	NA	up
5.949_309.1937	Metipranolol	C07915	HMDB0015345	down
5.989_226.1206	Butopyronoxyl	NA	NA	down
6.068_144.0575	1-naphthol	C11714	HMDB0012138	up
6.079_199.1208	Methyl (2r,3s)-3-hydroxy-8-methyl-8-azabicy	C12448	HMDB0006406	down
6.138_289.1346	Chloropyramine	null	HMDB0015690	up
6.16_274.041	Ensulizole	NA	NA	up
6.168_309.1938	Metipranolol	C07915	HMDB0015345	down
6.325_250.1205	Trolox	null	HMDB0038804	down
6.342_203.0946	Indole-3-butyric acid	C11284	HMDB0002096	down
6.346_170.0941	2-(diethoxymethyl)furan	NA	NA	down
6.358_136.0524	Phenyl acetate	C00548	NA	down
6.379_311.2095	(4s)-4-[(2e,4z)-2,4-decadienoyloxy]-4-(trimet	null	HMDB0013325	down
6.604_276.1724	Cyclandelate	null	HMDB0015586	up
6.797_212.1411	Mfcd18781916	null	HMDB0033601	up
6.799_150.068	4'-methoxyacetophenone	null	HMDB0032570	down
6.8_264.136	(±)-(2e)-abscisic acid	null	HMDB0036093	down
6.804_262.1204	Helenalin	NA	NA	down

6.875_313.225	9-decenoylcarnitine	null	HMDB0013205	down
7.136_226.084	Genipin	null	HMDB0035830	down
7.317_268.1308	2-(2-carboxyethyl)-4-methyl-5-pentyl-3-furoi	null	HMDB0061643	up
7.473_284.071	Diazepam	C06948	HMDB0014967	down
7.554_166.0993	Tbhq	null	HMDB0032062	down
7.554_284.0709	Diazepam	C06948	HMDB0014967	down
7.555_120.0939	Cumene	C14396	HMDB0034029	down
7.592_190.0992	Butylphthalide	C17854	HMDB0032064	up
7.638_120.0939	Cumene	C14396	HMDB0034029	down
7.65_341.2565	Trans-2-dodecenoylcarnitine	null	HMDB0013326	down
7.681_210.089	3-(3,5-dimethoxyphenyl)propanoic acid	null	HMDB0127493	down
7.717_263.1882	(+)-tramadol	C07153	HMDB0014339	up
7.758_592.326	Urobilinogen	C05790	HMDB0001898	up
7.761_273.2665	Hexadecasphinganine	NA	NA	down
7.776_317.2928	2-amino-1,3,4-octadecanetriol	C12144	HMDB0004610	down
7.781_263.1884	(+)-tramadol	C07153	HMDB0014339	up
7.785_286.0863	Ethofumesate	NA	NA	up
7.794_192.1151	Ibufenac	NA	NA	down
7.857_263.1883	(+)-tramadol	C07153	HMDB0014339	up
7.945_367.2721	3, 5-tetradecadiencarnitine	null	HMDB0013331	down
8.106_222.1982	(2e,6e)-farnesol	C06081	HMDB0004305	down
8.107_208.1826	2-decylfuran	null	HMDB0032215	down
8.112_134.1095	P-cymene	C06575	HMDB0005805	down
8.112_152.12	Citral	C01499	NA	down
8.113_120.0938	Cumene	C14396	HMDB0034029	down
8.118_302.2244	Eicosapentanoic acid	C06428	HMDB0001999	up
8.119_194.1306	Sedanolide	NA	NA	down
8.119_280.0761	Esonarimod	NA	NA	down
8.119_289.0763	Adrafinil	NA	NA	down
8.12_264.1037	2-(6'-methylthio)hexylmalic acid	NA	NA	down
8.146_214.1568	3-oxolauric acid	C02367	HMDB0010727	down
8.146_286.2141	1792831	C19615	HMDB0000672	down
8.17_190.1721	1,4-di-tert-butylbenzene	null	HMDB0094670	down
8.182_222.1982	(2e,6e)-farnesol	C06081	HMDB0004305	down
8.183_208.1826	2-decylfuran	null	HMDB0032215	down
8.223_256.0759	Benfuresate	NA	NA	down
8.349_301.2978	Sphinganine	C00836	HMDB0000269	down
8.417_328.225	(10e,15z)-9,12,13-trihydroxy-10,15-octadeca	null	HMDB0035919	up
8.455_240.1725	(1s,2r,5s)-2-isopropyl-5-methylcyclohexyl 3-	null	HMDB0032369	down
8.489_178.1356	Propofol	C07523	HMDB0014956	down
8.561_240.1722	(1s,2r,5s)-2-isopropyl-5-methylcyclohexyl 3-	null	HMDB0032369	down
8.582_285.1026	Probenecid	C07372	HMDB0015166	down
8.587_590.3097	Urobilin, (-)-	null	HMDB0004160	up
8.593_287.2457	N,n-bis(2-hydroxyethyl)dodecanamide	null	HMDB0032358	down
8.628_327.2772	N-heptadecanoylglycine	null	HMDB0013246	down
8.645_331.2145	Megastachine	NA	NA	down
8.681_236.1411	4-(heptyloxy)benzoic acid	NA	NA	down
8.811_238.1567	(2z)-3,7-dimethyl-2,6-octadien-1-yl 3-oxobuta	null	HMDB0038256	down

8.992_302.2244	Eicosapentanoic acid	C06428	HMDB0001999	down
9.027_298.2505	Ricinoleic acid	null	HMDB0034297	down
9.075_278.0968	Egualen	NA	NA	down
9.076_310.123	Porphine	NA	NA	down
9.182_282.198	Retinal 2	C05918	HMDB0035695	down
9.479_279.2559	Linoleamide	null	HMDB0062656	down
9.48_262.2293	Sl3675000	NA	NA	down
9.529_354.2765	1715064	null	HMDB0011538	up
9.537_402.2768	1,3-dihydroxy-2-propanyl (4z,7z,10z,13z,16z	null	HMDB0011557	up
9.551_378.2766	2-arachidonoyl glycerol	C13856	HMDB0004666	up
9.551_395.3033	9,12-hexadecadienoylcarnitine	null	HMDB0013334	up
9.583_408.1959	(6beta,8xi,11beta,14xi,16alpha)-9-fluoro-6,11	null	HMDB0061022	up
9.596_334.1439	Pimobendan	NA	NA	down
9.596_336.1393	Estra-1,3,5(10)-trien-3-yl hydrogen sulfate	NA	NA	down
9.597_332.1435	9-fluoro-17?-oxa-dextro-homoandrosta-1,4-di	NA	NA	down
9.598_330.1482	Gibberellin a7	NA	NA	down
9.617_418.308	Dinp	NA	NA	down
9.643_255.2559	Hexadecanamide	NA	NA	down
9.711_302.2243	Eicosapentanoic acid	C06428	HMDB0001999	up
9.715_281.2714	Oleamide	C19670	HMDB0002117	down
9.716_246.2345	Estrane	NA	NA	down
9.783_220.1461	Dk3970000	null	HMDB0013817	down
9.791_356.2922	1-oleoyl-rac-glycerol	NA	NA	up
9.793_264.245	2-[(5z)-5-tetradecen-1-yl]cyclobutanone	null	HMDB0037543	down
9.926_333.3028	(2e,4e,12z)-n-isobutyl-2,4,12-octadecatrienan	null	HMDB0032033	down
9.95_198.1617	4253	null	HMDB0029585	up
9.962_283.2871	Amide c18	C13846	HMDB0034146	down

Differential metabolites identified in negative mode (N 0d vs B 0d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
1.128_136.0383	Hypoxanthine	C00262	HMDB0000157	down
2.177_268.0806	Inosine	C00294	HMDB0000195	down
8.244_216.1723	12-hydroxydodecanoic acid	C08317	HMDB0002059	down
8.295_286.2142	Hexadecanedioic acid	C19615	HMDB0000672	down
9.121_320.2351	11,12-epoxy-(5z,8z,11z)-icosatrienoic acid	C14770	NA	down
9.219_200.1774	Lauric acid	C02679	HMDB0000638	down
6.63_166.0992	Perillic acid	C11924	HMDB0004586	down
0.738_115.0633	L-proline	C00148	HMDB0000162	up
10.092_328.2974	Glycol stearate	null	HMDB0032477	down
10.558_308.2713	Ethyl linoleate	NA	NA	down
5.057_246.0195	3-(3-sulfooxyphenyl)propanoic acid	null	HMDB0094710	up
5.433_230.0247	4-vinylguaiacol sulfate	null	HMDB0127980	up
5.532_382.0356	5-(5,7-dihydroxy-4-oxo-3,4-dihydro-2h-chron	null	HMDB0029202	up
6.03_250.0298	Bisphenol s	NA	NA	up
6.219_228.0456	(3e)-4-phenyl-3-buten-2-yl hydrogen sulfate	null	HMDB0133731	up
7.758_214.1567	2-hexyltetrahydrofuran-4-yl acetate	null	HMDB0037398	down
8.113_309.194	Metipranolol	C07915	HMDB0015345	up
8.308_240.1724	(1s,2r,5s)-2-isopropyl-5-methylcyclohexyl 3-(	null	HMDB0032369	down

8.38_499.9373	Perfluorooctanesulfonic acid	C18142	HMDB0059586	up
8.431_334.2143	1886839	NA	NA	down
8.627_331.2147	Megastachine	NA	NA	down
8.851_296.2349	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
9.095_661.852	Closantel	NA	NA	up
9.438_296.2349	13s-hydroxyoctadecadienoic acid	C14762	HMDB0004667	down
9.468_477.2852	2-linoleoyl-sn-glycero-3-phosphoethanolamir	null	HMDB0011477	up
9.501_300.2662	12-hsa	null	HMDB0061706	down
9.608_482.2431	2-hydroxy-3-(phosphonooxy)propyl (4z,7z,1(	null	HMDB0114755	up
9.817_278.2243	Elaidolinolenic acid	NA	NA	down

Differential metabolites identified in positive mode (A 0d vs A10d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.708_143.0583	Trimethadione	null	HMDB0014491	down
0.711_161.105	Dl-carnitine	NA	NA	down
0.717_228.1108	Tetraacetylethylenediamine	null	HMDB0040573	up
0.749_103.0997	Choline	C00114	HMDB0000097	down
0.763_262.0008	(2e)-4-hydroxy-3-methylbut-2-en-1-yl diphos	NA	NA	down
0.768_162.1083	(s)-1-methoxy-3-heptanethiol	null	HMDB0032380	down
0.769_115.0632	L-proline	C16435	NA	down
0.92_83.0735	1-piperideine	NA	NA	up
0.957_253.1174	Penciclovir	C07417	HMDB0014444	up
0.989_109.064	3,4-diaminopyridine	NA	NA	down
10.076_335.3183	(2e,4z)-n-isobutyl-2,4-octadecadienamide	null	HMDB0031678	up
10.12_269.2716	Capsi-amide	C17515	HMDB0040940	up
10.126_577.4104	Lysopc(22:1(13z))	null	HMDB0010399	up
10.139_323.3185	1-(14-methylhexadecanoyl)pyrrolidine	null	HMDB0034373	up
2.498_208.0847	L-kynurenine	C00328	HMDB0000684	down
2.547_191.0581	5-hydroxyindoleacetate	C05635	HMDB0000763	down
2.751_148.0523	Cinnamic acid	C10438	HMDB0000930	down
2.877_383.115	Acutumidine	NA	NA	down
3.119_141.0789	Hypoglycin a	NA	NA	down
3.14_159.0895	N-acetylvaline	null	HMDB0011757	down
3.271_333.1324	Oglufanide	null	HMDB0028830	up
3.388_143.0734	6-methylquinoline	null	HMDB0033115	up
3.784_230.163	Leu-val	null	HMDB0028942	down
3.887_282.1677	Mm3670000	null	HMDB0061822	up
3.9_355.0074	2-amino-4-hydroxy-6-pyrophosphoryl-methyl	NA	NA	down
3.982_109.0892	3662332	NA	NA	down
3.982_138.068	Veratrole	NA	NA	down
3.983_110.0731	Trans,trans-2,4-heptadienal	NA	NA	down
3.983_187.1207	Pivagabine	NA	NA	down
3.984_127.0996	Lq1825000	NA	NA	down
3.987_155.0945	Arecoline	C10129	HMDB0030353	down
4.332_244.1787	Leu-leu	C11332	HMDB0028933	down
4.397_217.1313	Propionylcarnitine	C03017	HMDB0000824	down
4.5_211.1207	Isoprenaline	C07056	HMDB0015197	down
4.508_200.1524	Hmba	null	HMDB0041901	down
4.615_227.1157	Dimetofrine	NA	NA	down

4.624_431.2731	Istamycin c1	NA	NA	up
4.78_169.1101	Aceclidine	NA	NA	down
4.781_124.0888	3721	null	HMDB0031686	down
4.782_123.1048	6-[(1z)-1-propen-1-yl]-2,3,4,5-tetrahydropyri	null	HMDB0033365	down
4.782_141.1154	8-methyl-8-azabicyclo[3.2.1]octan-3-ol	NA	NA	down
4.782_187.1207	Pivagabine	NA	NA	down
4.783_151.0996	Hydroxyamphetamine	null	HMDB0060765	down
4.783_201.1364	Capryloylglycine	null	HMDB0000832	down
4.784_152.0836	2128	null	HMDB0041326	down
4.79_231.1469	N-(tert-butoxycarbonyl)-l-leucine	NA	NA	down
4.809_475.2993	Netilmicin	null	HMDB0015090	up
4.951_243.1469	Tiglylcarnitine	null	HMDB0002366	down
5.163_185.1414	Atagabalin	NA	NA	down
5.233_153.1152	Pseudopelletierine	C10865	HMDB0034580	down
5.233_199.1207	Methyl (2r,3s)-3-hydroxy-8-methyl-8-azabicy	C12448	HMDB0006406	down
5.235_181.1102	3,4-dimethoxyphenethylamine (dmpea)	NA	NA	down
5.237_182.0918	(e)-dacarbazine	NA	NA	down
5.289_241.1312	Mfcd08277025	NA	NA	down
5.514_155.1309	To0127900	null	HMDB0031179	down
5.514_183.1259	Methyprylon	null	HMDB0015239	down
5.514_201.1364	Capryloylglycine	null	HMDB0000832	down
5.76_201.1363	Capryloylglycine	null	HMDB0000832	down
5.9_195.1259	4-(2-aminopropoxy)-3,5-dimethylphenol	null	HMDB0060954	down
5.901_167.1309	2-n-butyl-4-ethyl-5-methyloxazole	null	HMDB0037886	down
5.902_213.1363	C7-hsl	NA	NA	down
6.215_363.1891	9-[(5r)-5-ethyl-alpha-d-xylopyranosyl]-n-(3-n	null	HMDB0012240	down
6.316_182.0919	(e)-dacarbazine	NA	NA	up
6.336_360.1936	Cortisone	C00762	HMDB0002802	down
6.372_308.0796	Flazin	null	HMDB0033459	up
6.546_362.2091	Cortisol	C00735	HMDB0000063	down
6.88_329.2563	O-(4,8-dimethylnonanoyl)carnitine	null	HMDB0006202	down
6.927_211.1571	Elaeokanine c	NA	NA	down
7.002_346.2143	Corticosterone	C02140	HMDB0001547	down
7.075_220.1099	Precocene ii	NA	NA	down
7.225_228.1361	Traumatic acid	C16308	HMDB0000933	up
7.226_164.1201	Fenipentol	NA	NA	up
7.414_252.136	2,3-dimethoxy-5-methyl-6-(3-methyl-2-buten	null	HMDB0059661	down
7.419_234.1255	Stiripentol	NA	NA	down
7.42_230.1516	Dodecanedioic acid	C02678	HMDB0000623	up
7.508_327.2407	Cxa-10	null	HMDB0062737	down
7.661_329.2564	O-(4,8-dimethylnonanoyl)carnitine	null	HMDB0006202	down
7.76_329.2563	O-(4,8-dimethylnonanoyl)carnitine	null	HMDB0006202	down
7.871_329.2564	O-(4,8-dimethylnonanoyl)carnitine	null	HMDB0006202	down
7.977_327.2406	Cxa-10	null	HMDB0062737	down
8.182_313.2613	Palgly	null	HMDB0013034	down
8.183_208.1826	2-decylfuran	null	HMDB0032215	up
8.246_315.277	(8e)-2-amino-8-octadecene-1,3,4-triol	null	HMDB0038057	down
8.247_279.2558	Linoleamide	null	HMDB0062656	down

8.266_313.2614	Palgly	null	HMDB0013034	down
8.278_201.1362	Capryloylglycine	null	HMDB0000832	down
8.368_291.2198	Penbutolol	C07416	HMDB0015447	down
8.386_313.2614	Palgly	null	HMDB0013034	down
8.393_315.277	(8e)-2-amino-8-octadecene-1,3,4-triol	null	HMDB0038057	down
8.406_297.2666	Unii:out5yhb7bo	NA	NA	down
8.458_248.1774	3222	null	HMDB0037719	up
8.537_327.2771	N-heptadecanoylglycine	null	HMDB0013246	down
8.575_313.2613	Palgly	null	HMDB0013034	down
8.59_297.2664	Unii:out5yhb7bo	NA	NA	down
8.628_327.2772	N-heptadecanoylglycine	null	HMDB0013246	down
8.642_279.2559	Linoleamide	null	HMDB0062656	down
8.642_320.2517	3beta-fluoro-5beta-pregnan-20-one	NA	NA	down
8.643_262.2293	Sl3675000	NA	NA	down
8.68_299.2823	Threo-sphingosine, (-)-	null	HMDB0000252	up
8.704_262.2292	Sl3675000	NA	NA	down
8.704_279.2559	Linoleamide	null	HMDB0062656	down
8.705_300.2298	1,3-dihydroxy-2-propanyl (9z)-9-tetradecenoa	null	HMDB0011531	up
8.705_314.2456	Vs1150000	null	HMDB0041220	up
8.707_286.2142	1792831	C19615	HMDB0000672	up
8.734_316.261	9,10-dihydroxystearic acid	NA	NA	up
8.738_280.2398	2210856	null	HMDB0006270	up
8.739_298.2505	Ricinoleic acid	null	HMDB0034297	up
8.768_262.2293	Sl3675000	NA	NA	down
8.769_335.2224	[(4z,7z,11e,13z)-1-carboxy-4,7,11,13-nonade	null	HMDB0060099	down
8.776_423.3345	Linoleyl carnitine	null	HMDB0006469	up
8.783_279.2559	Linoleamide	null	HMDB0062656	down
8.835_297.2666	Unii:out5yhb7bo	NA	NA	down
8.852_262.2292	Sl3675000	NA	NA	down
8.892_297.2666	Unii:out5yhb7bo	NA	NA	down
8.926_252.2089	(8z)-oxacycloheptadec-8-en-2-one	null	HMDB0031086	up
8.964_297.2666	Unii:out5yhb7bo	NA	NA	down
8.981_425.3502	Mfcd22416941	null	HMDB0005065	up
9_280.24	2210856	null	HMDB0006270	down
9.02_171.1257	Gabapentin	C07018	HMDB0005015	down
9.022_262.2293	Sl3675000	NA	NA	down
9.022_297.2665	Unii:out5yhb7bo	NA	NA	down
9.027_155.1309	To0127900	null	HMDB0031179	down
9.027_298.2505	Ricinoleic acid	null	HMDB0034297	up
9.028_279.2558	Linoleamide	null	HMDB0062656	down
9.029_299.2822	Threo-sphingosine, (-)-	null	HMDB0000252	down
9.177_298.2505	Ricinoleic acid	null	HMDB0034297	up
9.585_479.3009	1-oleoyl-sn-glycero-3-phosphoethanolamine	null	HMDB0011506	up
9.611_299.282	Threo-sphingosine, (-)-	null	HMDB0000252	up
9.636_421.3189	(4s)-4-[(9z,12z,15z)-9,12,15-octadecatrienoyl	null	HMDB0006319	up
9.665_547.3636	1-[(11z,14z)]-icosadienoyl-sn-glycero-3-phos	null	HMDB0010392	up
9.711_302.2243	Eicosapentanoic acid	C06428	HMDB0001999	up
9.784_571.3613	Lysopc(22:4(7z,10z,13z,16z))	null	HMDB0010401	up

9.926_333.3028	(2e,4e,12z)-n-isobutyl-2,4,12-octadecatrienan	null	HMDB0032033	up

Differential metabolites identified in negative mode (A 0d vs A 10d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.629_134.0215	Dl-malic acid	C00711	NA	up
0.686_226.0689	(2xi)-d-gluco-heptonic acid	null	HMDB0240292	down
0.687_156.0188	Propanediol 1-phosphate	NA	NA	down
0.696_166.0475	D-xylonic acid	NA	NA	down
0.7_120.0422	D-(−)-threose	NA	NA	down
0.701_102.0317	2-oxobutyric acid	C00109	HMDB0000005	down
0.706_90.0317	L-(+)-lactic acid	C00186	HMDB0000190	up
0.708_162.0528	Diethylpyrocarbonate	C11592	HMDB0032873	down
0.714_129.0426	4-oxoproline	C01877	NA	up
0.726_254.0998	3-o-beta-d-galactosyl-sn-glycerol	NA	NA	up
10.066_479.301	1-oleoyl-sn-glycero-3-phosphoethanolamine	null	HMDB0011506	up
11.875_805.5826	O-{[(2r)-2-(docosanoyloxy)-3-(pentadecanoy	null	HMDB0112334	down
3.156_217.1311	Propionylcarnitine	C03017	HMDB0000824	down
3.326_187.1206	Pivagabine	NA	NA	down
3.373_187.1206	Pivagabine	NA	NA	down
4.36_201.1364	Capryloylglycine	null	HMDB0000832	down
5.196_208.0516	Cys-ser	null	HMDB0028784	down
6.041_252.1359	2,3-dimethoxy-5-methyl-6-(3-methyl-2-buten	null	HMDB0059661	down
6.331_242.1515	5-octyl-2-oxotetrahydro-3-furancarboxylic ac	null	HMDB0030987	up
6.36_184.1097	5,5-dimethyl-4-(3-oxobutyl)dihydro-2(3h)-fu	NA	NA	down
6.586_396.17	Mocetinostat	NA	NA	down
6.586_406.1987	1-(4-hydroxy-3,5-dimethoxyphenyl)-7-(4-hyd	null	HMDB0041091	down
6.807_408.2146	Cascarillin	null	HMDB0036836	down
6.968_256.1673	4-[(2-isopropyl-5-methylcyclohexyl)oxy]-4-o	null	HMDB0036143	up
7.273_188.1411	3-hydroxydecanoic acid	NA	NA	up
7.901_359.2669	3-hydroxydodecanoylcarnitine	null	HMDB0061638	down
7.944_284.1986	(10s)-juvenile hormone iii diol	NA	NA	up
8.198_359.2669	3-hydroxydodecanoylcarnitine	null	HMDB0061638	down
8.295_286.2142	Hexadecanedioic acid	C19615	HMDB0000672	up
8.67_300.2297	(2s)-2,3-dihydroxypropyl (9z)-9-tetradecenoa	null	HMDB0011562	up
8.684_312.2299	(10e,12z)-9-hydroperoxy-10,12-octadecadien	null	HMDB0006940	up
8.812_316.2611	9,10-dihydroxystearic acid	NA	NA	up
9.036_343.272	4147610	null	HMDB0002250	down
9.204_584.2633	Bilirubin	C00486	HMDB0000054	down
9.624_458.2435	1-arachidonoyl-sn-glycerol 3-phosphate	null	HMDB0062312	up
9.645_434.2447	1-linoleyl-sn-glycerol 3-phosphate	NA	NA	up

Differential metabolites identified in positive mode (S 0d vs S 10d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.749_103.0997	Choline	C00114	HMDB0000097	up
5.81_188.1048	Azelaic acid	C08261	HMDB0000784	down
3.347_187.0631	Indole-3-acrylic acid	NA	NA	down
3.388_143.0734	6-methylquinoline	null	HMDB0033115	down
6.182_164.0837	4-phenylbutyric acid	NA	NA	down
5.81_202.1204	Sebacic acid	C08277	HMDB0000792	down

9.699_505.353	C-8 ceramide-1-phosphate	NA	NA	up
10.094_561.4157	N-dodecanoylsphingosine 1-phosphate	null	HMDB0010699	up
11.774_723.5199	1-(1z-hexadecenyl)-2-arachidonoyl-sn-glycer	null	HMDB0011352	up
2.372_173.1416	Imagabalin	NA	NA	down
5.808_205.1315	Panthenol	null	HMDB0004231	down
5.81_124.0888	3721	null	HMDB0031686	down
5.811_216.1361	1780537	null	HMDB0000888	down
5.814_156.115	(2e)-4-hydroxy-2-nonenal	C21642	HMDB0004362	down
6.987_333.2293	Pentoxyverine	NA	NA	up
7.19_331.2137	Megastachine	NA	NA	up
9.56_302.2243	Eicosapentanoic acid	C06428	HMDB0001999	up
9.638_479.3373	1-(1z-hexadecenyl)-sn-glycero-3-phosphocho	null	HMDB0010407	up
9.65_437.2904	2-aminoethyl (2r)-3-[(1z)-1-hexadecen-1-ylox	null	HMDB0011152	up
9.704_481.3529	1-o-hexadecyl-lyso-sn-glycero-3-phosphocho	NA	NA	up
9.749_340.1777	3-hydroxyquinine	null	HMDB0001091	up
9.751_360.1595	2-{3-[2-(1h-imidazol-2-ylmethyl)-6-methoxyp	null	HMDB0033437	up
9.759_507.3687	Lysopc(p-18:0)	null	HMDB0013122	up
9.932_507.3687	Lysopc(p-18:0)	null	HMDB0013122	up
9.991_542.3946	Methyl 3-acetoxy-11-methoxyurs-12-en-28-o	null	HMDB0031675	up

Differential metabolites identified in negative mode (S 0d vs S 10d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.629_134.0215	Dl-malic acid	C00711	NA	up
1.098_181.0738	L-tyrosine	C00082	HMDB0000158	down
10.159_437.2904	2-aminoethyl (2r)-3-[(1z)-1-hexadecen-1-ylox	null	HMDB0011152	up
2.844_130.063	(hydroxyethyl)methacrylate	NA	NA	down

Differential metabolites identified in positive mode (B 0d vs B 10d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.552_109.0014	NA	NA	NA	down
0.607_203.9496	NA	NA	NA	down
0.609_271.9369	NA	NA	NA	down
0.611_339.9243	NA	NA	NA	down
0.611_407.9117	NA	NA	NA	down
0.774_114.0293	NA	NA	NA	up
0.846_112.0136	NA	NA	NA	down
0.957_147.0353	3-thiomorpholinecarboxylic acid	C03901	HMDB0059611	down
1.008_172.0347	NA	NA	NA	down
1.036_204.0214	NA	NA	NA	down
1.077_147.0353	3-thiomorpholinecarboxylic acid	C03901	HMDB0059611	down
1.157_153.04	NA	NA	NA	down
10.033_358.3079	1-stearoylglycerol	D01947	NA	up
10.068_406.3057	NA	NA	NA	up
10.076_335.3183	(2e,4z)-n-isobutyl-2,4-octadecadienamide	null	HMDB0031678	up
10.108_371.2855	NA	NA	NA	down
10.12_269.2716	Capsi-amide	C17515	HMDB0040940	up
10.12_326.2819	Mfcd00045988	NA	NA	up
10.139_323.3185	1-(14-methylhexadecanoyl)pyrrolidine	null	HMDB0034373	up
10.203_297.3029	Tridemorph	C11285	HMDB0031810	up

10.244_434.243	1-linoleyl-sn-glycerol 3-phosphate	NA	NA	up
10.261_311.3185	NA	NA	NA	up
10.303_337.3339	NA	NA	NA	up
10.35_434.243	1-linoleyl-sn-glycerol 3-phosphate	NA	NA	up
10.381_139.0609	NA	NA	NA	down
10.556_798.6609	NA	NA	NA	down
11.515_163.9771	NA	NA	NA	down
11.526_368.3441	NA	NA	NA	up
11.773_783.5771	1-oleoyl-2-linoleoyl-sn-glycero-3-phosphocho	null	HMDB0008105	up
12.027_733.5617	Dl-dipalmitoylphosphatidylcholine	NA	NA	up
2.192_161.051	S-allyl-l-cysteine	NA	NA	down
2.246_161.0509	S-allyl-l-cysteine	NA	NA	down
3.214_175.0666	NA	NA	NA	down
3.445_175.0666	NA	NA	NA	down
3.675_312.0777	Epithienamycin b	NA	NA	down
3.798_129.1517	Octylamine	NA	NA	down
3.984_218.1629	NA	NA	NA	up
4.237_193.0739	Phenylacetylglycine	C05598	HMDB0000821	up
4.264_189.0823	Prenisteine	NA	NA	down
4.508_200.1524	Hmba	null	HMDB0041901	up
4.534_244.1786	Leu-leu	C11332	HMDB0028933	up
4.558_316.1997	NA	NA	NA	other
4.951_243.1469	Tiglylcarnitine	null	HMDB0002366	up
5.292_184.1099	5,5-dimethyl-4-(3-oxobutyl)dihydro-2(3h)-fu	NA	NA	up
5.292_224.1022	NA	NA	NA	up
5.63_203.098	NA	NA	NA	down
5.9_195.1259	4-(2-aminopropoxy)-3,5-dimethylphenol	null	HMDB0060954	up
5.902_213.1363	C7-hsl	NA	NA	up
6.138_289.1346	Chloropyramine	null	HMDB0015690	down
6.319_228.1472	Leu-pro	null	HMDB0011175	up
6.76_313.2251	9-decenoylcarnitine	null	HMDB0013205	down
6.831_215.1885	NA	NA	NA	up
6.841_269.2101	Pramiracetam	NA	NA	up
7.298_252.1335	NA	NA	NA	up
7.569_305.166	NA	NA	NA	down
7.58_295.2509	NA	NA	NA	up
7.581_335.2433	NA	NA	NA	up
7.849_277.2404	NA	NA	NA	up
7.853_335.2433	NA	NA	NA	up
8.112_134.1095	P-cymene	C06575	HMDB0005805	up
8.17_190.1721	1,4-di-tert-butylbenzene	null	HMDB0094670	up
8.175_449.1854	NA	NA	NA	down
8.176_417.159	NA	NA	NA	other
8.182_222.1982	(2e,6e)-farnesol	C06081	HMDB0004305	up
8.183_208.1826	2-decylfuran	null	HMDB0032215	up
8.202_259.1604	NA	NA	NA	down
8.381_335.2433	NA	NA	NA	up
8.421_838.5572	(2r)-1-[(hydroxy{[(2r,3r,5s,6r)-2,3,4,5,6-pent	null	HMDB0062582	up

8.423_390.2767	Bis(2-ethylhexyl) phthalate	NA	NA	up
8.425_816.5743	Cholate	C00695	HMDB0000619	up
8.495_333.2281	NA	NA	NA	up
8.6_253.2403	NA	NA	NA	up
8.607_277.2404	NA	NA	NA	up
8.641_319.2485	NA	NA	NA	up
8.642_279.2559	Linoleamide	null	HMDB0062656	up
8.642_320.2517	3beta-fluoro-5beta-pregnan-20-one	NA	NA	up
8.643_262.2293	Sl3675000	NA	NA	up
8.643_280.2595	NA	NA	NA	up
8.644_616.5152	NA	NA	NA	up
8.646_381.2188	NA	NA	NA	up
8.646_594.5331	NA	NA	NA	up
8.776_423.3345	Linoleyl carnitine	null	HMDB0006469	down
8.783_279.2559	Linoleamide	null	HMDB0062656	up
8.839_377.2329	NA	NA	NA	down
8.893_110.1095	1733342	null	HMDB0061902	up
8.903_292.1674	Gingerdione	C10459	HMDB0039275	up
8.923_338.2608	3-(2,4-cyclopentadien-1-ylidene)-5alpha-andr	NA	NA	up
8.981_425.3502	Mfcd22416941	null	HMDB0005065	down
9.022_297.2665	Unii:out5yhb7bo	NA	NA	up
9.024_616.5152	NA	NA	NA	up
9.025_397.1913	NA	NA	NA	up
9.034_319.2485	NA	NA	NA	up
9.065_357.3604	NA	NA	NA	down
9.158_342.2769	NA	NA	NA	up
9.235_227.2248	NA	NA	NA	up
9.323_369.2878	Cis-5-tetradecenoylcarnitine	null	HMDB0002014	up
9.381_302.2454	Rac-glycerol 1-myristate	NA	NA	up
9.381_402.1703	NA	NA	NA	up
9.382_352.2611	Glyceryl 2-linolenate	null	HMDB0011540	up
9.476_301.2378	NA	NA	NA	up
9.479_244.219	NA	NA	NA	up
9.479_279.2559	Linoleamide	null	HMDB0062656	up
9.48_262.2293	Sl3675000	NA	NA	up
9.636_227.2247	NA	NA	NA	up
9.643_255.2559	Hexadecanamide	NA	NA	up
9.644_532.4942	NA	NA	NA	up
9.677_330.2765	1728235	NA	NA	up
9.697_402.2742	NA	NA	NA	up
9.699_380.2924	Persin	null	HMDB0041103	up
9.711_302.2243	Eicosapentanoic acid	C06428	HMDB0001999	down
9.715_281.2714	Oleamide	C19670	HMDB0002117	up
9.715_287.2798	NA	NA	NA	up
9.715_584.5253	NA	NA	NA	up
9.716_246.2345	Estrane	NA	NA	up
9.716_368.3399	NA	NA	NA	other
9.716_568.5515	NA	NA	NA	up

9.78_343.2541	NA	NA	NA	down
9.793_264.245	2-[(5z)-5-tetradecen-1-yl]cyclobutanone	null	HMDB0037543	up
9.793_424.3911	NA	NA	NA	down
9.826_347.2821	Anandamide	C11695	HMDB0004080	up
9.887_224.1775	2639	null	HMDB0030427	down
9.892_360.1748	NA	NA	NA	up
9.896_242.188	3-oxotetradecanoic acid	null	HMDB0010730	down
9.962_283.2871	Amide c18	C13846	HMDB0034146	up

Differential metabolites identified in negative mode (B 0d vs B10d):

Compound.ID	Name	KEGG.ID	HMDB.ID	label
0.686_202.0452	NA	NA	NA	down
0.687_149.9872	NA	NA	NA	down
0.687_156.0188	Propanediol 1-phosphate	NA	NA	up
0.719_226.0063	NA	NA	NA	down
0.727_293.9937	NA	NA	NA	down
0.737_147.9903	NA	NA	NA	down
10.204_330.2557	Ethyl eicosapentaenoic acid	C16184	HMDB0039530	up
10.238_306.2557	8z,11z,14z-eicosatrienoic acid	C03242	HMDB0002925	up
2.562_165.0789	L-phenylalanine	C02057	NA	up
3.156_217.1311	Propionylcarnitine	C03017	HMDB0000824	up
3.373_187.1206	Pivagabine	NA	NA	up
6.682_243.1833	N-undecanoylglycine	null	HMDB0013286	up
7.513_202.1568	1,3-nonanediol acetate	null	HMDB0032443	up
7.901_359.2669	3-hydroxydodecanoylcarnitine	null	HMDB0061638	up
7.903_349.2382	NA	NA	NA	up
8.199_349.2384	NA	NA	NA	up
8.426_408.2874	Cholic acid	C00695	HMDB0000619	up
8.953_438.298	NA	NA	NA	up
9.036_343.272	4147610	null	HMDB0002250	up
9.041_333.2433	NA	NA	NA	up
9.172_333.2433	NA	NA	NA	up
9.407_432.2273	1-(gamma-linolenoyl)-sn-glycero-3-phosphat	null	HMDB0062316	up
9.624_458.2435	1-arachidonoyl-sn-glycerol 3-phosphate	null	HMDB0062312	up
9.645_434.2447	1-linoleyl-sn-glycerol 3-phosphate	NA	NA	up
9.646_435.2475	NA	NA	NA	up
9.818_410.2433	1-palmitoyl lysophosphatidic acid	C04036	HMDB0007853	up

Table S4

Table S4 Detailed information about the differentially expressed proteins between groups

Differential proteins (N 0d vs A 0d):

Protein_ID	label
sp|P55058|PLTP_HUMAN	up
sp|P05546|HEP2_HUMAN	up
sp|P04278|SHBG_HUMAN	up
sp|Q96PD5|PGRP2_HUMAN	up
sp|O75636|FCN3_HUMAN	up
sp|P08519|APOA_HUMAN	up
sp|O14791|APOL1_HUMAN	up
sp|P02776|PLF4_HUMAN	down
sp|P07996|TSP1_HUMAN	down
sp|Q9H7E2|TDRD3_HUMAN	down
sp|P02775|CXCL7_HUMAN	down

Differential proteins (N 0d vs S 0d):

Protein_ID	label
sp|Q15166|PON3_HUMAN	up
sp|P62937|PPIA_HUMAN	up
sp|O00203|AP3B1_HUMAN	up
sp|P07996|TSP1_HUMAN	down
sp|Q03591|FHR1_HUMAN	down
sp|P26038|MOES_HUMAN	down
sp|P55056|APOC4_HUMAN	down
sp|P60709|ACTB_HUMAN	down
sp|P12814|ACTN1_HUMAN	down
sp|P04406|G3P_HUMAN	down

Differential proteins (N 0d vs B 0d):

Protein_ID	label
sp|P18428|LBP_HUMAN	up
sp|Q14520|HABP2_HUMAN	up
sp|Q15166|PON3_HUMAN	up
sp|Q9UNW1|MINP1_HUMAN	up
sp|Q8WUA8|TSK_HUMAN	up
sp|P05109|S10A8_HUMAN	up
sp|P03950|ANGI_HUMAN	up
sp|P13497|BMP1_HUMAN	up
sp|P26927|HGFL_HUMAN	up
sp|P09871|C1S_HUMAN	up
sp|P00736|C1R_HUMAN	up
sp|P02656|APOC3_HUMAN	up
sp|P61626|LYSC_HUMAN	up
sp|Q6Q788|APOA5_HUMAN	up
sp|P22352|GPX3_HUMAN	up
sp|P00748|FA12_HUMAN	up
sp|P02745|C1QA_HUMAN	up

sp|Q86UX7|URP2_HUMAN	up
sp|P04406|G3P_HUMAN	up
sp|P02655|APOC2_HUMAN	up
sp|Q9BXR6|FHR5_HUMAN	up
sp|P55774|CCL18_HUMAN	up
sp|P23528|COF1_HUMAN	up
sp|P06702|S10A9_HUMAN	up
sp|Q99969|RARR2_HUMAN	up
sp|O14791|APOL1_HUMAN	up
sp|P01876|IGHA1_HUMAN	down
sp|P00738|HPT_HUMAN	down
sp|P69905|HBA_HUMAN	down
sp|P20742|PZP_HUMAN	down
sp|P05543|THBG_HUMAN	down
sp|P02753|RET4_HUMAN	down
sp|P01011|AACT_HUMAN	down
sp|P0DOX2|IGA2_HUMAN	down
sp|P19827|ITIH1_HUMAN	down
sp|P51884|LUM_HUMAN	down
sp|P01859|IGHG2_HUMAN	down
sp|P05156|CFAI_HUMAN	down

Differential proteins (A 0d vs A 10d):

Protein_ID	label
sp|P02776|PLF4_HUMAN	up
sp|P08567|PLEK_HUMAN	up
sp|P05109|S10A8_HUMAN	up
sp|P04264|K2C1_HUMAN	up
sp|Q93079|H2B1H_HUMAN	up
sp|Q8WWA0|ITLN1_HUMAN	up
sp|Q9H7E2|TDRD3_HUMAN	up
sp|Q92743|HTRA1_HUMAN	up
sp|P02745|C1QA_HUMAN	up
sp|P04406|G3P_HUMAN	up
sp|P06702|S10A9_HUMAN	up
sp|Q96KK5|H2A1H_HUMAN	up
sp|P05543|THBG_HUMAN	down
sp|P02652|APOA2_HUMAN	down

Differential proteins (S 0d vs S 10d):

Protein_ID	label
sp|P02751|FINC_HUMAN	up
sp|P55056|APOC4_HUMAN	up
sp|P04278|SHBG_HUMAN	down
sp|P05154|IPSP_HUMAN	down
sp|O00203|AP3B1_HUMAN	down

Differential proteins (B 0d vs B 10d):

Protein_ID	label

sp|P02788|TRFL_HUMAN	down
sp|P05109|S10A8_HUMAN	down
sp|O95372|LYPA2_HUMAN	down
sp|P05160|F13B_HUMAN	down
sp|Q9NZP8|C1RL_HUMAN	down
sp|P60709|ACTB_HUMAN	down
sp|P80108|PHLD_HUMAN	down
sp|P20160|CAP7_HUMAN	down
sp|P00748|FA12_HUMAN	down
sp|Q15404|RSU1_HUMAN	down
sp|Q86UX7|URP2_HUMAN	down
sp|Q96PD5|PGRP2_HUMAN	down
sp|O94769|ECM2_HUMAN	down
sp|P05164|PERM_HUMAN	down
sp|P23528|COF1_HUMAN	down
sp|Q5T013|HYI_HUMAN	down
sp|P06702|S10A9_HUMAN	down
sp|P33908|MA1A1_HUMAN	up
sp|P04114|APOB_HUMAN	up

Table S5

Table S5 Migraine related targets collected from databases

Overview of migraine related targets collected from databases

Database	Key words	Number of Related targets
DrugBank	Migraine	84
TTD	Migraine	36
OMIM	Migraine	48
DisGeNET	Migraine disorders	81
Total		195

Note：

Therapeutic Target Database (TTD), Online Mendelian Inheritance in Man (OMIM).

Targets collected from DrugBank database (84):	**Targets collected from TTD database (36):**	**Targets collected from OMIM database (48):**	**Targets collected from ODisGeNET database (81):**
P35354	P80511	O00555	Q7Z2W7
P23219	P28221	P50993	Q9UM47
Q04828	Q8NER1	P48730	Q07954
P30542	P41143	P01258	Q9HAZ2
P29274	P28222	P06881	P37173
P29275	Q16602	P03372	Q5TD97
P0DMS8	P23219	P35498	Q9HAC7
Q01064	P35354	P25101	P03372
Q08499	P41586	P42898	P01258
Q13370	P08588	P31645	P06881
O76074	O95180	Q7Z418	P50993
P06881	O00555	P54098	P02462
P10092	P08908	P11166	P28223
Q16602	Q14524	P01375	Q9UN88
P28221	Q00975	P09172	P34969
P28222	P27338	P02462	O00555
P28223	P41595	P19838	Q8IWA4
P35348	P48167	P03915	Q7Z6L0
P35368	O75311	Q9UM47	Q14814
P25100	P23415	P06213	P08908
P23975	P23416	Q96QP1	P43003
P31645	P25103	Q7Z6L0	P01137
O43497	Q14416	P35228	O60313
O95180	Q9Y271	P12821	P54098
Q9P0X4	P28223	P09619	P00403
P0DP23	P10635	P30939	P22301
Q05940	P06881	P00846	P48730
P41595	P10092	P43003	P18507
P28335	P30939	P53985	Q96RR1
P08908	P35408	P08908	O75129
P34969	P29475	Q92889	Q9C0D0
P14867	P35372	P28222	P42336
P35498	P28335	P28221	Q8WWQ2
Q9Y5Y9	P14416	P28223	Q9NSU2

Q9UI33
Q99250
Q9NY46
P35499
Q14524
Q01118
Q9UQD0
Q15858
P39086
Q13002
Q13003
Q16099
Q16478
P00918
P22748
Q13936
Q01668
O60840
Q13698
Q02641
Q08289
P54284
O00305
PTGS2
P14416
P21728
P21918
P35462
Q9UKV0
P21917
P30939
P08588
P60880
Q8NER1
P07550
P56181
P31040
Q06432
P14555
P11229
Q13639
P46098
P41594
Q9UBS5
O00555
Q05586
P49841
P29218
O14732
P42263

P31645
P23975

P46098
P05026
P00558
P03897
P03905
Q04837
O96011
Q15738
Q13586
Q13733
Q86YV9
Q96RD7
O95140
Q4G176

Q9NS39
O14786
B7ZAP0
Q5R372
Q9HC58
Q9GZQ4
O00401
Q13976
Q9GZL7
Q9P2E8
Q63HN8
O95279
Q9UIG0
Q8NCD3
P29474
Q9P212
Q9BZE1
Q9H8M5
Q8N187
Q15777
Q96SD1
P31645
P01375
P35498
Q9H5I1
P80511
Q7Z5K2
P35556
Q8IW00
P14416
Q96PU5
O95214
Q9ULU4
P12821
P09172
Q8IUQ0
Q9UEE9
P46937
Q9Y6F6
Q96CS2
P21964
P18509
P42898
Q9ULZ9
Q7Z418
P28222
Q14642

Table S6

Table S6 Detailed information about the protein-metabolite interaction network

Node1	Node2
P41143	Q5JY77
P41143	P27824
P41143	P16615
P41143	Q96Q45-2
P28222	P22392
P28222	P35609
P28222	P59768
P28222	P09471-1
P28222	P62873-1
Q16602	O60895
P41586	P0DP25
P08588	Q86UL8
P08588	Q96QZ7
P08588	Q5TCQ9
P08588	P49407
P08588	P32121
O00555	Q9BZC7
O00555	O43681
O00555	Q96CW1
O00555	Q86SJ2
O00555	P04075
O00555	Q5XG79
O00555	Q96I11
O00555	O95153
O00555	Q9HCP6
O00555	P28799
O00555	Q92551
O00555	Q8TAS6
O00555	O75095
O00555	O00339
O00555	Q9NQG1
O00555	B9EG76
O00555	B7ZLY3
O00555	A8MQ03
O00555	P29122
O00555	O15034
O00555	P41222
O00555	Q9UHX1
O00555	P04275
O00555	P26640
O00555	Q9BVA1
O00555	Q9NP64
O00555	O00468
O00555	O75953
P08908	P11362
P08908	P28222
Q14524	O14744
Q14524	Q13424
Q14524	P0DP25
Q00975	P28702
P27338	Q96SB4
P27338	Q5RI15

P41595	O75970
P41595	Q9BUM1
P41595	Q8WUD6
P41595	O60238
P41595	Q12983
P41595	P05026
P41595	Q99758
P41595	P54368
P41595	O14929
P41595	Q9Y342
P41595	Q8N8Q9
P41595	Q6ZSY5
P41595	Q9UJH8
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O60391	Q05586
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29985	Q05586
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Q9BUH8	Q05586
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O94956	C04555
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32816	15422
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16827	44409
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17203	16015
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27823	28790
144308	28790
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C00735	18243
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27823	18265
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422	15996
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17596	15996
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16814	27974
16962	27974

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422 18420
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17712	17775
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18183	17590
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17203	17191
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27823	16796

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C00735	4903
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C00735	18258
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32816	15636
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30831	28718
17712	25858
16946	15793
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C00735	16962
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32816	16320
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17203	16414
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30831	17626
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17203	15611
15724	6359
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17596	17821
17368	17712
17596	17712
18072	17712
17368	17256
17596	17256
17596	17172
17712	17172
17368	28542
17596	28542
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17596	28997

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32816	15961
30831	15961
32816	16319
32816	16717
32816	16878
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32816	C00193
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17368	52617
16946	18377
16814	17474
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15354	17203
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32816	27978
27823	18397
144308	18397
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144308	15760
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17203	35280
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C00735	18332
15354	16424
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32816	16992
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144308	144365
C00735	5132

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30831	15684
32816	48052
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17712	15652
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P22748	16827
P35354	16827
P11229	16827
P46098	16827
P09172	16827

P21964	16827
P08908	16827
P28222	16827
P11229	15354
P28222	15354
P35354	17351
P23219	17351
P14555	17351
P04264	17351
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O95140	28364
P25101	28364
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Q96RR1	422
P53985	422
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P29474	C00735
P01258	C00735
P35354	C00735
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O95140	17368
P04406	17368
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P31645	27823
P46098	27823
P09172	27823
P21964	27823
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P28222	27823
P10635	51209
P07550	51209
P08588	51209
P31645	51209
P23975	51209
P35348	51209
P39086	16946
P41143	16962
P29275	17712
P27338	144308
P21964	144308
P35354	9349
P27338	28281

Table S7

Table S7 Detailed information about the enriched pathways in acupuncture group

Pathways	Hits	Raw p	FDR	Impact	Matched_features
Steroid hormone biosynthesis	5	0.001089	0.18018	0.079812	cpd:C00735; cpd:C00762; cpd:C13713; cpd:C04555; cpd:C02140
Bile secretion	5	0.007142	0.28528	0	cpd:C00486; cpd:C04555; cpd:C00318; cpd:C00735; cpd:C00114
Linoleic acid metabolism	4	0.000173	0.057257	0.31707	cpd:C14827; cpd:C00157; cpd:C01595; cpd:C14762
Cysteine and methionine metabolism	4	0.002225	0.24553	0.1165	cpd:C08276; cpd:C03145; cpd:C00109; cpd:C00022
Glycerophospholipid metabolism	4	0.006177	0.28528	0.1619	cpd:C04230; cpd:C00114; cpd:C00157; cpd:C01210
Purine metabolism	4	0.024754	0.39689	0.084158	cpd:C11821; cpd:C00294; cpd:C00262; cpd:C00385
Cholesterol metabolism	3	0.003192	0.26416	0	hsa:4018; hsa:336; hsa:5360
Phenylalanine metabolism	3	0.006433	0.28528	0	cpd:C00022; cpd:C04148; cpd:C02765
PPAR signaling pathway	3	0.0074	0.28528	0.084746	hsa:336; hsa:5360; cpd:C14762
Glycine, serine and threonine metabolism	3	0.009877	0.32693	0.035294	cpd:C00114; cpd:C00109; cpd:C00022
Glycolysis or Gluconeogenesis	3	0.012783	0.38466	0.21538	hsa:2597; cpd:C00186; cpd:C00022
Central carbon metabolism in cancer	3	0.015348	0.39079	0	cpd:C00022; cpd:C00186; cpd:C00148
Choline metabolism in cancer	3	0.01653	0.39082	0	cpd:C00114; cpd:C00157; cpd:C04230
HIF-1 signaling pathway	3	0.023191	0.39689	0.036585	cpd:C00022; cpd:C00186; hsa:2597
Tryptophan metabolism	3	0.023191	0.39689	0.064	cpd:C00328; cpd:C05635; cpd:C05660
Arginine and proline metabolism	3	0.02518	0.39689	0.051282	cpd:C00022; cpd:C01877; cpd:C00148
Systemic lupus erythematosus	3	0.029427	0.44274	0.057692	hsa:712; hsa:85235; hsa:8345
ABC transporters	3	0.061431	0.70555	0	cpd:C00148; cpd:C00114; cpd:C00294
Valine, leucine and isoleucine biosynthesis	2	0.007757	0.28528	0.038462	cpd:C00022; cpd:C00109
Prion diseases	2	0.015008	0.39079	0	hsa:712; cpd:C02140
Sulfur metabolism	2	0.018977	0.39689	0	cpd:C11142; cpd:C08276
African trypanosomiasis	2	0.020676	0.39689	0	hsa:8542; cpd:C00328
Aldosterone-regulated sodium reabsorption	2	0.020676	0.39689	0.10714	cpd:C00735; cpd:C00762
Terpenoid backbone biosynthesis	2	0.043113	0.61769	0	cpd:C06081; cpd:C00022
alpha-Linolenic acid metabolism	2	0.045462	0.61769	0.038462	cpd:C00157; cpd:C16308
Pyruvate metabolism	2	0.046654	0.61769	0.22642	cpd:C00186; cpd:C00022
Biosynthesis of unsaturated fatty acids	2	0.057883	0.70555	0.015152	cpd:C01595; cpd:C06428
Complement and coagulation cascades	2	0.059183	0.70555	0.059701	hsa:3053; hsa:712
Propanoate metabolism	2	0.061815	0.70555	0.041667	cpd:C00109; cpd:C00186
IL-17 signaling pathway	2	0.078404	0.86506	0	hsa:6279; hsa:6280
Viral protein interaction with cytokine and cytokin	2	0.087168	0.93073	0.013158	hsa:5473; hsa:5196
Prostate cancer	2	0.099284	1	0.032258	cpd:C00735; cpd:C00762
Tyrosine metabolism	2	0.10867	1	0.024194	cpd:C00022; cpd:C05589

Glucagon signaling pathway	2	0.13809	1	0	cpd:C00022; cpd:C00186
Arachidonic acid metabolism	2	0.14826	1	0.042017	cpd:C14770; cpd:C00157
Serotonergic synapse	2	0.18138	1	0	cpd:C05635; cpd:C14770
Necroptosis	2	0.20826	1	0.021277	cpd:C00319; hsa:85235
Chemokine signaling pathway	2	0.24835	1	0.015625	hsa:5196; hsa:5473
Alcoholism	2	0.24835	1	0.02	hsa:85235; hsa:8345
Cytokine-cytokine receptor interaction	2	0.42796	1	0.006928	hsa:5196; hsa:5473
Pathways in cancer	2	0.77284	1	0.003086	cpd:C00735; cpd:C00762
Caffeine metabolism	1	0.12517	1	0	cpd:C00385
Taurine and hypotaurine metabolism	1	0.15082	1	0	cpd:C00022
Bladder cancer	1	0.18387	1	0	hsa:7057
Thiamine metabolism	1	0.20783	1	0	cpd:C00022
Pantothenate and CoA biosynthesis	1	0.20783	1	0	cpd:C00022
Citrate cycle (TCA cycle)	1	0.21955	1	0.045455	cpd:C00022
Type II diabetes mellitus	1	0.22727	1	0.032258	cpd:C00022
Malaria	1	0.23491	1	0	hsa:7057
Phosphonate and phosphinate metabolism	1	0.2684	1	0	cpd:C00022
Primary bile acid biosynthesis	1	0.27203	1	0.020833	cpd:C05446
Alanine, aspartate and glutamate metabolism	1	0.27203	1	0.04918	cpd:C00022
Pentose phosphate pathway	1	0.27564	1	0	cpd:C00022
Regulation of lipolysis in adipocytes	1	0.28992	1	0.016667	cpd:C02140
Butanoate metabolism	1	0.29344	1	0	cpd:C00022
p53 signaling pathway	1	0.30044	1	0.015152	hsa:7057
Sphingolipid metabolism	1	0.30044	1	0.098361	cpd:C00319
Ovarian steroidogenesis	1	0.30392	1	0	cpd:C14770
Ascorbate and aldarate metabolism	1	0.31424	1	0	cpd:C00022
Cortisol synthesis and secretion	1	0.31764	1	0	cpd:C00735
Galactose metabolism	1	0.31764	1	0.028169	cpd:C05401
Pertussis	1	0.34757	1	0.044118	hsa:712
Fructose and mannose metabolism	1	0.35081	1	0	cpd:C00186
Mineral absorption	1	0.35081	1	0	cpd:C00148
N-Glycan biosynthesis	1	0.35404	1	0.012658	cpd:C06081
Pentose and glucuronate interconversions	1	0.35725	1	0	cpd:C00022
ECM-receptor interaction	1	0.35725	1	0.0625	hsa:7057
Nicotinate and nicotinamide metabolism	1	0.3668	1	0	cpd:C00022
Glyoxylate and dicarboxylate metabolism	1	0.3668	1	0.022727	cpd:C00022
TGF-beta signaling pathway	1	0.37308	1	0.0125	hsa:7057

Glutathione metabolism	1	0.37308	1	0.043478	cpd:C01879
Thyroid hormone synthesis	1	0.3762	1	0	hsa:6906
Insulin secretion	1	0.38547	1	0	cpd:C00022
Staphylococcus aureus infection	1	0.38547	1	0.046512	hsa:712
Glycerolipid metabolism	1	0.38853	1	0	cpd:C05401
Chagas disease (American trypanosomiasis)	1	0.41539	1	0.013699	hsa:712
Aminoacyl-tRNA biosynthesis	1	0.44389	1	0.010309	cpd:C00148
Aldosterone synthesis and secretion	1	0.44942	1	0	cpd:C02140
Cholinergic synapse	1	0.46032	1	0	cpd:C00114
Insulin resistance	1	0.47102	1	0	cpd:C00022
Sphingolipid signaling pathway	1	0.48666	1	0	cpd:C00319
Apoptosis	1	0.50186	1	0	cpd:C00319
Protein digestion and absorption	1	0.50682	1	0	cpd:C00148
AMPK signaling pathway	1	0.50929	1	0	cpd:C00022
Vascular smooth muscle contraction	1	0.52143	1	0.014085	cpd:C14770
Phagosome	1	0.53328	1	0	hsa:7057
Adrenergic signaling in cardiomyocytes	1	0.54711	1	0.028169	cpd:C07056
Retrograde endocannabinoid signaling	1	0.56494	1	0	cpd:C00157
Cushing syndrome	1	0.56712	1	0	cpd:C00735
Alzheimer disease	1	0.58833	1	0.014925	hsa:2597
Porphyrin and chlorophyll metabolism	1	0.60056	1	0.012346	cpd:C00486
Viral carcinogenesis	1	0.63331	1	0	hsa:8345
Focal adhesion	1	0.63331	1	0.032258	hsa:7057
Pathogenic Escherichia coli infection	1	0.63881	1	0.008	hsa:2597
Proteoglycans in cancer	1	0.65133	1	0.015	hsa:7057
Rap1 signaling pathway	1	0.65829	1	0.010638	hsa:7057
cAMP signaling pathway	1	0.70032	1	0.008197	cpd:C00186
Thermogenesis	1	0.71939	1	0	cpd:C00318
MicroRNAs in cancer	1	0.78879	1	0.002227	hsa:7057
Human papillomavirus infection	1	0.81213	1	0.01875	hsa:7057
PI3K-Akt signaling pathway	1	0.83463	1	0.029412	hsa:7057
Neuroactive ligand-receptor interaction	1	0.86103	1	0.005618	cpd:C00735

Table S8

Table S8 Detailed information about the enriched pathways in sham acupuncture group

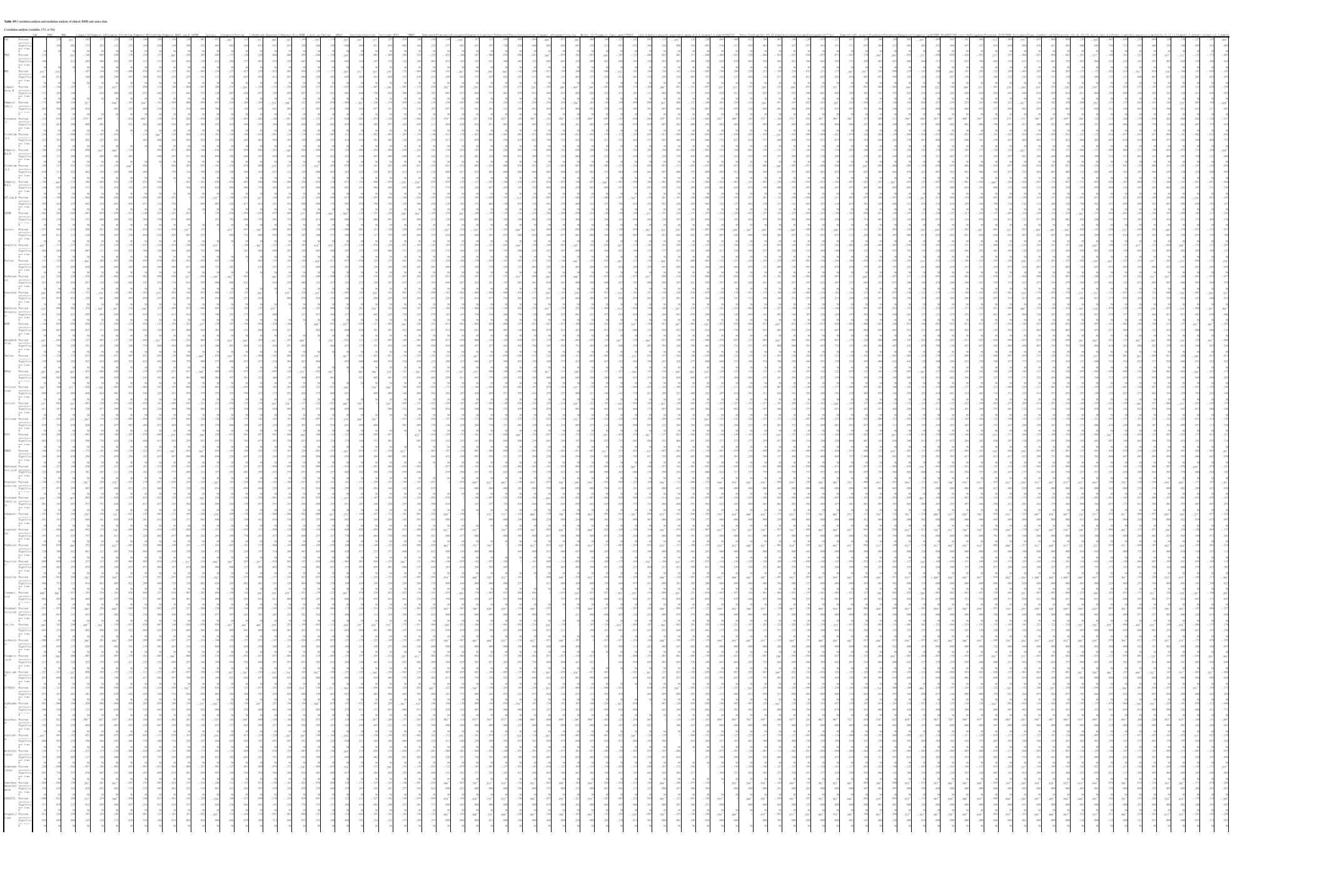
Pathways	Hits	Raw p	FDR	Impact	Matched_features
Focal adhesion	4	0.002614	0.25055	0.25806	hsa:87; hsa:2335; hsa:7057; hsa:60
Proteoglycans in cancer	4	0.003115	0.25055	0.085	hsa:60; hsa:7057; hsa:4478; hsa:2335
Regulation of actin cytoskeleton	4	0.003502	0.25055	0.13253	hsa:87; hsa:4478; hsa:2335; hsa:60
Linoleic acid metabolism	3	0.000589	0.19499	0.02439	cpd:C14827; cpd:C00157; cpd:C14762
Choline metabolism in cancer	3	0.003814	0.25055	0	cpd:C00114; cpd:C00157; cpd:C04230
Leukocyte transendothelial migration	3	0.004542	0.25055	0.087912	hsa:60; hsa:4478; hsa:87
Glycerophospholipid metabolism	3	0.009073	0.429	0.1619	cpd:C04230; cpd:C00114; cpd:C00157
Tight junction	3	0.012963	0.53634	0.096296	hsa:87; hsa:60; hsa:4478
ABC transporters	3	0.015783	0.57021	0	cpd:C00114; cpd:C01606; cpd:C00294
Adherens junction	2	0.017983	0.57021	0.29333	hsa:60; hsa:87
Bacterial invasion of epithelial cells	2	0.01895	0.57021	0.16279	hsa:60; hsa:2335
ECM-receptor interaction	2	0.027436	0.75676	0.21528	hsa:2335; hsa:7057
Cysteine and methionine metabolism	2	0.04179	0.96725	0.009709	cpd:C08276; cpd:C03145
Tyrosine metabolism	2	0.043148	0.96725	0.096774	cpd:C00082; cpd:C05576
Amoebiasis	2	0.043833	0.96725	0	hsa:2335; hsa:87
Yersinia infection	2	0.050907	1	0.052083	hsa:2335; hsa:60
Arachidonic acid metabolism	2	0.06067	1	0.02521	cpd:C14773; cpd:C00157
Phagosome	2	0.072666	1	0	hsa:60; hsa:7057
Steroid hormone biosynthesis	2	0.077665	1	0.065728	cpd:C00535; cpd:C03681
Retrograde endocannabinoid signaling	2	0.084496	1	0.035714	cpd:C13856; cpd:C00157
Porphyrin and chlorophyll metabolism	2	0.099593	1	0	cpd:C05794; cpd:C05790
Pathogenic Escherichia coli infection	2	0.11824	1	0.048	hsa:60; hsa:2597
Rap1 signaling pathway	2	0.12886	1	0.053191	hsa:60; hsa:7057
Purine metabolism	2	0.1387	1	0.049505	cpd:C00294; cpd:C00262
Thermogenesis	2	0.16812	1	0.036145	hsa:60; cpd:C13856
Human papillomavirus infection	2	0.25237	1	0.01875	hsa:2335; hsa:7057
PI3K-Akt signaling pathway	2	0.27956	1	0.029412	hsa:2335; hsa:7057
Pathways in cancer	2	0.49149	1	0.009259	hsa:2335; cpd:C00535
Phenylalanine, tyrosine and tryptophan biosynthesis	1	0.11014	1	0.14634	cpd:C00082
Bladder cancer	1	0.11274	1	0	hsa:7057
Sulfur metabolism	1	0.11791	1	0	cpd:C08276
Thiamine metabolism	1	0.12816	1	0	cpd:C00082
Pantothenate and CoA biosynthesis	1	0.12816	1	0	cpd:C05944

Malaria	1	0.14583	1	0	hsa:7057
Cocaine addiction	1	0.1533	1	0	cpd:C00082
Vibrio cholerae infection	1	0.15824	1	0.035714	hsa:60
Viral myocarditis	1	0.1607	1	0.030303	hsa:60
Endocrine and other factor-regulated calcium reabsorptior	1	0.16316	1	0.017857	cpd:C01673
Shigellosis	1	0.18254	1	0.02381	hsa:60
alpha-Linolenic acid metabolism	1	0.18254	1	0.038462	cpd:C00157
p53 signaling pathway	1	0.18969	1	0.015152	hsa:7057
Sphingolipid metabolism	1	0.18969	1	0.14754	cpd:C00836
Ovarian steroidogenesis	1	0.19206	1	0	cpd:C00535
GnRH secretion	1	0.19206	1	0.021277	cpd:C00535
Phenylalanine metabolism	1	0.20148	1	0.013889	cpd:C00082
Steroid biosynthesis	1	0.20148	1	0.020408	cpd:C01673
Amphetamine addiction	1	0.20382	1	0	cpd:C00082
Arrhythmogenic right ventricular cardiomyopathy (ARVC	1	0.20615	1	0	hsa:60
Biosynthesis of unsaturated fatty acids	1	0.20615	1	0.007576	cpd:C06428
Complement and coagulation cascades	1	0.20848	1	0.029851	hsa:5104
Prolactin signaling pathway	1	0.21079	1	0	cpd:C00082
PPAR signaling pathway	1	0.21079	1	0.016949	cpd:C14762
Salmonella infection	1	0.21771	1	0.061224	hsa:60
Mineral absorption	1	0.22456	1	0.011765	cpd:C01673
Gastric acid secretion	1	0.2291	1	0.019231	hsa:60
Glycine, serine and threonine metabolism	1	0.23136	1	0.011765	cpd:C00114
Hypertrophic cardiomyopathy (HCM)	1	0.2381	1	0.043478	hsa:60
TGF-beta signaling pathway	1	0.24034	1	0.0125	hsa:7057
Small cell lung cancer	1	0.24256	1	0.039216	hsa:2335
Dilated cardiomyopathy (DCM)	1	0.25141	1	0.06383	hsa:60
Glycolysis or Gluconeogenesis	1	0.25141	1	0.12308	hsa:2597
Ubiquinone and other terpenoid-quinone biosynthesis	1	0.26016	1	0.011628	cpd:C00082
Central carbon metabolism in cancer	1	0.26665	1	0	cpd:C00082
Melanogenesis	1	0.26881	1	0.022727	cpd:C00082
Endocrine resistance	1	0.27095	1	0	cpd:C00535
Prostate cancer	1	0.27095	1	0.032258	cpd:C00535
AGE-RAGE signaling pathway in diabetic complications	1	0.27309	1	0	hsa:2335
Parathyroid hormone synthesis, secretion and action	1	0.28791	1	0.012195	cpd:C01673
Aminoacyl-tRNA biosynthesis	1	0.29208	1	0.010309	cpd:C00082
Cholinergic synapse	1	0.30448	1	0	cpd:C00114

HIF-1 signaling pathway	1	0.30448	1	0.036585	hsa:2597
Lysosome	1	0.31059	1	0	hsa:8546
Thyroid hormone signaling pathway	1	0.31666	1	0.009434	hsa:60
Sphingolipid signaling pathway	1	0.32467	1	0	cpd:C00836
Systemic lupus erythematosus	1	0.32864	1	0	hsa:87
Platelet activation	1	0.33258	1	0.022989	hsa:60
Measles	1	0.33455	1	0.011236	hsa:4478
Apoptosis	1	0.33651	1	0.026549	hsa:60
Protein digestion and absorption	1	0.34041	1	0	cpd:C00082
Dopaminergic synapse	1	0.34235	1	0	cpd:C00082
Fluid shear stress and atherosclerosis	1	0.35006	1	0.009524	hsa:60
Hippo signaling pathway	1	0.36335	1	0.009804	hsa:60
Serotonergic synapse	1	0.36897	1	0	cpd:C14773
Parkinson disease	1	0.36897	1	0	cpd:C00082
Adrenergic signaling in cardiomyocytes	1	0.37268	1	0.028169	cpd:C07056
Oxytocin signaling pathway	1	0.38371	1	0.013158	hsa:60
Necroptosis	1	0.39633	1	0.010638	hsa:5478
Influenza A	1	0.39811	1	0	hsa:60
Alzheimer disease	1	0.40695	1	0.014925	hsa:2597
Hepatocellular carcinoma	1	0.41392	1	0.067797	hsa:60
Alcoholism	1	0.43438	1	0	cpd:C00082
Metabolism of xenobiotics by cytochrome P450	1	0.43939	1	0	cpd:C11714
Tuberculosis	1	0.43939	1	0.007194	cpd:C01673
Viral carcinogenesis	1	0.446	1	0	hsa:87
Bile secretion	1	0.51532	1	0	cpd:C00114
MicroRNAs in cancer	1	0.59962	1	0.002227	hsa:7057
Neuroactive ligand-receptor interaction	1	0.68706	1	0.005618	cpd:C13856

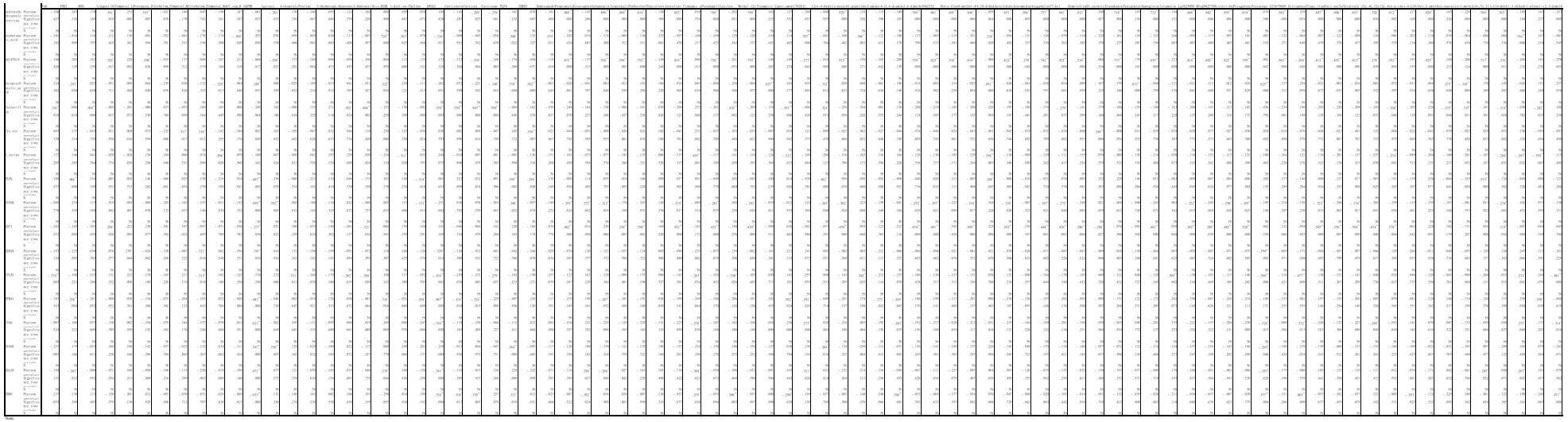
Table S9 Correlation analysis and mediation analysis of clinical, fMRI and omics data

Correlation analysis (variables 153, n=56)



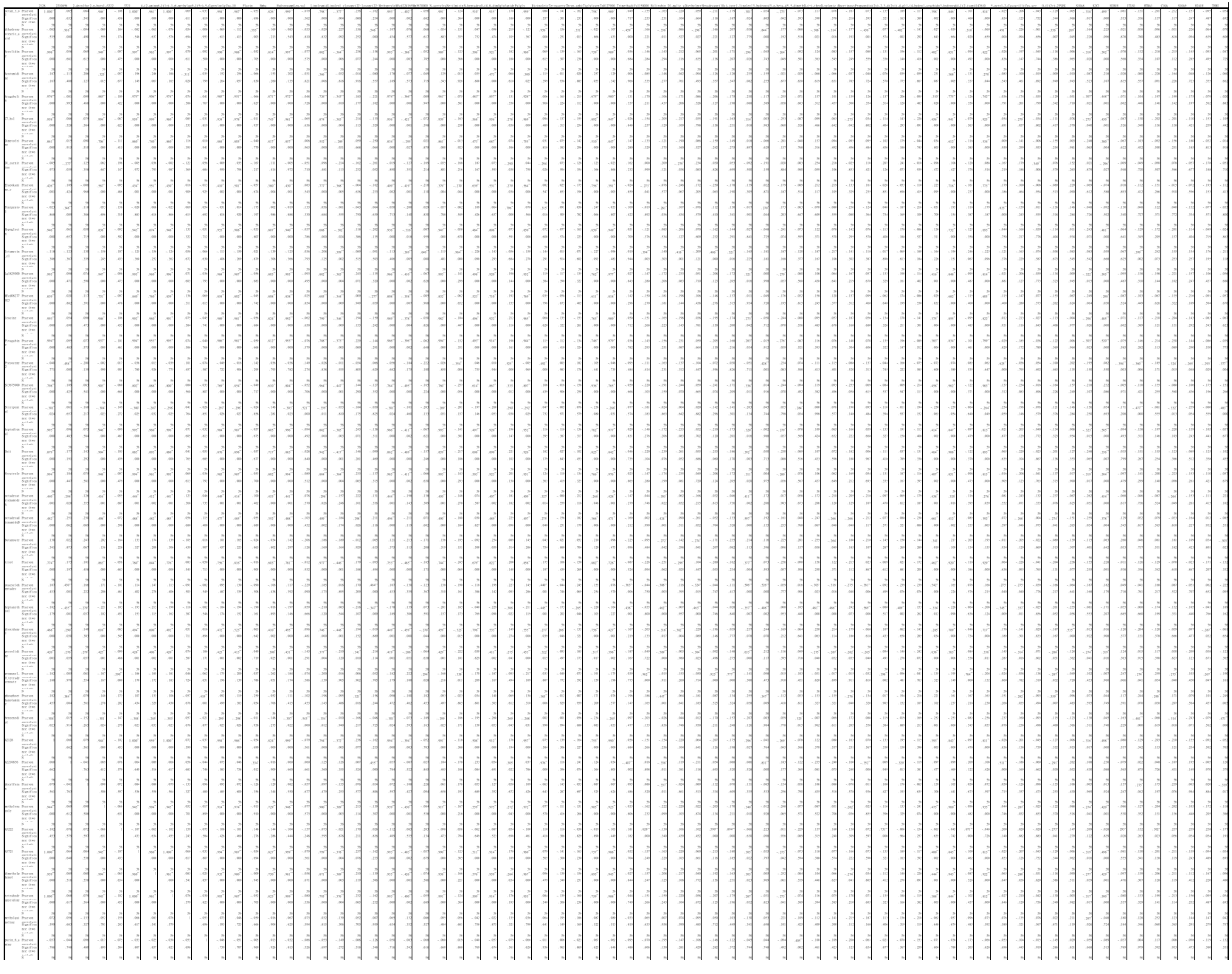
		VAS	PSQI	MSQ	Lingual Gy	Temporal L	Precuneus_	Cerebelum_	Temporal_M	Cerebelum_	Temporal_M	ACC_sup_R	GAPDH	Lactate	4-Oxoproli	Proline	2-Oxobutan	L-Kynureni	5-Hydroxyi	9(s)-HODE	1-Acyl-sn-	Choline	APOA2	Corticoste	Cortisol	Cortisone	PLF4	TDRD3	Dodecanedi	Propionylc
octan_3_ol	Pearson correlation	-.100	-.048	.212	.299*	.264*	.373**	-.039	.176	.009	-.045	.201	-.237	-.290*	.154	-.210	.103	-.175	-.199	.013	.005	.121	.131	-.138	-.217	-.127	-.153	-.090	-.042	.974**
	Significance (two-tailed)	.465	.726	.118	.025	.049	.005	.777	.195	.949	.740	.138	.079	.030	.257	.121	.451	.198	.142	.925	.972	.374	.335	.311	.107	.352	.259	.508	.759	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
dihydroxystearic_acid	Pearson correlation	-.007	-.010	-.150	.132	.071	-.104	-.276*	-.131	-.340*	-.230	-.132	.126	.146	.074	-.230	-.181	-.180	-.227	.445**	.565**	-.053	-.181	.067	-.101	-.152	.319*	.201	.098	-.094
	Significance (two-tailed)	.959	.942	.271	.331	.601	.445	.040	.337	.010	.088	.333	.354	.285	.587	.089	.182	.186	.092	.001	.000	.700	.181	.626	.460	.263	.017	.137	.474	.489
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Aceclidine	Pearson correlation	-.106	-.031	.216	.300*	.247	.372**	-.055	.171	-.007	-.045	.199	-.235	-.280*	.164	-.207	.106	-.169	-.188	.012	.005	.126	.143	-.130	-.208	-.122	-.151	-.093	-.043	.979**
	Significance (two-tailed)	.437	.821	.109	.025	.066	.005	.690	.209	.957	.742	.141	.082	.037	.228	.126	.437	.214	.164	.930	.968	.356	.294	.341	.124	.372	.266	.496	.756	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Acutumidine	Pearson correlation	-.238	.038	-.032	.072	.025	.054	.049	.145	-.071	-.074	-.054	-.054	-.049	.193	.001	-.082	-.085	-.139	-.170	.041	.104	.167	-.140	-.121	-.087	-.214	-.089	-.050	.230
	Significance (two-tailed)	.077	.784	.813	.598	.856	.695	.719	.287	.602	.587	.692	.694	.721	.153	.991	.547	.535	.307	.210	.761	.444	.219	.302	.375	.522	.114	.514	.715	.088
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Atagabalin	Pearson correlation	-.079	-.055	.231	.235	.243	.391**	-.064	.191	-.006	-.023	.143	-.254	-.261	.101	-.158	.109	-.154	-.164	-.015	-.079	.073	.142	-.145	-.183	-.094	-.145	-.095	-.008	.928**
	Significance (two-tailed)	.563	.685	.087	.081	.072	.003	.637	.158	.965	.864	.293	.059	.052	.460	.245	.422	.259	.228	.913	.563	.591	.297	.286	.176	.490	.288	.488	.955	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
C7_hsl	Pearson correlation	-.127	.073	.173	.371**	.285*	.384**	-.021	.174	.026	-.104	.211	-.156	-.286*	.182	-.244	.093	-.162	-.186	.026	.047	.122	.122	-.177	-.288*	-.235	-.164	-.026	-.071	.985**
	Significance (two-tailed)	.351	.593	.203	.005	.033	.004	.877	.200	.852	.447	.118	.250	.033	.180	.070	.497	.233	.169	.847	.732	.370	.370	.191	.031	.081	.228	.849	.603	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Dimetofrine	Pearson correlation	.051	-.047	.283*	.139	.224	.382**	-.079	.203	.010	-.007	.065	-.182	-.214	-.082	-.106	.121	-.142	-.176	-.002	-.176	-.138	.039	-.086	-.145	-.054	-.059	-.035	.003	.755**
	Significance (two-tailed)	.711	.731	.034	.309	.097	.004	.563	.134	.939	.957	.635	.178	.112	.550	.438	.375	.298	.195	.989	.195	.310	.776	.528	.287	.692	.666	.797	.983	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Dl_carnitine	Pearson correlation	.239	.170	.355**	.091	-.036	.157	.126	.186	.295*	-.023	.075	.050	-.143	-.194	-.076	.269*	.133	.091	-.006	-.228	-.101	.125	.095	.157	.022	-.023	.000	-.057	-.006
	Significance (two-tailed)	.075	.209	.007	.503	.791	.247	.354	.170	.027	.865	.581	.714	.294	.152	.579	.045	.330	.505	.968	.091	.459	.359	.485	.247	.873	.867	1.000	.679	.967
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Elaeokanine_c	Pearson correlation	.140	.394**	.243	.044	.117	.099	.028	.147	.096	-.247	.106	.021	-.251	-.045	-.102	.220	.011	.037	-.025	.080	.033	.183	-.021	-.098	-.088	-.197	.125	-.131	.453**
	Significance (two-tailed)	.304	.003	.072	.747	.388	.466	.836	.281	.480	.066	.438	.881	.062	.744	.455	.103	.937	.788	.856	.560	.808	.178	.878	.471	.520	.145	.358	.336	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Fenipentol	Pearson correlation	.169	.296*	.090	-.081	.128	.117	-.159	.157	-.060	-.385**	-.071	.149	.093	-.007	-.036	-.057	.075	.014	.246	.099	-.067	-.178	.188	-.114	-.215	.281*	.434**	-.003	-.023
	Significance (two-tailed)	.213	.027	.509	.555	.348	.390	.243	.249	.662	.003	.602	.272	.497	.957	.791	.677	.584	.920	.067	.467	.622	.189	.164	.402	.111	.036	.001	.984	.865
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Hypoglycin	Pearson correlation	.003	-.055	.219	.304*	.192	.386**	-.040	.165	.005	.019	.138	-.197	-.245	-.036	-.165	.117	-.126	-.153	-.015	-.107	-.064	.095	-.101	-.172	-.092	-.118	-.091	-.019	.904**
	Significance (two-tailed)	.983	.686	.105	.023	.155	.003	.770	.226	.970	.891	.312	.145	.068	.791	.225	.388	.356	.261	.912	.432	.641	.485	.459	.206	.499	.386	.507	.892	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Istamycin_cl	Pearson correlation	-.435**	-.271*	-.165	.068	.026	.280*	-.018	.183	-.109	.125	-.283*	.113	.330*	.176	.274*	-.218	-.121	-.131	.166	-.022	-.210	-.303*	-.181	-.219	-.176	-.032	-.153	.574**	-.121
	Significance (two-tailed)	.001	.044	.224	.616	.850	.037	.893	.176	.423	.357	.034	.405	.013	.195	.041	.106	.374	.337	.221	.870	.120	.023	.183	.105	.195	.813	.259	.000	.375
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Lq1825000	Pearson correlation	-.098	-.050	.204	.322*	.253	.367**	-.035	.170	.018	-.047	.213	-.238	-.299*	.167	-.232	.097	-.179	-.210	.025	.036	.139	.127	-.110	-.215	-.129	-.154	-.092	-.045	.974**
	Significance (two-tailed)	.472	.717	.132	.016	.060	.005	.800	.211	.897	.731	.116	.077	.025	.220	.085	.478	.187	.121	.855	.790	.308	.351	.418	.112	.345	.257	.501	.744	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Mfcd08277025	Pearson correlation	.093	.050	.296*	.146	.259	.403**	-.081	.247	.079	-.072	.068	-.127	-.227	-.110	-.110	.144	-.119	-.147	.023	-.201	-.171	.024	-.060	-.152	-.102	-.058	.073	-.010	.748**
	Significance (two-tailed)	.494	.713	.027	.282	.054	.002	.555	.067	.563	.600	.616	.351	.092	.420	.418	.288	.384	.279	.865	.138	.206	.862	.661	.264	.453	.672	.593	.941	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
leucine	Pearson correlation	-.101	-.028	.191	.309*	.253	.400**	-.053	.185	.006	-.061	.154	-.213	-.262	.151	-.196	.082	-.160	-.177	.013	-.013	.098	.126	-.137	-.222	-.145	-.146	-.069	-.052	.974**
	Significance (two-tailed)	.457	.835	.158	.020	.060	.002	.698	.173	.963	.654	.259	.116	.051	.266	.147	.548	.240	.192	.925	.925	.472	.356	.314	.101	.285	.284	.613	.704	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Pivagabine	Pearson correlation	-.086	-.052	.203	.315*	.243	.365**	-.045	.177	.006	-.038	.188	-.244	-.293*	.143	-.215	.103	-.165	-.192	.013	.025	.122	.142	-.096	-.190	-.104	-.146	-.101	-.042	.971**
	Significance (two-tailed)	.527	.704	.133	.018	.072	.006	.741	.191	.966	.783	.166	.070	.028	.292	.111	.451	.224	.157	.927	.853	.370	.297	.483	.160	.447	.282	.459	.757	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56

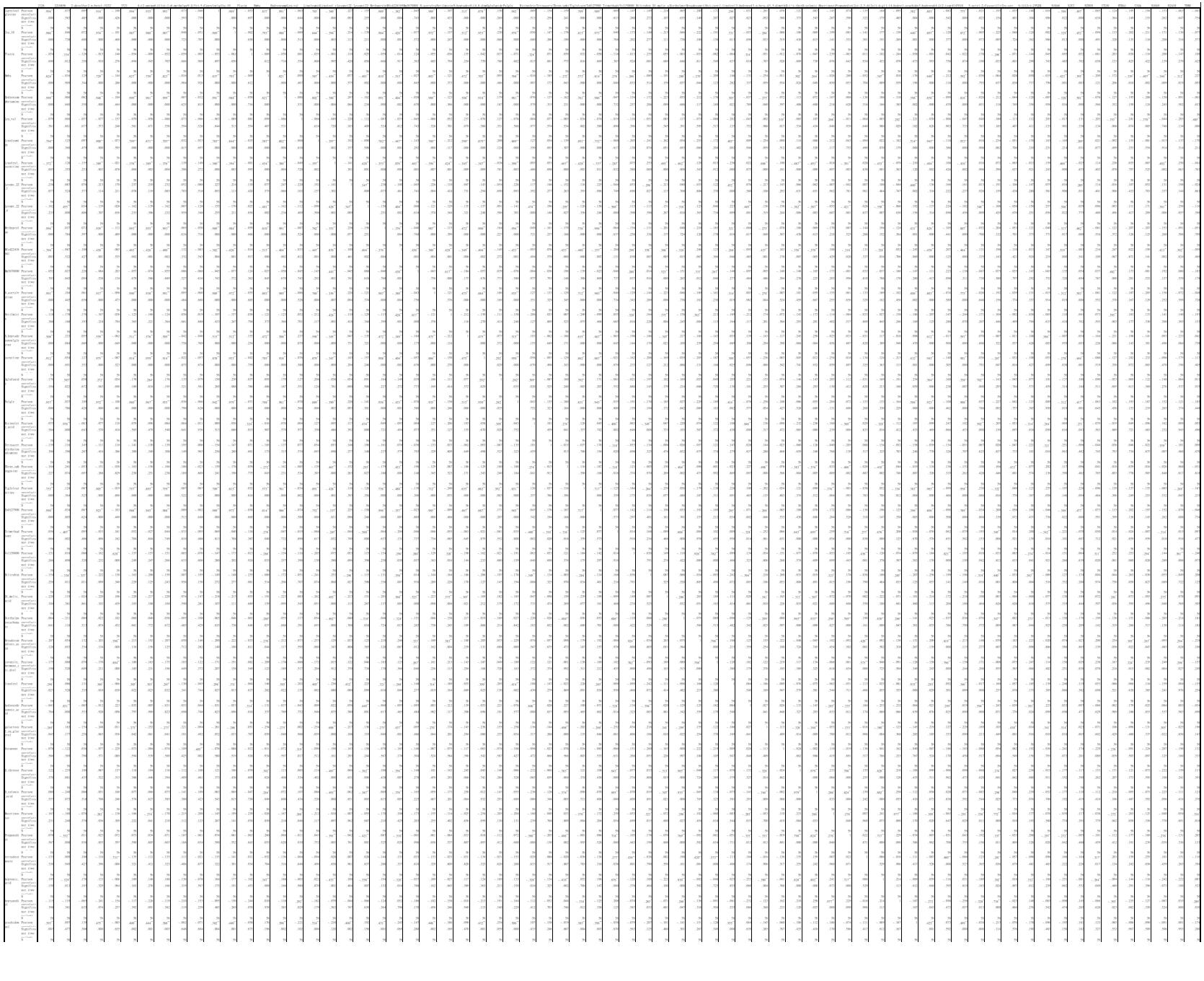
		VAS	PSQI	MSQ	Lingual Gy	Temporal L	Precuneus_	Cerebelum_	Temporal_M	Cerebelum_	Temporal_M	ACC_sup_R	GAPDH	Lactate	4-Oxoproli	Proline	2-Oxobutan	L-Kynureni	5-Hydroxyi	9(s)-HODE	1-Acyl-sn-	Choline	APOA2	Corticoste
Capryloyl glycine	Pearson correlation	-.085	-.065	.221	.267*	.262	.368**	-.056	.162	-.006	-.048	.169	-.235	-.276*	.149	-.193	.108	-.166	-.186	.037	.010	.120	.124	-.135
	Significance (two tailed)	.535	.632	.102	.047	.051	.005	.679	.233	.967	.726	.213	.081	.039	.273	.154	.428	.222	.171	.786	.943	.378	.364	.323
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Cxa_10	Pearson correlation	-.111	.002	.213	.326*	.251	.366**	-.018	.190	.029	-.055	.219	-.231	-.311*	.172	-.227	.083	-.176	-.196	-.009	.010	.151	.147	-.141
	Significance (two tailed)	.413	.988	.115	.014	.062	.006	.897	.161	.831	.688	.105	.087	.020	.205	.092	.545	.195	.147	.949	.942	.268	.280	.299
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Flazin	Pearson correlation	.052	.071	-.099	.042	.216	.084	-.135	.179	-.307*	.057	.017	-.079	.032	-.053	.015	-.059	-.058	-.142	.017	.134	-.030	-.051	-.255
	Significance (two tailed)	.702	.605	.467	.757	.109	.537	.322	.186	.021	.674	.902	.563	.817	.696	.914	.665	.671	.298	.903	.326	.825	.708	.058
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Hmba	Pearson correlation	.038	.005	.243	.135	.185	.416**	-.031	.220	.039	.018	.109	-.493**	-.292*	-.025	-.104	.286*	-.146	-.151	-.071	-.198	.138	.376**	-.085
	Significance (two tailed)	.782	.970	.071	.320	.173	.001	.820	.103	.773	.893	.425	.000	.029	.855	.444	.033	.284	.267	.605	.144	.310	.004	.534
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Hydroxyamphetamine	Pearson correlation	-.106	-.048	.211	.296*	.267*	.372**	-.040	.179	.008	-.045	.204	-.236	-.291*	.156	-.214	.099	-.177	-.202	.013	-.001	.117	.124	-.140
	Significance (two tailed)	.436	.728	.118	.027	.047	.005	.770	.188	.953	.743	.131	.080	.030	.251	.112	.470	.192	.135	.925	.996	.391	.361	.304
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Leu_val	Pearson correlation	.342**	.158	.117	-.175	-.306*	-.013	.073	-.127	-.003	-.154	-.183	-.225	.062	-.172	.271*	.085	.029	.062	-.113	.002	-.073	.328*	.255
	Significance (two tailed)	.010	.246	.389	.198	.022	.927	.595	.350	.981	.259	.176	.096	.648	.206	.043	.531	.834	.648	.408	.987	.593	.014	.058
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Linoleamide	Pearson correlation	-.149	.120	.137	.287*	.197	.252	-.054	.128	.025	-.162	.203	-.070	-.306*	.198	-.239	.129	-.079	-.141	-.031	.149	.123	.114	-.119
	Significance (two tailed)	.274	.378	.314	.032	.145	.061	.691	.347	.855	.234	.134	.608	.022	.143	.076	.344	.560	.300	.822	.272	.365	.401	.384
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Linoleyl_carnitine	Pearson correlation	-.257	-.021	-.314*	.124	-.060	-.024	-.116	-.061	-.209	.052	-.392**	.288*	.806**	.357**	-.010	-.484**	-.153	-.068	.124	.231	-.151	-.181	.008
	Significance (two tailed)	.056	.877	.018	.364	.660	.860	.395	.657	.121	.704	.003	.032	.000	.007	.940	.000	.259	.619	.361	.087	.266	.182	.954
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Lysopc_22_1	Pearson correlation	-.308*	-.190	.044	-.210	.142	-.031	-.265*	.009	-.266*	-.058	.277*	.056	-.203	.248	-.193	.084	-.209	-.191	.220	.352**	.198	-.112	-.026
	Significance (two tailed)	.021	.160	.746	.121	.295	.822	.049	.945	.048	.669	.039	.683	.134	.065	.154	.536	.123	.159	.103	.008	.143	.413	.850
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Lysopc_22_4	Pearson correlation	-.219	-.012	-.162	.016	-.016	-.215	-.251	-.178	-.309*	-.009	-.137	.393**	.217	.253	-.306*	-.256	-.210	-.256	.260	.720**	.028	-.275*	.131
	Significance (two tailed)	.104	.929	.234	.906	.907	.111	.062	.190	.021	.946	.314	.003	.109	.060	.022	.056	.120	.057	.053	.000	.835	.040	.337
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Methyprylon	Pearson correlation	-.127	-.068	.184	.312*	.250	.367**	-.038	.165	.009	-.017	.202	-.248	-.284*	.186	-.199	.082	-.169	-.183	-.002	.006	.160	.145	-.152
	Significance (two tailed)	.353	.621	.174	.019	.063	.005	.779	.225	.949	.903	.136	.066	.034	.171	.141	.548	.214	.176	.986	.967	.239	.286	.265
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Mfcd22416941	Pearson correlation	-.211	-.022	-.122	.107	-.063	-.045	-.059	-.080	-.220	.114	-.288*	.339*	.683**	.214	-.007	-.343**	-.139	-.037	.098	.199	-.272*	-.175	.114
	Significance (two tailed)	.118	.871	.369	.431	.645	.742	.668	.556	.104	.403	.031	.011	.000	.113	.957	.010	.306	.787	.470	.141	.043	.196	.403
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Mm3670000	Pearson correlation	-.520**	-.150	-.317*	.224	.016	.336*	-.108	.184	-.136	.186	-.306*	.115	.318*	.157	-.034	-.174	-.227	-.266*	.271*	.168	-.171	-.280*	-.115
	Significance (two tailed)	.000	.269	.017	.097	.908	.011	.428	.174	.316	.171	.022	.397	.017	.247	.803	.200	.093	.047	.043	.216	.208	.037	.397
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
N_acetylvaline	Pearson correlation	-.090	-.072	.197	.315*	.243	.372**	-.050	.152	.008	-.034	.186	-.242	-.285*	.171	-.224	.086	-.173	-.196	.044	.038	.143	.116	-.103
	Significance (two tailed)	.512	.600	.146	.018	.072	.005	.713	.263	.951	.802	.170	.072	.034	.206	.098	.527	.203	.148	.747	.781	.292	.395	.448
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Netilmicin	Pearson correlation	-.404**	-.277*	-.165	.032	.003	.252	-.011	.222	-.091	.158	-.245	.087	.361**	.174	.265*	-.180	-.092	-.083	.064	-.046	-.235	-.249	-.171
	Significance (two tailed)	.002	.038	.223	.813	.984	.060	.933	.099	.503	.244	.069	.524	.006	.200	.048	.183	.498	.544	.640	.734	.081	.064	.208
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
N_heptadecanoylglycine	Pearson correlation	.156	.505**	.430**	-.013	.264*	.181	.029	.114	.046	-.197	.073	.010	-.195	-.087	-.100	.289*	-.045	-.047	.132	.093	-.040	.150	-.028
	Significance (two tailed)	.250	.000	.001	.924	.049	.182	.829	.401	.735	.146	.591	.940	.149	.522	.464	.031	.741	.731	.332	.495	.771	.270	.840
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
carnitine	Pearson correlation	-.166	.060	.132	.384**	.225	.370**	-.002	.217	.023	-.087	.164	-.170	-.275*	.185	-.226	.031	-.166	-.207	-.041	.037	.132	.160	-.155
	Significance (two tailed)	.221	.660	.332	.003	.095	.005	.988	.107	.866	.524	.226	.210	.040	.172	.094	.823	.221	.126	.764	.788	.331	.238	.253
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Oglufanide	Pearson correlation	.045	.302*	.000	.153	.200	.194	-.059	.071	-.051	-.384**	-.094	.030	.124	.251	-.112	-.193	-.061	-.045	.219	.202	.147	-.007	.178
	Significance (two tailed)	.743	.024	.997	.261	.139	.152	.666	.605	.711	.004	.490	.828	.364	.062	.411	.154	.653	.739	.105	.136	.278	.960	.189
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Palgly	Pearson correlation	-.152	.031	.195	.287*	.250	.354**	-.050	.183	.014	-.103	.178	-.202	-.290*	.235	-.211	.064	-.158	-.177	.004	.045	.184	.134	-.136
	Significance (two tailed)	.265	.819	.150	.032	.063	.007	.715	.176	.918	.448	.188	.135	.030	.081	.118	.642	.246	.191	.977	.742	.175	.324	.316
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Ricinoleic_acid	Pearson correlation	.058	.061	-.096	.164	.089	-.072	-.213	-.112	-.272*	-.251	-.105	.052	.088	.109	-.276*	-.124	-.144	-.219	.445**	.567**	.026	-.119	.093
	Significance (two tailed)	.672	.655	.483	.227	.516	.598	.116	.412	.042	.062	.443	.702	.519	.424	.040	.364	.291	.105	.001	.000	.847	.382	.495
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Tetraacetylethylenediamine	Pearson correlation	.028	.024	-.136	.009	-.316*	.003	.011	-.116	.052	-.016	.073	.203	.096	-.111	.019	.046	.185	.162	-.218	.127	-.206	-.089	.366**
	Significance (two tailed)	.836	.859	.319	.945	.018	.985	.934	.396	.702	.907	.594	.133	.480	.414	.888	.735	.172	.234	.107	.351	.128	.513	.006
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Threo_sphingosine	Pearson correlation	-.090	-.063	-.225	.242	.035	-.002	-.200	-.093	.011	-.131	-.269*	.145	.469**	.160	-.224	-.340*	-.086	-.032	.335*	.257	-.142	-.153	.153
	Significance (two tailed)	.509	.645	.096	.072	.799	.989	.140	.494	.936	.334	.045	.286	.000	.238	.097	.010	.528	.817	.012	.056	.298	.260	.260
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Tiglylcarnitine	Pearson correlation	-.045	.266*	.165	.364**	.302*	.348**	.008	.190	.106	-.216	.235	.004	-.287*	.073	-.259	.142	-.114	-.143	.020	.055	.020	.091	-.162
	Significance (two tailed)	.739	.047	.225	.006	.024	.008	.954	.161	.436	.110	.081	.979	.032	.595	.054	.296	.405	.295	.882	.687	.886	.507	.234
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
To0127900	Pearson correlation	-.106	-.067	.196	.306*	.250	.383**	-.048	.155	-.006	-.021	.188	-.239	-.269*	.167	-.191	.083	-.161	-.172	.011	-.014	.136	.134	-.147
	Significance (two tailed)	.438	.625	.147	.022	.063	.004	.728	.255	.968	.878	.166	.076	.045	.220	.159	.542	.236	.205	.937	.918	.319	.325	.281
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Trimethadione	Pearson correlation	.091	-.067	.211	-.159	-.022	.142	-.019	.083	.148	.214	.133	-.296*	-.225	-.094	.086	.461**	.335*	.269*	-.061	-.417**	.083	.159	.071
	Significance (two tailed)	.505	.623	.119	.241	.871	.298	.888	.545	.275	.113	.330	.027	.095	.492	.530	.000	.012	.045	.653	.001	.542	.242	.604
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Vs1150000	Pearson correlation	-.203	-.125	.185	.181	.099	.061	-.043	.078	-.176	-.075	-.266*	.245	-.006	-.082	.038	-.039	-.147	-.062	.519**	.180	-.253	-.285*	.006
	Significance (two tailed)	.133	.360	.173	.181	.468	.658	.751	.569	.195	.585	.048	.068	.964	.548	.780	.777	.279	.650	.000	.184	.060	.033	.964
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Bilirubin	Pearson correlation	.083	.084	.252	.024	-.129	.084	.124	-.012	.082	.211	.056	-.174	.279*	.005	.218	-.063	.170	.235	-.252	-.210	.017	.268*	.198
	Significance (two tailed)	.544	.537	.061	.862	.342	.539	.362	.928	.550	.119	.680	.200	.037	.971	.106	.644	.211	.081	.061	.121	.901	.046	.143
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Dl_malic_acid	Pearson correlation	-.332*	-.106	-.274*	.217	.088	.122	-.047	.115	-.173	.211	-.345**	.031	.494**	.234	.228	-.375**	-.233	-.159	.088	.223	.049	-.083	-.010
	Significance (two tailed)	.013	.436	.041	.108	.519	.371	.732	.400	.203	.118	.009	.819	.000	.082	.091	.004	.084	.242	.521	.099	.721	.542	.941
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Diethylpyrocarbonate	Pearson correlation	.351**	.181	.266*	-.261	-.195	-.080	-.056	.061	.062	.114	.311*	-.160	-.269*	-.287*	.067	.935**	.419**	.255	-.066	-.271*	-.019	.197	.195
	Significance (two tailed)	.008	.181	.048	.052	.151	.556	.680	.656	.650	.405	.020	.237	.045	.032	.625	.000	.001	.057	.627	.043	.891	.146	.150
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Hexadecanedioic_acid	Pearson correlation	-.222	-.048	.095	.165	.087	.106	-.084	.164	-.157	-.063	-.383**	.270*	.086	-.077	.137	-.015	-.100	-.034	.552**	.160	-.248	-.335*	-.019
	Significance (two tailed)	.100	.724	.487	.225	.523	.436	.537	.228	.249	.642	.004	.044	.530	.572	.312	.910	.464	.804	.000	.240	.066	.011	.890
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
juvenile_hormone_iii_diol	Pearson correlation	-.177	.008	.097	.112	.044	.109	-.027	.080	-.080	-.123	-.272*	.316*	.006	-.116	.081	.143	.079	.067	.566**	.081	-.215	-.339*	.082
	Significance (two tailed)	.192	.956	.475	.409	.745	.425	.843	.558	.556	.365	.043	.018	.963	.395	.555	.292	.565	.622	.000	.554	.112	.011	.548
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
linoleyl	Pearson correlation	-.325*	-.197	-.058	-.019	.178	-.049	-.089	-.077	-.036	-.107	.176	-.148	-.202	.675**	-.217	-.101	-.180	-.165	.170	.438**	.661**	.000	-.100
	Significance (two tailed)	.014	.145	.669	.892	.189	.717	.516	.571	.791	.431	.195	.277	.136	.000	.108	.458	.183	.223	.211	.001	.000	.998	.463
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
hydroxydecanoic_acid	Pearson correlation	.090	.056	-.041	.093	.043	-.107	-.114	-.129	-.153	-.205	.019	.198	-.015	.017	-.286*	-.010	-.136	-.137	.444**	.458**	-.022	-.246	-.027
	Significance (two tailed)	.509	.682	.763	.494	.752	.433	.405	.343	.260	.130	.887	.143	.914	.898	.032	.941	.316	.313	.001	.000	.871	.068	.842
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
galactosyl_sn_glycerol	Pearson correlation	.017	.220	-.151	.148	.085	.084	-.125	.045	.028	-.174	-.380**	.184	.855**	.326*	.076	-.322*	.078	.133	.211	.017	-.090	-.027	.045
	Significance (two tailed)	.904	.104	.268	.278	.533	.537	.359	.741	.837	.200	.004	.174	.000	.014	.578	.015	.568	.328	.118	.899	.510	.846	.742
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
furanone	Pearson correlation	.201	-.289*	-.160	.000	-.064	-.087	.179	-.126	.381**	-.091	.207	-.149	-.135	-.173	.002	-.038	.171	.076	-.272*	-.229	-.035	.104	-.040
	Significance (two tailed)	.138	.031	.240	1.000	.637	.525	.186	.356	.004	.505	.127	.274	.321	.203	.988	.778	.207	.580	.043	.089	.798	.446	.769
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
D_threose	Pearson correlation	.301*	.188	.252	-.254	-.146	-.052	-.054	.118	.113	.115	.321*	-.120	-.335*	-.299*	.110	.958**	.403**	.211	-.003	-.271*	-.029	.168	.129
	Significance (two tailed)	.024	.166	.061	.059	.283	.702	.691	.386	.407	.399	.016	.377	.012	.025	.422	.000	.002	.119	.983	.043	.832	.216	.342
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
D_xylonic_acid	Pearson correlation	.297*	.196	.235	-.288*	-.146	-.104	-.035	.099	.141	.123	.271*	-.126	-.368**	-.323*	.134	.912**	.441**	.273*	.010	-.279*	-.006	.173	.114
	Significance (two tailed)	.026	.147	.081	.031	.284	.447	.798	.468	.300	.366	.043	.354	.005	.015	.326	.000	.001	.042	.942	.037	.964	.203	.403
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Mocetinostat	Pearson correlation	.233	-.014	.258	-.318*	-.204	-.294*	-.072	-.078	-.023	.024	.021	-.281*	.016	-.152	.206	.185	.212	.226	-.129	-.111	.016	.315*	.552**
	Significance (two tailed)	.084	.919	.055	.017	.132	.028	.600	.570	.867	.859	.879	.036	.909	.264	.127	.172	.116	.095	.343	.417	.909	.018	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
Propanediol	Pearson correlation	.147	.089	.148	-.234	-.104	-.136	.018	.169	.118	.303*	.153	-.329*	-.338*	-.258	.140	.654**	.343**	.273*	-.161	-.271*	.120	.289*	.054
	Significance (two tailed)	.278	.513	.277	.082	.445	.319	.894	.212	.386	.023	.259	.013	.011	.054	.304	.000	.010	.042	.236	.044	.379	.031	.691
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
tetradecenoate	Pearson correlation	.063	.041	.294*	.209	.074	.202	.102	-.068	-.021	-.008	-.118	.163	-.012	-.082	-.190	.181	.016	.092	.246	.034	-.168	-.106	.305*
	Significance (two tailed)	.643	.765	.028	.122	.590	.136	.456	.618	.877	.954	.386	.231	.933	.548	.161	.181	.908	.501	.067	.806	.216	.437	.022
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
heptonic_acid	Pearson correlation	.217	.038	.237	-.162	-.107	.071	.017	.121	.152	.258	.381**	-.220	-.342**	-.195	.097	.750**	.298*	.140	-.134	-.333*	.032	.168	.128
	Significance (two tailed)	.108	.780	.078	.233	.435	.602	.901	.372	.264	.055	.004	.104	.010	.150	.475	.000	.026	.302	.326	.012	.812	.215	.345
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
heptanediol	Pearson correlation	.265*	-.059	.243	-.286*	-.205	-.295*	-.029	-.086	.022	-.006	.093	-.289*	-.054	-.207	.212	.178	.177	.159	-.109	-.110	.011	.292*	.551**
	Significance (two tailed)	.048	.668	.071	.032	.129	.027	.830	.529	.875	.968	.497	.031	.692	.125	.117	.189	.192	.242	.425	.418	.937	.029	.000
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56
arachidonoyl	Pearson correlation	-.348**	-.161	-.105	.167	.236	.005	-.077	-.074	-.072	-.084	.180	-.126	-.161	.713**	-.263*	-.137	-.186	-.151	.127	.439**	.642**	.058	-.161
	Significance (two tailed)	.009	.236	.443	.219	.080	.972	.573	.589	.599	.538	.184	.356	.236	.000	.050	.312	.170	.267	.351	.001	.000	.673	.236
	N	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56	56

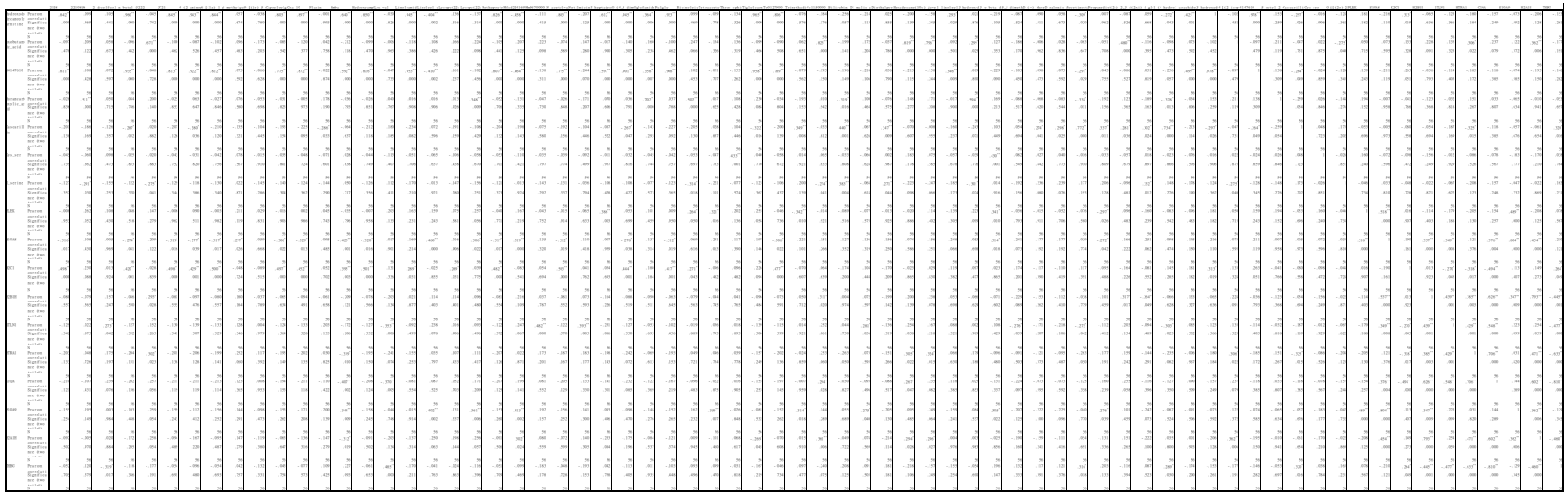


Note:
* significant correlation, $p < 0.05$
** significant correlation, $p < 0.001$

		2128	2210856	2-decylfur	2-n-butyl-	3222	3721	4-(2-amino	6-[(1z)-1-	6-methylqu	9-[(5r)-5-	Capryloylg	Cxa-10
VAS	Pearson correlation	-.099	.055	-.286*	-.149	-.136	-.101	-.116	-.095	.051	.078	-.085	-.111
	Significance (two-tailed)	.468	.687	.033	.273	.316	.459	.393	.485	.706	.567	.535	.413
	N	56	56	56	56	56	56	56	56	56	56	56	56
PSQI	Pearson correlation	-.046	.086	-.060	.078	.075	-.048	.081	-.049	-.020	-.180	-.065	.002
	Significance (two-tailed)	.737	.531	.660	.570	.583	.726	.553	.722	.882	.183	.632	.988
	N	56	56	56	56	56	56	56	56	56	56	56	56
MSQ	Pearson correlation	.215	-.097	-.147	.167	.175	.213	.184	.210	-.028	-.069	.221	.213
	Significance (two-tailed)	.112	.477	.280	.219	.197	.115	.176	.121	.840	.614	.102	.115
	N	56	56	56	56	56	56	56	56	56	56	56	56
Lingual Gyrus_R	Pearson correlation	.298*	.155	.030	.374**	.167	.297*	.369**	.307*	.119	.160	.267*	.326*
	Significance (two-tailed)	.025	.253	.828	.004	.219	.026	.005	.022	.382	.238	.047	.014
	N	56	56	56	56	56	56	56	56	56	56	56	56
Temporal Lobe_L	Pearson correlation	.263*	.063	-.006	.283*	.074	.265*	.288*	.262	-.036	.290*	.262	.251
	Significance (two-tailed)	.050	.647	.966	.035	.588	.048	.031	.051	.789	.030	.051	.062
	N	56	56	56	56	56	56	56	56	56	56	56	56
Precuneus_L	Pearson correlation	.375**	-.083	.013	.380**	.159	.373**	.389**	.372**	.181	.027	.368**	.366**
	Significance (two-tailed)	.004	.541	.927	.004	.243	.005	.003	.005	.183	.845	.005	.006
	N	56	56	56	56	56	56	56	56	56	56	56	56
Cerebelum_6_L	Pearson correlation	-.041	-.214	.079	-.015	.000	-.040	-.018	-.036	-.198	.307*	-.056	-.018







Mediation analysis (variables 7, n=56)

Model : 4
Y : PSQI
X : Temporal_Mid_L
M : Traumatic acid
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
-0.166	0.0719	-2.3085	0.0248	-0.3102	-0.0218	-0.2997

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
-0.1214	0.0754	-1.6108	0.1132	-0.2727	0.0298	-0.2192

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Traumatic acid	-0.0446	0.0583	-0.1811	0.0347

Model : 4
Y : PSQI
X : Traumatic acid
M : Temporal_Mid_L
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
0.3633	0.1529	2.3761	0.0211	0.0568	0.6699	0.3077

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
0.2733	0.1607	1.7003	0.0949	-0.0491	0.5957	0.2314

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Temporal_Mid_L	0.09	0.0857	-0.0805	0.2511

Model : 4
Y : PSQI
X : Temporal_Mid_L
M : Fenipentol
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
-0.166	0.0719	-2.3085	0.0248	-0.3102	-0.0218	-0.2997

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
-0.1208	0.077	-1.5698	0.1224	-0.2752	0.0336	-0.2181

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Fenipentol	-0.0452	0.066	-0.1936	0.0584

Model : 4
Y : PSQI
X : Fenipentol
M : Temporal_Mid_L
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
0.4067	0.1786	2.2772	0.0268	0.0486	0.7647	0.296

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
0.2914	0.1909	1.5263	0.1329	-0.0915	0.6743	0.2121

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Temporal_Mid_L	0.1153	0.1188	-0.087	0.388

Model : 4
Y : PSQI
X : Temporal_Mid_L
M : Precocene ii
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
-0.166	0.0719	-2.3085	0.0248	-0.3102	-0.0218	-0.2997

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
-0.1225	0.0807	-1.5175	0.1351	-0.2844	0.0394	-0.2211

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Precocene ii	-0.0435	0.0536	-0.1677	0.0455

Model : 4
Y : PSQI
X : Precocene ii
M : Temporal_Mid_L
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
0.4066	0.1953	2.0819	0.0421	0.015	0.7981	0.2726

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
0.2549	0.2173	1.1728	0.2461	-0.181	0.6908	0.1709

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Temporal_Mid_L	0.1517	0.1309	-0.1294	0.3981

Model : 4
Y : PSQI
X : Temporal_Mid_L
M : Oglufanide
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
-0.166	0.0719	-2.3085	0.0248	-0.3102	-0.0218	-0.2997

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
-0.1195	0.0768	-1.556	0.1257	-0.2736	0.0346	-0.2158

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Oglufanide	-0.0465	0.0647	-0.1869	0.0559

Model : 4
Y : PSQI
X : Oglufanide
M : Temporal_Mid_L
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
0.1377	0.0593	2.3239	0.0239	0.0189	0.2565	0.3015

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
0.0999	0.0633	1.5772	0.1207	-0.0271	0.2269	0.2187

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Temporal_Mid_L	0.0378	0.0346	-0.0271	0.108

Model : 4
Y : PSQI
X : Temporal_Mid_L
M : 5-octyl-2-oxotetrahydro-3-furancarboxylic acid
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
-0.166	0.0719	-2.3085	0.0248	-0.3102	-0.0218	-0.2997

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
-0.1262	0.075	-1.6821	0.0984	-0.2768	0.0243	-0.2279

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
5-octyl-2-oxotetrahydro-3-fura	-0.0398	0.055	-0.1753	0.0357

Model : 4
Y : PSQI
X : 5-octyl-2-oxotetrahydro-3-furancarboxylic acid
M : Temporal_Mid_L
Sample
Size: 56
Total effect of X on Y

Effect	se	t	p	LLCI	ULCI	c_cs
0.3982	0.1765	2.2554	0.0282	0.0442	0.7521	0.2934

Direct effect of X on Y

Effect	se	t	p	LLCI	ULCI	c'_cs
0.2965	0.1838	1.6129	0.1127	-0.0722	0.6652	0.2185

Indirect effect(s) of X on Y:

	Effect	BootSE	BootLLCI	BootULCI
Temporal_Mid_L	0.1017	0.094	-0.0956	0.2705