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Integrative Omics Analysis for Amyotrophic Lateral Sclerosis

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St. Olaf College

2017

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Abstract

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By Shihua Wang

Introduction: Integrative omics analysis is useful for investigating the complex problems of molecular interactions in a biological system. The R package, xMWAS provides an automated workflow for integrative analysis of more than two datasets, differential network analysis, and community detection. In our study, we utilized the integrative omics analysis to explore the etiology and pathophysiology of ALS (amyotrophic lateral sclerosis).

Method: We applied the xMWAS package to analyze three types of omics data, microbiome, metabolites and cytokines, from 10 ALS patients and 10 control subjects. We conducted integrative omics analysis for all samples and then separately for patients and control subjects. We also generate 500 bootstrap samples from our data and repeated the same analysis to investigate the significant features that are associated with ALS.

Result: There is one more community of features in ALS compared than control subjects. The communities for ALS patients are clearer and the nodes in the communities are more closely connected. There are some 87 features whose normalized centrality indices differ by more than 0.2 between patient and controls. From the bootstrap samples, we found that there are 12 features whose centrality features are significantly different between patients and control subjects.

Discussion: Our result about microbiome verifies previous findings in the literature that gut microbiota has a significant association with ALS disease. The centrality change for cytokines can also be explained by an increased level of blood inflammatory cytokines for ALS patients. Future studies can focus on the association between ALS etiology and gut microbiota to address the decrease in centrality.

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Acknowledgement

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1 Introduction

Nowadays, multi-assay molecular profiling of biological samples is being widely used to investigate the molecular mechanisms for diseases and host responses to environmental factors, enabled by technological advances[5]. Since most cellular processes in a biological system are dependent on complex molecular interactions[1], integrative omics analysis allows researchers to address the complexity and answer challenging biological questions, such as the function of unknown metabolites, signaling, and metabolic pathway responses to infection[5].

There are a few data-driven/unsupervised and knowledge-based tools used to integrate data from different omics and other molecular assays [11][8]. However, most existing data integration tools allow integration of only two datasets and do not allow identification of community structure and evaluation of network changes between different conditions[10]. In 2018, Dr. Uppal from Emory University developed a R package xMWAS which provides an automated workflow for integrative analysis of more than two datasets, differential network analysis, and community detection to improve our understanding of complex molecular interactions and disease mechanisms of disease.

In our study, we want to explore the etiology and pathophysiology of ALS (Amyotrophic lateral sclerosis) which is well understood. There are 10 ALS patients and 10 control subjects who are the spouses of the patients in our study. We sequenced their microbiome and cytokines and measured their metabolites. Several studies have suggested that there is an associations of gut microbial communities and ALS [4]

and we also want to investigate their associations with cytokines and metabolites. Therefore, we used integrative omics analysis by xMWAS package to compare the networks of ALS and their spouse control subjects in order to better understand the pathophysiology of ALS.

2 Method

2.1 Data Description

The data we used come from 10 ALS patients with their spouses. For each of them, we sequenced their gut microbiota and cytokines and measured their metabolites and the cytokines. For microbiome data, we had an amplicon sequence variant (ASV) table containing the count for the number of observations of each ASV sequence in each sample, with ASVs labelled by their taxonomic classification. For microbiome, we converted our data to an OTU table where the rows represents the species of bacteria and the columns represent the samples - ALS patients or control subjects.

Similarly for metabolites and cytokines, each row represent a metabolite or cytokine and each column represents a sample. For metabolites, we have 7819 in total but only 3313 (40%) of them can be identified. For the ones that are unidentified, their names will be represented by m/z value (mass-to-charge ratio) combined with time by an underscore. For example, "299.1385157_23.12535687" represents a metabolites whose m/z value is 299.1385157 and time is 23.1253568.

Totally, we had 149 taxa of bacteria, 28 cytokines and 7819 metabolites respectively for these three matrices. Therefore, we have a total of 7996 features for each

subject in our analysis. We standardized the measurements for each of them into a value between 0 and 1, which is required to run xMWAS.

2.2 Overview of xMWAS

xMWAS is a package that provides an automated framework for integrative and differential network analysis which can take more than two omics datasets [10]. There are three stages of xMWAS for three matrices of omics data. These results include graph representation of the network, table of overall centrality of each feature and the cluster assignment of each feature.

2.2.1 Stage I: Integrative and Association Analysis

In stage one, xMWAS first conducted dimension reduction for each pair of matrices by sparse Partial Least Squares (sPLS) [3]. For each pair of matrices X and Y, we want to maximize the objective function which is:

$$\underset{||u||,||v||}{\text{argmax}} \ cov(X_h U_h, Z_h V_h) \quad h = 1, \ 2, \ ...H$$

In order to reduces the complexity of the network, sPLS applied L_1 LASSO (Least Absolute Shrinkage and Selection Operator) penalty on u and v [7]. Then an association matrix A_{xy} was generated from the output of sPLS for each pair, followed by a student's t-test to evaluate the statistical significance of association scores. If the absolute value of association score was > 0.7 and the p-value was < 0.01, the association score was then used for further analysis.

The resulting graph for each pair of matrices was $G_i = (V_i, E_i)$ where V_i is a set of nodes and E_i is a set of edges. Then xMWAS imported the information in G_i and converted the edges between each two nodes to an edge list matrix L_i. For L_i, each row represented an edge between the input matrices pair, such as X and Y.

2.2.2 Stage II: Generate the Integrative Network Graph

In stage two, xMWAS took the union of the individual edge list matrices to generate a combined edge list matrix $L_e = \bigcup_{i=1}^{3} L_i$. The matrix L_e was used to generate the overall integrative network graph, $G = (V, E)$. V corresponds to nodes and E corresponds to edges between the nodes, representing positive or negative associations between multiple datasets [10].

2.2.3 Stage III: Community Detection

In stage three, xMWAS used a multilevel community detection algorithm [2] to identify communities of nodes. Nodes that are tightly connected with each other but sparsely connected with the rest of the network were assigned to the same cluster[10]. The centrality of each node was calculated by the Page Rank Algorithm[9].

2.3 Bootstrapping

We first applied xMWAS for all the data which contained both patients and control subjects. Then we ran xMWAS separately for the patients and control subjects. After doing that, we bootstrapped our samples to generate new data. For the 20 samples, we randomly chose one with replacement for 20 times to generate 20 new

samples. We assigned the first 10 selected samples to be patients and the second 10 selected samples to be control subjects. Then we used the microbiome, metabolites and cytokines data for each sample as the new matrices input to xMWAS and run xMWAS on data from the bootstrap sample. We repeated this procedure for 500 times and compared the results from bootstrap samples to the result from our real data.

2.4   Analyzing xMWAS Output

After we ran xMWAS on the matrices separately for patient and control each time, we first found the common features in the ALS patient and control outputs. We calculated the differences in overall centrality to compare each feature's change in centrality for patient and control. We first calculated the differences for the real data and then compared them to the distribution of differences in the 500 bootstrap samples.

We also did a composite analysis for the clusters from xMWAS output. For every xMWAS output, we extracted the pairs of features that were assigned to the same cluster in patient and control. We repeated this analysis for the 500 bootstrap samples and calculated the frequencies of being assigned to the same cluster in patient and control for each pair of features.

3 Result

3.1 Network and Clusters of Real Data

3.1.1 Network Visualization

Figure 1 shows the communities network for all the data, including patients and controls. There are four clusters in this network and three of them are very dense (blue, orange and yellow) while one of them is relatively sparse (green). Also, in the visualization we can see that these clusters are very closely related to each other.
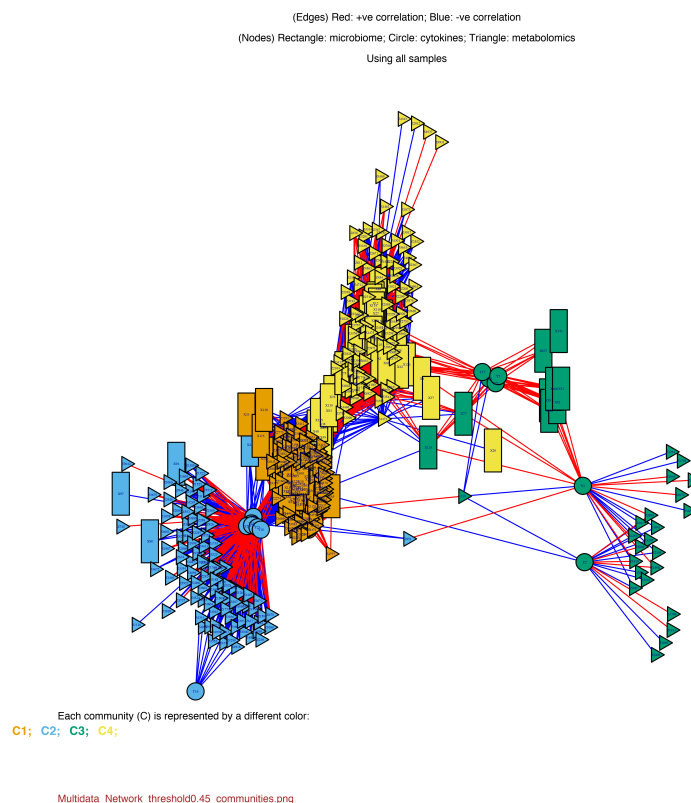
Figure 1: **Communities Network for All Subjects** Rectangles represent microbiome, circles represent cytokines and triangles represent metabolites. The four different colors represent four clusters. Red edges indicate positive correlation and blue edges represent negative correlation.

Figure 2 and Figure 3 show the communities network for ALS patients and control subjects respectively. There are four clusters for ALS patients where cluster 1 (orange) is relatively distant from the other three clusters. In contrast, there are only three clusters in control subjects and each cluster is more closely connected to the other two.
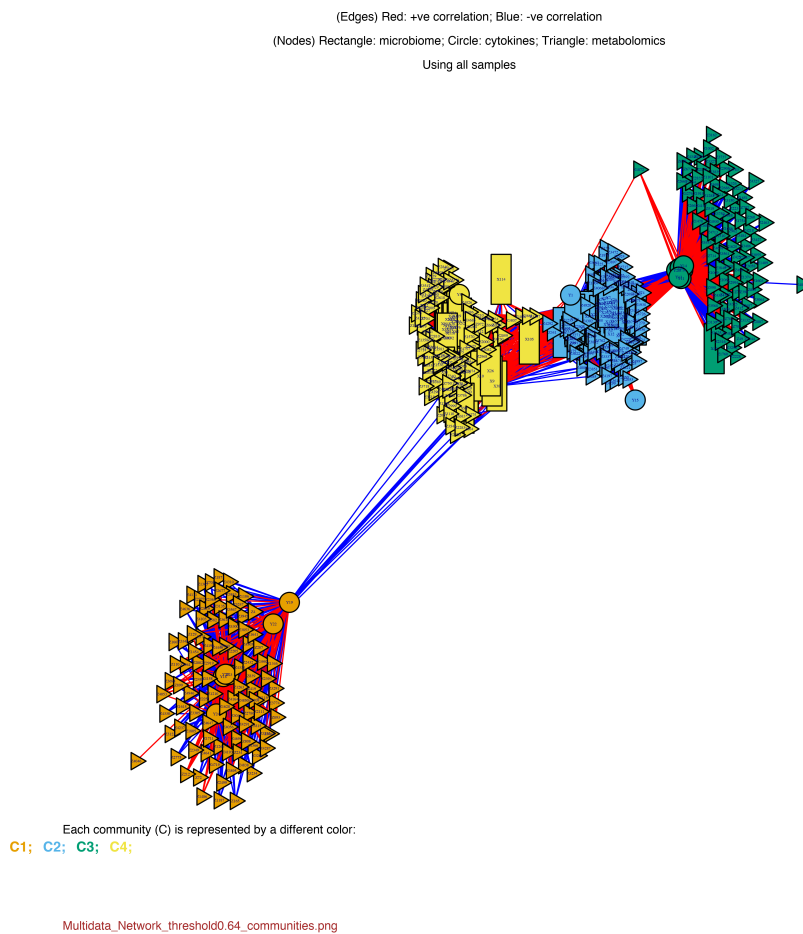
Figure 2: **Communities Network for ALS Patients** Rectangles represent microbiome, circles represent cytokines and triangles represent metabolites. The four different colors represent four clusters. Red edges indicate positive correlation and blue edges represent negative correlation.
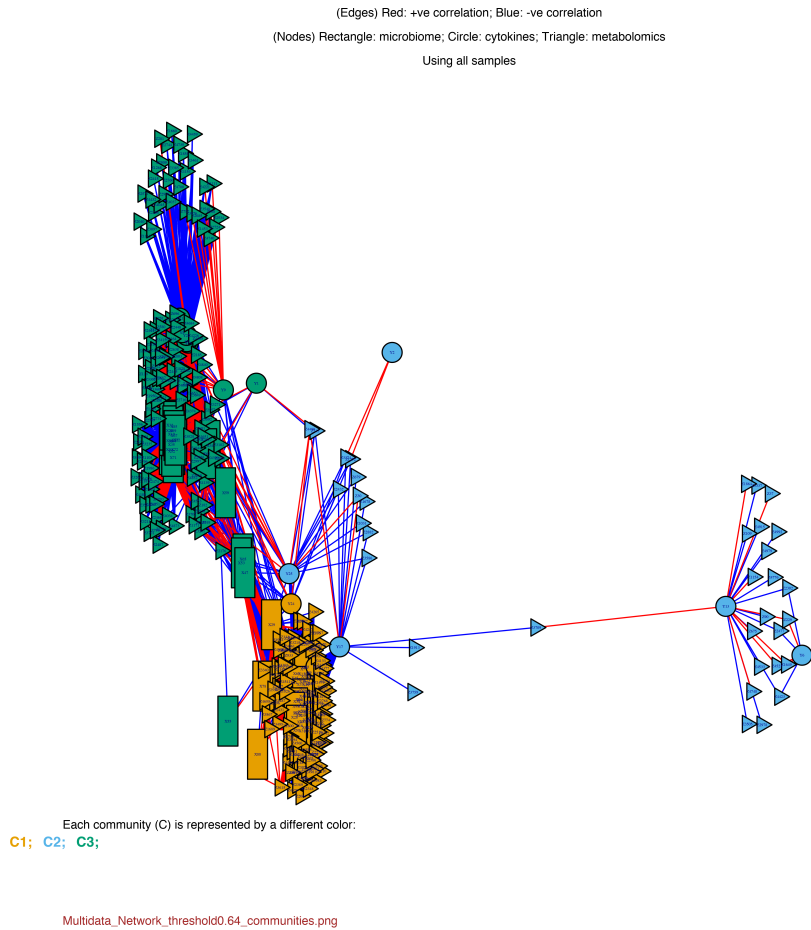
Figure 3: **Communities Network for control subjects** Rectangles represent microbiome, circles represent cytokines and triangles represent metabolites. The three different colors represent three clusters. Red edges indicate positive correlation and blue edges represent negative correlation.

3.1.2 Cluster Assignment of Patients and control subjects

In Figure 4, we illustrate the difference in assigning features to clusters between patients and control subjects. Each cell in the matrices represents the number of features assigned to the corresponding patients' cluster and control subjects' cluster. For microbiome, most of the features in cluster 2 and 4 for patients were assigned to cluster A for control subjects. For cytokines and metabolites, there was more discrepancy in cluster assignment between patients and control subjects.

10

Microbiome			
	A	B	C
1	0	0	0
2	28	0	7
3	0	0	0
4	17	0	5

Cytokines			
	A	B	C
1	2	1	0
2	0	0	1
3	0	1	3
4	0	0	1

Metabolites			
	A	B	C
1	2	0	3
2	3	0	5
3	1	1	0
4	3	0	3

Figure 4: **Cluster Assignment for ALS Patients and control subjects**. Each row represent the cluster in patient and each column represents a cluster in control.

3.1.3 Comparing the Centrality of Patients and control subjects

We found there were 87 features existing in both ALS patients and control subjects network. Among these 87 features, 44 of them had absolute values of difference in centrality larger than 0.2 (Table 1). Features from microbiome data had relatively larger difference in centrality and most of them had lower centrality in ALS patients compared to the centrality in control.

Table 1: Difference in Centrality Between ALS Patients and control subjects

Class	Centrality_Patient	Centrality_Control	Difference	Indicator
Ruminococcaceae	0.013	1.000	-0.987	-
Peptostreptococcus	0.981	0.009	0.972	+
Solobacterium	0.965	0.007	0.958	+
Victivallis	0.040	0.997	-0.957	-
Dorea	0.043	0.998	-0.955	-
Eisenbergiella	0.032	0.987	-0.955	-
Clostridiales	0.044	0.997	-0.953	-
Negativibacillus	0.047	0.998	-0.951	-
Phascolarctobacterium	0.047	0.996	-0.949	-
Anaeroglobus	0.043	0.981	-0.938	-
LachnospiraceaeNKAgroup	0.051	0.987	-0.936	-
Fusobacterium	0.047	0.945	-0.898	-
Gardnerella	0.043	0.939	-0.896	-
Mobiluncus	0.015	0.903	-0.888	-
Methanobrevibacter	0.113	0.999	-0.886	-
Eubacterium	0.881	0.009	0.872	+
Flavonifractor	0.033	0.903	-0.870	-
283.175178_278.9540313*	0.022	0.889	-0.867	-
Alistipes	0.149	0.997	-0.848	-
Parasutterella	0.158	0.996	-0.838	-
Negativicoccus	0.840	0.021	0.819	+

Class	Centrality_Patient	Centrality_Control	Difference	Indicator
Klebsiella	0.814	0.009	0.805	+
il13_stool	0.810	0.025	0.785	+
ifng_stool	0.804	0.026	0.778	+
il2_stool	0.780	0.006	0.774	+
Fusicatenibacter	0.143	0.879	-0.736	-
Metabolite84[†]	0.724	0.002	0.722	+
Gemella	0.969	0.256	0.713	+
Metabolite1[†]	0.000	0.706	-0.706	-
tnfa_plasma	0.678	0.000	0.678	+
553.7238317_45.82948904 [*]	0.649	0.000	0.649	+
Hungatella	0.618	0.009	0.609	+
Christensenellaceae	0.436	0.996	-0.560	-
Metabolite223[†]	0.489	0.010	0.479	+
Paraprevotella	0.547	0.995	-0.448	-
Barnesiella	0.962	0.536	0.426	+
Campylobacter	0.679	0.995	-0.316	-
crp_plasma	0.252	0.001	0.251	+
Lachnospira	0.246	0.009	0.237	+
Faecalitalea	0.748	0.978	-0.230	-

Class	Centrality_Patient	Centrality_Control	Difference	Indicator
Lachnospiraceae Uncultured Genus002	0.742	0.971	-0.229	-
Sarcina	0.044	0.270	-0.226	-
Jonquetella	0.780	0.994	-0.214	-
LachnospiraceaeNDgroup	0.787	0.997	-0.210	-

[†] represents targeted metabolite and the exact name is available in Table 4 in Appendix.

[⋆] represents untargeted metabolites.

3.2   Comparing Real Data to Bootstrap Samples

For the 44 features in Table 1, we obtained the distribution of the difference in the 500 bootstrap samples and used a 0.05 percentile to decide whether the difference is significantly lower or higher. The distributions of the difference for the 44 features were normally distributed around 0. There were 12 features with difference lower than 5% of the bootstrap samples or higher than 95% of the bootstrap samples. There were two targeted metabolites - Metabolite1 and Metabolite84 whose exact name is available in Table 4 in Appendix. The last two plots in figure 5 show the distributions for untargeted metabolites.

Figure 5: **Distribution of Features' Centrality Difference**
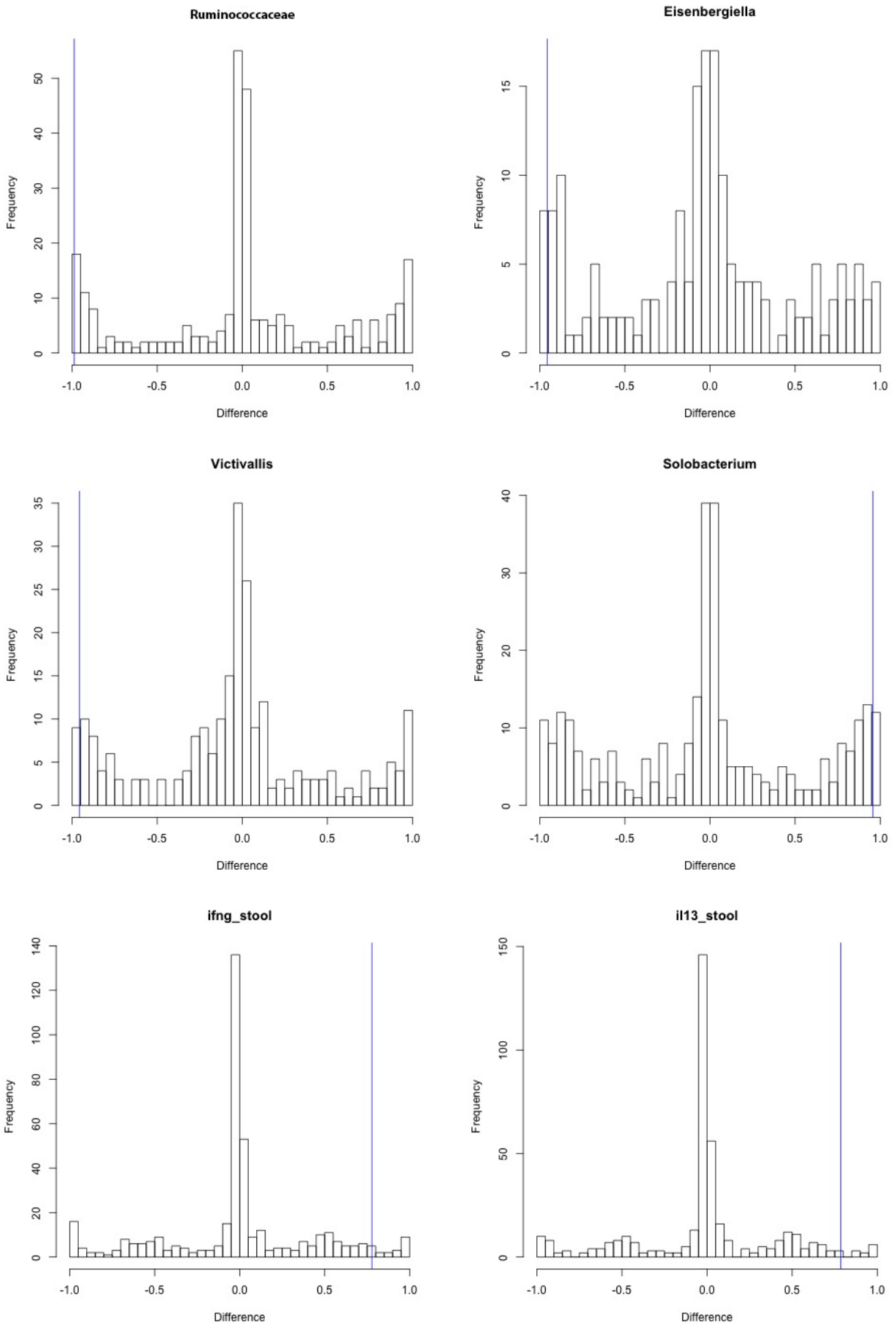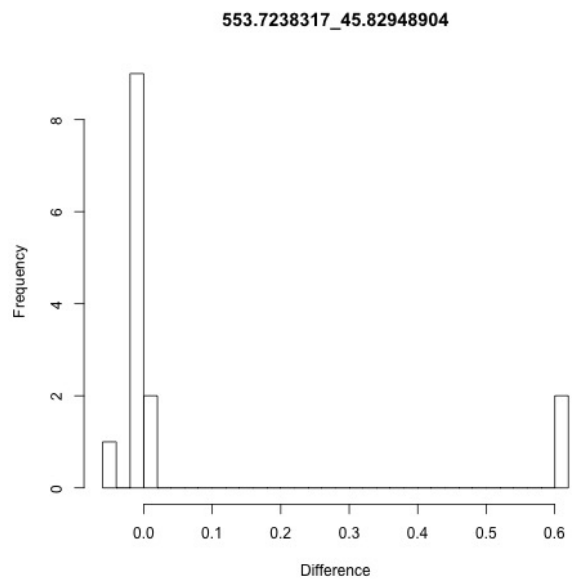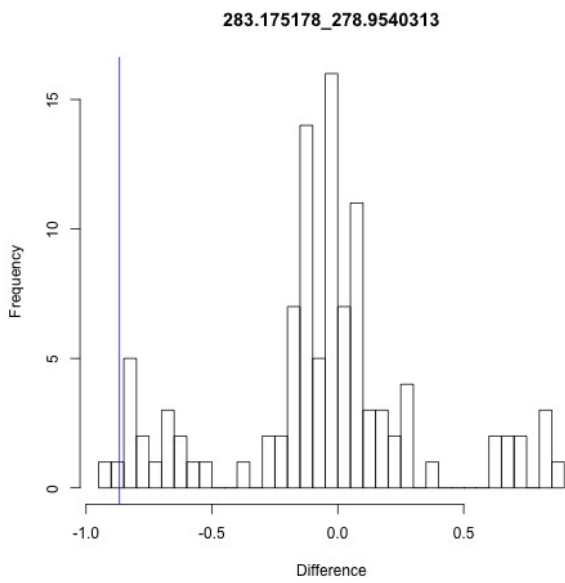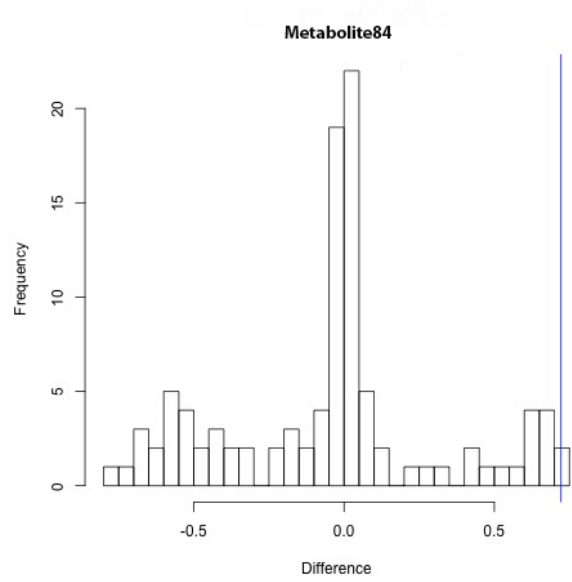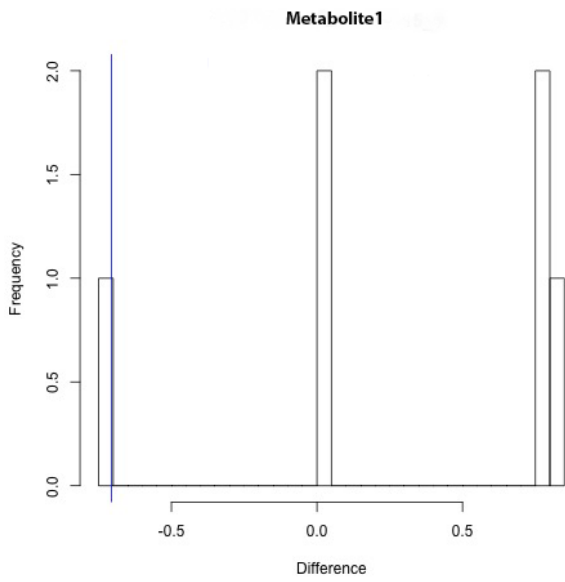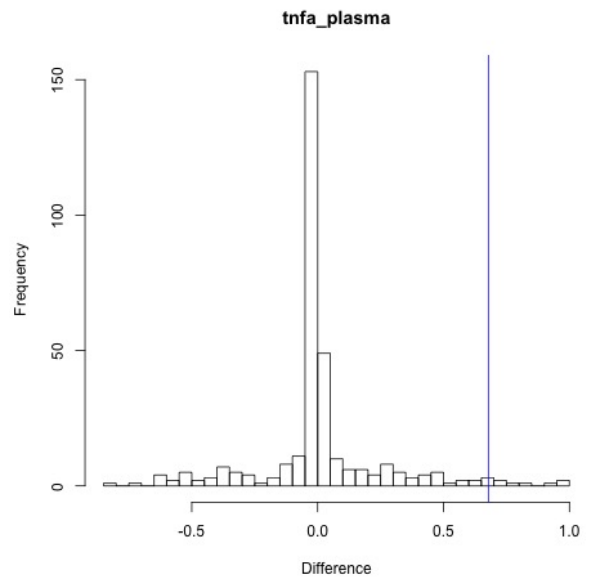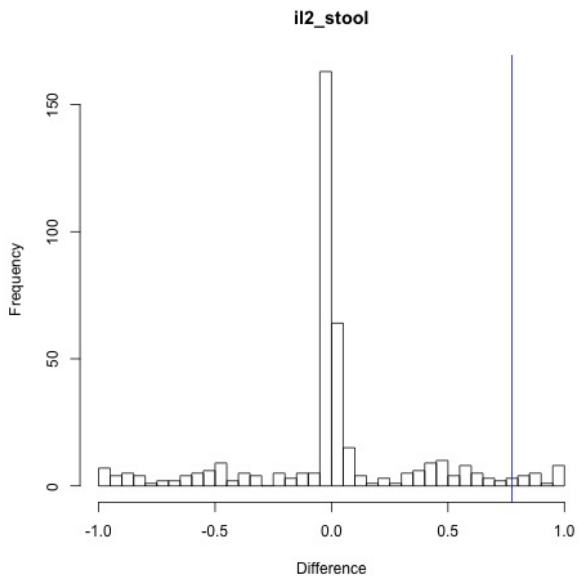
4   Discussion

From our integrative analysis on microbiome data, cytokine data and metabolites data, we found that for ALS patients there was one more cluster than the control subjects had. The nodes in patients' clusters were more closely connected with each other and more sparsely connected with other clusters. Therefore, the omics for ALS patients was more diverse than the control subjects'.

Most of the features whose centrality changed considerably were from microbiome (35 out of 44) while there were only a few cytokines (4) and metabolites (5) whose centrality changed considerably. This result verifies the previous finding that gut microbiota has a significant association with ALS disease [4]. By comparing the result to bootstrap samples, we found that among the nine features whose centrality was significantly different between patients and control subjects, the two microbiome features (Ruminococcaceae and Eisenbergiella) had significantly lower centrality in patients while the other three cytokine features (ifngstool, il13stool and il2stool) had significantly higher centrality in patients. The centrality change for cytokines could also be explained by an increase level of blood inflammatory cytokines for ALS patients [6]. Future studies can focus on the association between ALS pathophysiology and gut microbiota to address the decrease in centrality.

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5   Appendix

Table 4 lists all the features of the control subjects with the node ID shown in the network, the cluster each feature belongs to, the name of each feature and the global centrality. Table 5 lists the same information for ALS patients. Table 6 shows the metabolites with the metabolite ID we used in the results section as well as the matching names of the metabolite. One metabolite can have multiple possible matchings which result in multiple names.

Table 2: **Names for Identified Metabolites**

ID	MZ_Time	Name
Metabolite1	100.0756415_33.22355974	1-Pyrrolidinecarboxaldehyde
		N-Methyl-2-pyrrolidinone;1-Methyl-2-pyrr
		~~olidinone;N-Methylpyrrolidone
		(2R)-2-Hydroxy-2-methylbutanenitrile
		25-Dihydro-24-dimethyloxazole
		2-Piperidinone
Metabolite2	100.1121195_267.3263044	2-Methylpiperidine
		Cyclohexylamine
		Cyclohexylamine;Cyclohexamine
Metabolite3	101.034535_61.77970592	Hydantoin;Glycolylurea
Metabolite4	104.1070002_47.33711003	Neurine
Metabolite5	1044.706568_30.61476831	N-(eicosanoyl)-4R-hydroxyeicosasphingani
		~~ne-1-O-D-mannopyranosyl-alpha1-2-myo-ino
		~~sitol-1-phosphate
		N-(2-hydroxydocosanoyl)-sphinganine-1-O-
		~~D-mannopyranosyl-alpha1-2-myo-inositol-1
		~~-phosphate
		N-(2-hydroxyeicosanoyl)-eicosasphinganin
		~~e-1-O-D-mannopyranosyl-alpha1-2-myo-inos
		~~itol-1-phosphate
		N-(docosanoyl)-4R-hydroxysphinganine-1-O
		~~-D-mannopyranosyl-alpha1-2-myo-inositol-
		~~1-phosphate
Metabolite6	105.0697997_25.42452132	Styrene;Phenylethylene
		Styrene
Metabolite7	108.0443778_50.08327836	Nitrosobenzene
		alpha-Fluoro-beta-alanine;3-Amino-2-fluo
		~~ropropionic acid
		3-Fluoro-D-alanine;(S)-3-Fluoroalanine
		6-Iminocyclohexa-24-dienone;12-Benzoquin
		~~one monoimine
		3-Pyridildehyde;Pyridine-3-aldehyde;3-
		~~Pyridinecarboxaldehyde;Nicotildehyde
Metabolite8	1086.053593_278.6753715	TG(24:020:024:1(15Z))
		TG(22:022:024:1(15Z))
		TG(22:024:1(15Z)22:0)
		TG(24:024:020:1(11Z))
		TG(22:024:022:1(13Z))
Metabolite9	1086.428363_279.623132	13Z16Z-docosadienoyl-CoA
		(13Z16Z)-Docosadi-1316-enoyl-CoA
		Docosanoyl-CoA
Metabolite10	109.0633222_45.03556619	Anisole
		m-Cresol
		o-Cresol;2-Hydroxytoluene;o-Methylphenol
		Aromatic primary alcohol;Aromatic alcoho
		~~l
		3-Cresol;m-Cresol;3-Hydroxytoluene

ID	MZ_Time	Name
Metabolite11	110.0349469_277.5951096	p-Benzosemiquinone;4-Hydroxyphenoxy radi ~~cal
		o-Benzosemiquinone;2-Hydroxyphenoxy radi ~~cal
Metabolite12	111.0804055_17.22343399	2E4Z-Heptadiel
		2-Isopropylfuran
		3-Methyl-2-cyclohexen-1-one
		24-heptadiel
		2-Ethyl-5-methylfuran
Metabolite13	112.0869547_79.15587854	Betazole
		Histamium
		Histamine;1H-Imidazole-4-ethamine;2-(4 ~~-Imidazolyl)ethylamine
		Histamine
Metabolite14	113.0960976_36.23331657	xi-3-Methyl-3-cyclohexen-1-ol
		(Z)-4-Heptel
		2-Heptel
		4-Methyl-1-hexen-3-one
		(R)-3-Methylcyclohexanone
Metabolite15	114.0549856_276.1903119	1-Pyrroline-2-carboxylate;1-Pyrroline-2- ~~carboxylic acid;delta1-Pyrroline 2-carbo ~~xylate;1-Pyrroline 2-carboxylate
		1-Pyrroline-5-carboxylic acid
		1-Pyrroline-2-carboxylic acid
		Glutarimide;Piperidine-26-dione;26-Diket ~~opiperidine
		delta-1-Pyrroline-5-carboxylate;34-Dihyd ~~ro-2H-Pyrrole-2-carboxylate
Metabolite16	115.0389974_130.0844245	cis-Acetylacrylate
		3-oxo-4-pentenoic acid
		Tulipalin B;(4S)-4-Hydroxy-3-methylidene ~~oxolan-2-one
		2-Hydroxy-24-pentadienoate;cis-2-Hydroxy ~~penta-24-dienoate;Oxopent-4-enoate;2-Oxo ~~pent-4-enoate;2-Hydroxypenta-24-dienoate
Metabolite17	115.0754331_274.0691716	22-dimethyl-3-butenoic acid
		Ethyl crotote
		5-hexenoic acid
		(2Z)-2-methylpent-2-enoic acid
		2-Hydroxycyclohexan-1-one;2-Hydroxycyclo ~~hexanone;Adipoin
Metabolite18	118.0604132_262.0736413	Guanidinoacetate;Guanidinoacetic acid;Gl ~~ycocyamine;N-Amidinoglycine;Guanidoaceti ~~c acid
		N-Nitroso-N-ethylurea
		Guanidoacetic acid
Metabolite19	119.0160775_53.23379689	Dihydro-4-mercapto-3(2H)-furanone

ID	MZ_Time	Name
Metabolite20	119.0853706_25.89055982	Indane
		alpha-Methylstyrene
		Vinyl toluene
		alpha-Methylstyrene;1-Methyl-1-phenyleth
		∼∼ylene;2-Phenylpropene
Metabolite21	123.0553669_273.0350179	Niacimide
		Nicotimide;Nicotinic acid amide;Niacin
		∼∼amide;Vitamin PP
		2-Acetylpyrazine
		Picolimide
		Isonicotineamide;Isonicotimide
Metabolite22	124.0758303_268.2042133	ortho-Anisidine;o-Anisidine
		4-Hydroxybenzylamine
		p-Anisidine
		para-Anisidine;1-Amino-4-methoxybenzene
		2-Acetyl-1-methylpyrrole
Metabolite23	126.0298108_53.4239191	2-Aminoethylphosphote;(2-Aminoethyl)ph
		∼∼osphote;Ciliatine
		Ciliatine
		D-(1-Aminoethyl)phosphote;D-(1-Aminoet
		∼∼hyl)phosphonic acid
Metabolite24	126.0662632_269.871915	3-Methylcytosine
		2-O-Methylcytosine
		5-Methylcytosine
Metabolite25	127.0614116_17.85277005	5-Amino-4-imidazolecarboxyamide
		5-Aminoimidazole-4-carboxamide
		24-Diamino-6-hydroxypyrimidine
Metabolite26	129.0346989_169.498307	4-Fluorocatechol
		2-nonene-468-triyl
		3-Fluorocatechol
Metabolite27	130.0498701_77.00001118	5-Oxoprolite
		dimethadione
		Pyrrolidonecarboxylic acid
		N-Acryloylglycine
		1-Pyrroline-4-hydroxy-2-carboxylate
Metabolite28	130.1226825_266.4769854	N-methyl hexanoyl amine
		N-Methylhexamide
Metabolite29	130.9664179_39.18501884	22-Dichloro-11-ethanediol
		Calcium formate;Formic acid calcium salt
Metabolite30	131.0339083_66.24304779	2-Hydroxyglutaric acid lactone
		(2Z)-4-methoxy-4-oxobut-2-enoic acid
		(E)-Glutacote;trans-Glutacote;trans-
		∼∼Glutaconic acid;Glutaconic acid
		Citraconic acid
		Acetylpyruvate;Acetylpyruvic acid;24-Dio
		∼∼xopentanoate

ID	MZ_Time	Name
Metabolite31	133.101803_39.83950082	Dicyclopentadiene
		p-Mentha-1358-tetraene
		Tetralin;1234-Tetrahydrophthalene
Metabolite32	134.0811916_68.16763006	14-Dideoxy-14-imino-D-ribitol
		N-Lactoyl ethanolamine
		L-2-Amino-5-hydroxypentanoic acid
		N-Hydroxy-L-valine
Metabolite33	134.0945634_107.7805766	Tranylcypromine
		1234-Tetrahydroisoquinoline
Metabolite34	138.0549869_59.48651816	m-Aminobenzoic acid
		4-Aminobenzoate;ABEE;4-Aminobenzoic acid
		∼∼;p-Aminobenzoate
		Anthranilate;Anthranilic acid;o-Aminoben
		∼∼zoic acid;Vitamin L1;2-Aminobenzoate
		2-Aminobenzoic acid
		Trigonelline
Metabolite35	140.0536904_226.3703561	24-Dimethyl-5-vinylthiazole
Metabolite36	141.0184979_212.75819	trans-4-Carboxymethylenebut-2-en-4-olide
		cis-4-Carboxymethylenebut-2-en-4-olide;4
		∼∼-Carboxymethylenebut-2-en-4-olide
		cis-4-Carboxymethylenebut-2-en-4-olide
		5-Formyl-2-furoate;5-Formyl-2-furancarbo
		∼∼xylate;5-Formylfuran-2-carboxylate
Metabolite37	141.0714947_59.77032705	34-Diethylthiophene
		5-Phenyl-13-pentadiyne
		Norcapillene
Metabolite38	141.1274703_266.4822124	24-Dimethyl-2E4E-heptadien-1-ol
		(Z)-6-Nonel
		3E-Nonen-2-one
		(3E6Z)-no-36-dien-1-ol
		8-Nonen-3-one
Metabolite39	143.1067056_216.2861138	Ethyl 5-hexenoate
		propan-2-yl (2Z)-2-methylbut-2-enoate
		trans-2-Octenoic acid
		(3Z)-2-propylpent-3-enoic acid
		7-octenoic acid
Metabolite40	145.049581_37.19921588	2-methyl-2E-pentenedioic acid
		(2Z)-4-ethoxy-4-oxobut-2-enoic acid
		3-Hexenedioic acid
		Methylitacote;2-Methylene-3-methylsucc
		∼∼ite
		2-Methyleneglutarate;alpha-Methylene glu
		∼∼tarate
Metabolite41	145.0971581_70.03299618	4-Amino-1-piperidinecarboxylic acid
		adipamide
Metabolite42	147.0241535_129.9190303	ZAPA;(Z)-3-((Aminoiminomethyl)thio)-2-pr
		∼∼openoic acid

ID	MZ_Time	Name
Metabolite43	147.0441826_250.7399794	Chromone
		2-Benzofurancarboxaldehyde
		Coumarin;Coumarine;Cumarin;2H-1-Benzopyr
		~~an-2-one;12-Benzopyrone;2-Propenoic acid
		~~3-(2-hydroxyphenyl)- delta-lactone;56-B
		~~enzo-2-pyrone;Benzo-alpha-pyrone;cis-o-C
		~~oumarinic acid lactone;Coumarinic anhydr
		~~ide;o-Hydroxycinmic acid lactone;Ratte
		~~x;Tonka bean camphor
		Coumarin
		Phenylpropiolic acid
Metabolite44	148.0425503_41.63051475	Thiomorpholine 3-carboxylate
Metabolite45	149.0636146_67.62618086	3-Mercapto-3-methylbutyl formate
		Ethyl 3-(methylthio)propanoate
		Methylthiomethyl butyrate
		methyl 4-(methylsulfanyl)butanoate
		Methyl 4-(methylthio)butyrate
Metabolite46	149.0950297_45.23961258	4-Phenyl-3-buten-2-ol
		1-Methoxy-4-(2-propenyl)benzene
		2-(4-Methylphenyl)propal
		Anethole
		246-Trimethylbenzaldehyde
Metabolite47	149.0961937_279.6069524	Estragole;1-Methoxy-4-(2-propenyl)benzen
		~~e;Methylchavicol
		4-Isopropylbenzaldehyde;p-Cumic aldehyde
		~~;Cumildehyde
		1-Methoxy-4-(2-propenyl)benzene
		Anethole;t-Anethole;trans-Anethole
		246-Trimethylbenzaldehyde
Metabolite48	150.0766456_58.60377347	7-Methyladenine
		3-Methyladenine
		4-Amino-4-deoxy-L-arabinose;L-Ara4N
		6-Methylaminopurine;N6-Methyladenine
		1-Methyladenine
Metabolite49	150.0914201_261.9530434	Venoterpine
		5-Acetyl-23-dihydro-1H-pyrrolizine
		23-Dihydro-6-methyl-1H-pyrrolizine-5-car
		~~boxaldehyde
		D-Cathinone;Cathinone
		3-Phenylpropioldoxim
Metabolite50	151.0615914_39.97365617	Diisopropyl disulfide
		beta-D-Apiose
		D-Xylulose
		L-Xylulose;L-threo-Pentulose;L-Lyxulose
		D-Lyxose

ID	MZ_Time	Name
Metabolite51	151.0753367_265.5548362	4-Methoxyacetophenone
		4-Ethoxybenzaldehyde
		4-Hydroxy-3-methylacetophenone
		2-Ethyl-4-(2-furanyl)-2-propel
		Methyl phenylacetate
Metabolite52	151.086473_19.77301555	2-Acetyl-3-ethylpyrazine
		78-Dihydro-3-methylpyrrolo12-apyrimidin-
		~~2(6H)-one
		N-Methylanthranilamide;N-Methyl-2-aminob
		~~enzamide
		NN-Dimethyl-4-nitrosoaniline;Accelerine
		2-Acetyl-35-dimethylpyrazine
Metabolite53	153.1275048_271.8666215	(R)-Ipsdienol;(4R)-2-Methyl-6-methyleneo
		~~cta-27-dien-4-ol
		(1S4S)-Dihydrocarvone
		Dehydro-18-cineole
		Pinocarveol
		()-cis-Isopulegone
Metabolite54	154.0494112_49.05688262	4-Aminosalicylate;4-Aminosalicylic acid
		2-Nitro-p-cresol
		Mesalazine
		3-Amino-4-hydroxybenzoate;3-Amino-4-hydr
		~~oxybenzoic acid;34-AHBA
		(5R)-Carbapen-2-em-3-carboxylate;1-Carba
		~~pen-2-em-3-carboxylic acid;(5R)-Carbapen
		~~em-3-carboxylic acid;(5R)-Carbapenem-3-c
		~~arboxylate;(5R)-7-Oxo-1-azabicyclo320hep
		~~t-2-ene-2-carboxylate
Metabolite55	154.074217_57.5568992	FAPy-adenine
		46-Diamino-5-formamidopyrimidine;46-Diam
		~~ino-5-N-formamidopyrimidine
Metabolite56	155.0451164_66.58684397	Diethylphosphoric acid;OO-Diethylphospho
		~~ric acid
		2-Amino-5-nitrophenol
		Diethylphosphate
		4-Amino-2-nitrophenol
		3-Imidazole-2-oxopropanoate
Metabolite57	160.0253384_69.57499715	(E)-4-Isothiocyato-1-(methylthio)-1-bu
		~~tene
		(E)-Raphanusanin
Metabolite58	160.0758354_272.5560522	Echinopsine
		3-Methyl-quinolin-2-ol
		Indoleacetaldehyde
		Indole-3-acetaldehyde;2-(Indol-3-yl)acet
		~~aldehyde;Indoleacetaldehyde
		N-Hydroxy-1-aminophthalene;1-phthylh
		~~ydroxylamine
Metabolite59	160.1154535_273.6074586	()-2-Pentylthiazolidine

ID	MZ_Time	Name
Metabolite60	160.1331467_36.54004876	3-amino-octanoic acid
		2-amino-octanoic acid
		Pregabalin
		8-aminocaprylic acid
		DL-2-Aminooctanoic acid
Metabolite61	163.0977438_64.65031799	Oleandrose;beta-L-Oleandropyranose
		2-(1-Ethoxyethoxy)propanoic acid
		beta-Cymaropyranose;D-Cymarose;Cymarose;
		~~26-Dideoxy-3-O-methyl-D-ribo-hexose
		Dimethicone
Metabolite62	163.1329087_280.7491753	(3R7R)-137-Octanetriol
Metabolite63	166.1227113_142.0710616	Atoxin a;Ethanone 1-(9-azabicyclo(421)
		~~non-2-en-2-yl)- (1R)-
		Perilla sugar
		Hordenine;4-2-(Dimethylamino)ethylphenol
		Ephedrine;(-)-Ephedrine;L-Ephedrine
		2-(5-Methyl-2-furanyl)piperidine
Metabolite64	167.0872736_53.86261152	3-(4-Methyl-3-pentenyl)thiophene
		1-Phenyl-5-heptene-13-diyne;Benzene 5-he
		~~ptene-13-diynyl-
		Fluorene;Diphenylenemethane;22-Methylene
		~~biphenyl
		(3E5Z)-135-Tridecatriene-7911-triyne
		1311-Tridecatriene-579-triyne
Metabolite65	167.1067386_277.1221859	Borne-26-dione;6-Oxocamphor
		8-Dimethyl-3E8E-decadien-10-olide
		Epinepetalactone
		4-(4-Hydroxyphenyl)-2-butanol;4-HPB;Rhod
		~~odendrol;Betuligenol
Metabolite66	168.0813779_116.8544098	Carbazole;9H-Carbazole
Metabolite67	168.9607232_182.5891642	Methyl 1-propene-1-sulfenoselenoate
		Methyl (2-propenylthio) selenide
Metabolite68	168.9803708_235.9469174	3-Sulfopyruvate;3-Sulfopyruvic acid
		3-Sulfotopyruvate
		3-Sulfopyruvic acid
Metabolite69	169.0969903_37.77340052	Pyridoxamine;PM
		Pyridoxamine
		Cyclo(deltaAla-L-Val)
		4-PIOL;5-(4-Piperidyl)isoxazol-3-ol
Metabolite70	172.096794_157.1050358	Crotanecine
		N-Butyryl-L-homoserine lactone
		N-butanoyl-lhomoserine lactone
Metabolite71	172.1331658_100.40671	Gabapentin
Metabolite72	172.1696336_23.56156206	decamide
		N23-trimethyl-2-(propan-2-yl)butamide
		N23-Trimethyl-2-(1-methylethyl)butamid
		~~e

ID	MZ_Time	Name
Metabolite73	173.1325899_278.73048	12-Dihydro-116-trimethylphthalene
Metabolite74	175.1189533_111.9589915	D-Arginine;D-2-Amino-5-guanidinovaleric ~~acid
		L-Arginine
		D-Arginine
		Amino acid(Arg-);Arginine;2-Amino-5-guan ~~idinovaleric acid
		L-Arginine;(S)-2-Amino-5-guanidinovaleri ~~c acid;L-Arg
Metabolite75	176.0703906_26.59489622	Indole-3-acetate;Indole-3-acetic acid;(I ~~ndol-3-yl)acetate;Indoleacetate;Indoleac ~~etic acid;IAA
		Indoleacetic acid
		5-Hydroxyindoleacetaldehyde
		2-Methylquinoline-34-diol
		(Indol-3-yl)glycolaldehyde;3-Indoleglyco ~~laldehyde
Metabolite76	176.1163331_95.9288709	Debrisoquin;Debrisoquine
		Debrisoquine
Metabolite77	179.0694419_192.4843435	9-oxo-2457-decatetraenoic acid
		Coniferyl aldehyde;Coniferaldehyde;4-Hyd ~~roxy-3-methoxycinmaldehyde;Ferulaldehy ~~de
		8S-hydroxy-2-Decene-46-diynoic acid
		2-Oxo-4-phenylbutyric acid;2-Oxo-4-pheny ~~lbutanoic acid;2-Oxo-4-phenylbutanoate
		10-hydroxy-8Z-Decene-46-diynoic acid
Metabolite78	183.1380953_268.7191545	4-undecynoic acid
		9-undecynoic acid
		Geranyl formate
		(2E6Z)-26-Nodien-1-Yl acetate
		10-undecynoic acid
Metabolite79	186.9227892_217.4884614	Iodoethanoic acid
Metabolite80	187.0412093_203.2498126	Psoralen;Ficusin
		Angelicin;Isopsoralen
		Psoralen
		Angelicin
Metabolite81	188.119738_220.0672542	Amantadine hydrochloride
Metabolite82	191.0662592_81.59190726	Aspartyl-Glycine
		Glycyl-Aspartate
		Carglumic acid
		N-Carbamyl-L-glutamate;Carglumic acid
		L-alpha-Amino-gamma-oxalylaminobutyric a ~~cid
Metabolite83	191.1795459_275.5768916	2-Methyl-2-phenyl-undecane
		7-Ethyl-35-dimethyl-2E4E6E8E-decatetraen ~~e
		468-Trimethyl-2E4E6E8E-undecatetraene
		357-Trimethyl-2E4E6E8E-undecatetraene
		1-Ethyl-35-diisopropyl-benzene

ID	MZ_Time	Name
Metabolite84	193.0683198_68.8963676	2-epi-5-epi-Valiolone;(2S3S4S5R)-2345-Te ~~trahydroxy-5-(hydroxymethyl)cyclohexan-1 ~~-one Quite;Quinic acid;Kinic acid;Chinic ac ~~id;L-Quinic acid;L-Quite;(-)-Quinic ac ~~id 2-epi-Valiolone;(2S3S4S5S)-2345-Tetrahyd ~~roxy-5-(hydroxymethyl)cyclohexan-1-one 2-(Methylthiomethyl)-3-phenyl-2-propel Quinic acid
Metabolite85	194.117691_271.6399092	Ethyl N-ethylanthranilate (-)-Salsoline (S)-N-Methylsalsolinol 2-Methylpropyl 2-aminobenzoate
Metabolite86	197.066722_33.02317231	37-Dimethyluric acid Gluconic acid 19-Dimethyluric acid Galactonic acid 13-Dimethyluric acid
Metabolite87	199.1476875_24.4268888	14-dimethyl-7-(propan-2-yl)azulene 4-Isopropyl-16-dimethylphthalene Cadalene 7-Isopropyl-14-dimethylazulene Guaiazulene;14-Dimethyl-7-isopropylazule ~~ne
Metabolite88	200.1017934_30.08666059	gamma-Glutamyl-beta-aminopropiononitrile gamma-Glutamyl-beta-aminopropiononitrile ~~;gamma-Glutamyl-3-aminopropiononitrile
Metabolite89	201.0907649_270.1012906	4-(Benzyloxyl)phenol;Monobenzone;4-(Phen ~~ylmethoxy)phenol (3-Phenoxyphenyl)methanol;3-Phenoxybenze ~~nemethanol (2R3E11E)-trideca-311-dien-579-triyne-12 ~~-diol ()-(3S4R)-cis-34-Dihydroxy-34-dihydroflu ~~orene Safynol;(2R3E11E)-311-Tridecadiene-579-t ~~riyne-12-diol
Metabolite90	201.1635832_23.32668369	(S)-gamma-Calacorene beta-Calacorene alpha-Corocalene 34-Dihydrocadalene Isolongifolene 45910-dehydro-
Metabolite91	202.1188087_44.48899796	Heteropyrithiamine;1-(4-Amino-2-methylpy ~~rimidin-5-yl)methylpyridinium
Metabolite92	203.0856158_274.4400499	Pyrene Fluoranthene

ID	MZ_Time	Name
Metabolite93	203.1394105_38.39122048	Alanyl-Leucine
		Alanyl-Isoleucine
		Isoleucyl-Alanine
		Leucyl-Alanine
Metabolite94	203.143031_253.9576079	Feniculin
		Dictagymnin
		2-Pentyl-3-phenyl-2-propel
		()-Anisoxide
		alpha-Amylcinmaldehyde;alpha-Pentylcin ∼∼maldehyde
Metabolite95	205.1258189_35.93039371	hexyl 3-sulfanylbutanoate
		Hexyl 3-mercaptobutanoate
		(S)-3-Mercaptohexyl butyrate
		3-Mercaptohexyl butyrate
Metabolite96	208.0556603_58.25423421	Benzthiazuron
Metabolite97	208.1189012_16.54244465	N-Ethylglycocyamine
		Miglitol
		2-Deoxy-2-dimethylamino-alpha-D-Glucose
Metabolite98	209.0159941_42.98294885	(1S3R)-3-(22-Dichloroethenyl)-22-dimethy ∼∼lcyclopropanecarboxylate
		Lactyltrimethylammonium betaine
Metabolite99	209.059471_223.1899111	Cysteinyl-Serine
		910-Phenthroquinone;910-Phenthrenedi ∼∼one;Phenthraquinone;Phenthrenequinon ∼∼e
		Serinyl-Cysteine
		Anthraquinone;910-Anthraquinone
		4-(12-Epoxyethyl)-89-epoxy-enediyne
Metabolite100	210.1124677_244.9429312	Propoxur;Aprocarb;2-Isopropoxyphenyl N-m ∼∼ethylcarbamate
		p-Lactophenetide;4-Ethoxylactanilide;Lac ∼∼tylphenetidin
		Anhalamine;N-Demethylanhalidine
		Tyr-OEt
Metabolite101	211.1439169_27.42303071	LL-Cyclo(leucylprolyl)
Metabolite102	212.0428642_98.90626461	Phosphocreatine;N-Phosphocreatine;Creati ∼∼ne phosphate
		Phosphocreatine
Metabolite103	212.1472767_28.46414003	2-Heptyl-45-dimethylthiazole
		4-Ethyl-2-heptylthiazole
Metabolite104	213.0150977_65.35879531	2-Phosphinomethylmalate;2-Phosphinomethy ∼∼lmalic acid
		(4S)-4-Hydroxy-5-phosphonooxypentane-23- ∼∼dione;Phospho-DPD;P-DPD
		3-Hydroxy-5-phosphonooxypentane-24-dione ∼∼;3-Hydroxy-24-pentadione-5-phosphate;P-H ∼∼PD

ID	MZ_Time	Name
Metabolite105	213.1486442_272.9265085	(1R2S)-3-oxo-2-pentyl-cyclopentaneacetic ~~acid (1R2S3S)-3-hydroxy-2-(2Z)-pent-2-en-1-yl ~~cyclopentylacetic acid (1S2S)-3-oxo-2-pentylcyclopentylacetic a ~~cid 8-oxo-37-Dimethyl-6E-octenyl acetate 3-Ethenyl-4-hydroxy-25-dimethylhex-5-en- ~~2-yl acetate
Metabolite106	214.2166348_273.5124209	Tridecamide
Metabolite107	215.1388438_55.86631735	Prolyl-Valine Dethiobiotin;Desthiobiotin Dethiobiotin Valyl-Proline
Metabolite108	216.1596843_276.6806558	Ethyl 3-(N-butylacetamido)propiote;Eth ~~yl butylacetylaminopropiote N-Nonoylglycine
Metabolite109	217.1193567_23.55714097	gamma-Glutamyl-gamma-aminobutyraldehyde Threoninyl-Proline Prolyl-Threonine 10E12E-tetradecadiene-46-diynoic acid Sakacin P
Metabolite110	220.1010666_64.31336935	N(omega)-Nitro-L-arginine;N(G)-Nitro-L-a ~~rginine
Metabolite111	221.0767318_89.74719913	Dehydroxyzyleuton Brassitin L-beta-aspartyl-L-serine Carbamorph Aspartyl-Serine
Metabolite112	221.1899396_243.0377349	(5R)-Albaflavenol 26-Di-tert-butyl-4-methylphenol 3711-trimethyldodeca-2Z6E10-triel
Metabolite113	222.0059001_47.27084613	Fluoromidine
Metabolite114	223.0634848_23.9757886	224466-Hexamethyl-135-trithiane (E)-1-Propenyl 1-(propylthio)propyl disu ~~lfide 2-(3-Methylthio)propylmalic acid;2-(3-Me ~~thylthio)propylmalate 3-(3-Methylthio)propylmalic acid;3-(3-Me ~~thylthio)propylmalate 246-Triethyl-135-trithiane
Metabolite115	226.1449423_22.99120823	N-Methylmescaline Prelterol Terbutaline
Metabolite116	228.1593905_263.2521089	N-Octanoyl-L-homoserine lactone;C8-HSL;N ~~-(3S)-Tetrahydro-2-oxo-3-furanyloctami ~~de

ID	MZ_Time	Name
Metabolite117	230.1145763_22.43679091	Propazine;2-Chloro-46-bis(isopropylamino ~~)-135-triazine
		Terbuthylazine
		Asparaginyl-Proline
		Trietazine
		Prolyl-Asparagine
Metabolite118	233.0871787_63.28205961	Fluometuron
		Parafluron
Metabolite119	235.2055533_24.36889468	4611-hexadecatriel
		26-Di-tert-butyl-4-ethylphenol
		13Z-Hexadecen-11-yl
		7Z11Z13E-Hexadecatriel
		4E6E11Z-Hexadecatriel
Metabolite120	236.1646733_147.1297389	Stovaine;Amylocaine
		NO-Didesmethyltramadol
Metabolite121	236.1724812_172.760009	Procaimide
Metabolite122	237.0873371_43.84481292	L-Formylkynurenine
		NN-Dihydroxy-L-tryptophan
		Serinyl-Methionine
		Methionyl-Serine
		N-Formyl-D-kynurenine
Metabolite123	237.0969327_160.3952573	Didanosine
		Purine deoxyribonucleoside;Purine 2-deox ~~yribonucleoside
Metabolite124	238.9994352_202.1625924	2-Hydroxy-35-dichlorobiphenyl;35-Dichlor ~~o-2-hydroxybiphenyl;24-Dichloro-6-phenyl ~~phenol
		26-Dichloro-4-biphenylol;26-Dichloro-(11 ~~-biphenyl)-4-ol
		4-Hydroxy-35-dichlorobiphenyl;35-Dichlor ~~o-4-hydroxybiphenyl
		25-Dichloro-2-biphenylol;25-Dichloro-2-h ~~ydroxybiphenyl
		25-Dichloro-4-biphenylol;25-Dichloro-(11 ~~-biphenyl)-4-ol
Metabolite125	240.0746908_46.54104939	9-Carboxymethoxymethylguanine
Metabolite126	241.0491872_148.2790569	Dantron
		Alizarin;Dihydroxyanthraquinone;12-Dihyd ~~roxyanthraquinone;Dihydroxy-910-anthrace ~~nedione
		Danthron;Chrysazin;18-Dihydroxyanthraqui ~~none
		Xanthopurpurin
		Anthrafravic acid;Anthraflavin;26-Dihydr ~~oxyanthraquinone
Metabolite127	243.1591096_283.5541932	(3S5R6R7E)-356-Trihydroxy-7-megastigmen- ~~9-one
		2-Carboxy-4-dodecanolide

ID	MZ_Time	Name
Metabolite128	245.1857664_29.38673179	N-(6-Aminohexanoyl)-6-aminohexanoate
		6-(6-aminohexamido)hexanoic acid
		Isoleucyl-Leucine
		Leucyl-leucine
		Leucyl-Leucine
Metabolite129	246.1626131_31.54645758	Desmethyl frovatriptan
Metabolite130	247.0286384_56.42924568	Busulfan
Metabolite131	248.1569085_169.6416897	Threoninyl-Lysine
		Lysyl-Threonine
Metabolite132	248.1643711_199.634382	Ketobemidone
		beta-Eucaine
		Meperidine
		Meperidine;Pethidine
Metabolite133	252.997131_19.18085603	Cartilagineal
Metabolite134	253.2157075_24.52115516	7Z10Z-hexadecadienoic acid
		9E12E-Tetradecadienyl acetate
		8Z10E-Tetradecadienyl acetate
		3-oxo-9Z-Hexadecel
		Hydnocarpic acid
Metabolite135	253.2161429_223.4999538	10Z12E-Tetradecadienyl acetate
		(Z)-7-Hexadecen-116-olide
		7Z10Z-Hexadecadienoic acid
		10-hexadecynoic acid
		10Z12E-hexadecadienoic acid
Metabolite136	253.2161551_280.4516919	10E12E-Tetradecadienyl acetate
		9E11Z-Tetradecadienyl acetate
		11-Methyl-9Z12-tridecadienyl acetate
		7E10E-hexadecadienoic acid
		9Z12Z-hexadecadienoic acid
Metabolite137	256.1459846_243.3091435	Diethylenetriamine crosslinked with epic
		∼∼hlorohydrin
Metabolite138	257.1469329_57.59100644	Pulcherriminic acid;25-Dihydroxy-36-bis(
		∼∼2-methylpropyl)pyrazine bis-N-oxide
Metabolite139	260.1140991_119.4960468	Proacacipetalin;3-Butenenitrile 2-(beta-
		∼∼D-glucopyranosyloxy)-3-methyl- (S)-
		Fumarycarnitine
		(3S)-3-(2E)-3-carboxyprop-2-enoyloxy-4-(
		∼∼trimethylazaniumyl)butanoate
		Osmaronin
Metabolite140	262.1652371_36.22342058	3-(3-hydroxy-3-methylbutanoyl)oxy-4-(tri
		∼∼methylazaniumyl)butanoate
		3-hydroxy-3-isovaleryloxy-4-(trimethylam
		∼∼monio)butyrate
Metabolite141	263.073591_60.34878772	Carbadox
		Furano23:67aurone
Metabolite142	263.0877348_86.65191513	-L-Glutamyl-L-aspartic acid
		L-beta-aspartyl-L-glutamic acid
		Ng-L-Glutamyl-L-aspartic acid
		Dorsteniol
		(S)-Rutaretin

ID	MZ_Time	Name
Metabolite143	263.1627782_38.08065156	3-Hydroxy-geranylhydroquinone
Metabolite144	263.1640202_245.6969479	3-Hydroxy-geranylhydroquinone
Metabolite145	264.1959355_242.2537927	Hydroxy-alpha-sanshool
		Dendrobine
		Desvenlafaxine
		N-Desmethylvenlafaxine
		O-Desmethylvenlafaxine
Metabolite146	265.0812206_41.93964821	11-bromo-undecanoic acid
Metabolite147	265.1181341_28.9415658	Alpha-N-Phenylacetyl-L-glutamine
		Acetyl-N-formyl-5-methoxykynuremine
		di-Hydroxymelatonin
		Phenylacetylglutamine;alpha-N-Phenylacet
		∼∼yl-L-glutamine;N2-(2-Phenylacetyl)-L-glu
		∼∼tamine
		Formyl-N-acetyl-5-methoxykynuremine
Metabolite148	266.1598092_49.8457619	Esprocarb
Metabolite149	267.0587683_153.8231895	Methoxybrassinin
		4-Methoxybrassinin
Metabolite150	267.1719106_24.38465976	Tributyl phosphate;TBP
		(3xi6E)-17-Diphenyl-6-hepten-3-ol
		Practolol
		Atenolol
Metabolite151	267.1741406_271.5048621	Atenolol
		(3xi6E)-17-Diphenyl-6-hepten-3-ol
		Practolol
		Tributyl phosphate;TBP
Metabolite152	268.1025109_138.6489943	Zidovudine;Azidothymidine;3-Azido-3-deox
		∼∼ythymidine;AZT
		Adenosine
		Deoxyguanosine
		Miserotoxin
Metabolite153	268.1394681_29.98248278	Voglibose
Metabolite154	268.1473339_262.9479803	Ergine;Lysergamide
Metabolite155	268.1482513_35.70628463	Ergine;Lysergamide
Metabolite156	268.2271515_158.0892218	Allopumiliotoxin 267A
Metabolite157	269.1748072_282.0032101	1-(3-Furanyl)-67-dihydroxy-48-dimethyl-1
		∼∼-nonone
		Bisacurone epoxide
		31112-Trihydroxy-1(10)-spirovetiven-2-on
		∼∼e
		Acoric acid
		N-(p-Hydroxyphenethyl)actinidine
Metabolite158	271.1903216_280.4492261	Ethylene brassylate
		(10S)-Juvenile hormone III acid diol
Metabolite159	271.1905111_149.8910105	(10S)-Juvenile hormone III acid diol
		Ethylene brassylate
Metabolite160	272.053742_163.3350026	35-Dinitro-L-tyrosine
Metabolite161	273.0392843_241.8811386	5-(Hydroxyphenyl)-gamma-valerolactone-O-
		∼∼sulphate
		2-epi-5-epi-Valiolone 7-phosphate
		5-epi-Valiolone 7-phosphate

ID	MZ_Time	Name
Metabolite162	273.1846629_247.9658111	Estradiol-17alpha;17alpha-Estradiol
		Estra-135(10)-triene-217beta-diol;2-Hydr
		~~oxy-3-deoxyestradiol
		19-Norandrostenedione;delta4-Estrene-317
		~~-dione
		17a-Estradiol
		Lilyl phenylacetate
Metabolite163	277.1798116_273.6542266	Paquinquecol 2
		Sugeonyl acetate
		Onchidal;E()-2-(E)-2-Acetoxyethenyl-4-(2
		~~2-dimethyl-6-methylenecyclohexyl)-2-bute
		~~l
		8-Shogaol
		Paquinquecol 7
Metabolite164	279.1590198_263.8489868	Alpha-CEHC
		Monoethylhexyl phthalic acid
		Diisobutyl phthalate;DIBP
		Dibutyl phthalate
Metabolite165	280.1542979_29.28158682	Metalaxyl-M
		Metalaxyl
		()-Metalaxyl
Metabolite166	280.2634847_25.19325191	9Z12Z-octadecadiemide
Metabolite167	281.1381942_23.71856619	(1beta4alpha5alpha6beta8alpha10b)-110:45
		~~-Diepoxy-6-hydroxy-7(11)-germacren-128-o
		~~lide
		Artabsinolide A
		()-67-epoxy-5-hydroxy-4(15)-hirusten-12-
		~~oic acid
		Nigellic acid
		Vulgarolide
Metabolite168	281.1748318_275.226904	6b-Hydroxy-8a-methoxy-7(11)-eremophilen-
		~~128-olide
		1-(34-Dihydroxyphenyl)-5-hydroxy-3-decan
		~~one
		3b-Hydroxy-6b-methoxy-7(11)-eremophilen-
		~~128a-olide
		Prehumulinic acid
		34-Epoxy-6-methylcyclohexylmethyl-34-epo
		~~xy-6-methylcyclo-hexanecarboxylate
Metabolite169	281.2110167_225.4472108	12-hydroxy-5810-heptadecatrienoic acid
		Juvenile hormone I acid;(2E6E10R11S)-101
		~~1-Epoxy-7-ethyl-311-dimethyl-26-tridecad
		~~ienoate
		heptadeca-46-diyne-3910-triol
		Dihydropaxacol
		methyl (2E6E10R11S)-1011-epoxy-3711-trim
		~~ethyltrideca-26-dienoate
Metabolite170	282.2423582_18.33577261	Methyl 15-cyanopentadecanoate
Metabolite171	282.2511006_230.830527	Petroselinic acid

ID	MZ_Time	Name
Metabolite172	283.2631607_281.3995544	2-methyl-16-heptadecenoic acid
		13E-octadecenoic acid
		11Z-octadecenoic acid
		2Z-octadecenoic acid
		5Z-Hexadecenyl acetate
Metabolite173	284.1275894_25.01886544	N-2-Hydroxy-2-(4-hydroxyphenyl)ethylcinn ~~amide
		Axagoreine
		N-(p-Hydroxyphenyl)ethyl p-hydroxycinm ~~ide
		2-Methyl(3-phenylpropanoyl)aminobenzoic ~~acid
		Morphinone
Metabolite174	285.1190242_140.0449253	Coformycin
Metabolite175	285.2061008_183.1038283	(10S)-Juvenile hormone III diol
Metabolite176	286.1437304_24.51808299	Apohyoscine
		Hydromorphone
		Norcodeine;N-Desmethylcodeine
		HC Blue No 2;22-4-(2-Hydroxyethyl)amino- ~~3-nitrophenyliminobis-ethanol
		Piperine;N-(EE)-Piperoylpiperidine;1-Pip ~~eroyl-piperidine
Metabolite177	286.2007906_29.40836124	2-Octenoylcarnitine
		(3S)-3-(2E)-oct-2-enoyloxy-4-(trimethyla ~~zaniumyl)butanoate
		3-(2E)-oct-2-enoyloxy-4-(trimethylazaniu ~~myl)butanoate
Metabolite178	286.3099289_23.43766505	1-deoxy-sphinganine
Metabolite179	288.0038621_277.6878914	5-(Aminomethyl)furan-3-ylmethyl diphosph ~~ate;5-(Aminomethyl)-3-furanmethanol diph ~~osphate
Metabolite180	291.0121846_280.8545666	5-(4-Acetoxy-3-oxo-1-butynyl)-22-bithiop ~~hene
		Furocaespitane
Metabolite181	293.0343078_56.07587177	2-Hydroxychlorpropamide
		5-(3-Hydroxy-4-acetoxybut-1-ynyl)-22-bit ~~hiophene
		Citreovirone
		3-Hydroxychlorpropamide
Metabolite182	295.1291332_40.71645416	Aspartame
		Glutamylphenylalanine
		L-gamma-Glutamyl-beta-phenyl-beta-L-alan ~~ine
		4-tert-Butyl-26-dimethyl-35-dinitroaceto ~~phenone
Metabolite183	296.2580789_20.40639836	sphinga-4E8E10E-trienine
Metabolite184	297.0799678_59.69647821	7-Methoxy-34-methylenedioxyflavone
		4-Methoxy-78-methylenedioxyisoflavone
		39-Dimethylcoumestan
		Aspulvinone E;(5Z)-4-Hydroxy-3-(4-hydrox ~~yphenyl)-5-(4-hydroxyphenyl)methylene-2(~~5H)-furanone

ID	MZ_Time	Name
Metabolite185	298.143644_31.59066217	3-Hydroxyestra-135(10)7-tetraene-1617-di ~~one 16-oxime
		Glaziovine
		(-)-Apoglaziovine
		Tuduranine
		Codeinone;(5alpha)-78-Didehydro-45-epoxy ~~-3-methoxy-17-methylmorphin-6-one
Metabolite186	298.2735433_24.11989046	5S-(5S-hydroxyoctyl)-2S-methyldecahydroq ~~uinolin-3R-ol
		3-Ketosphingosine
		3-keto-sphing-4-enine
		sphinga-4E8Z-dienine
		2S-amino-octadeca-4E6E-diene-13R-diol
Metabolite187	299.147916_23.69601636	Neoilludin A
		Toxin T2 tetrol
		Sesamex
		37815-Scirpenetetrol
Metabolite188	299.22163_281.1824008	8E-Heptadecenedioic acid
		Plakortic acid
Metabolite189	301.1800287_278.6096092	3-oxo-1317-secoandrosta-14-dieno-1713alp ~~ha-lactone
		9alpha-Hydroxyandrosta-14-diene-317-dion ~~e
		11alpha-Hydroxyandrosta-14-diene-317-dio ~~ne
		3-Hydroxy-910-secoandrosta-135(10)-trien ~~e-917-dione;Secophenol
		19-Oxoandrost-4-ene-317-dione
Metabolite190	303.2317902_24.22334679	Mibolerone;17-beta-Hydroxy-7-alpha17-dim ~~ethylestr-4-en-3-one
		ent-8(17)13(16)14-Labdatrien-18-oic acid
		813-Abietadien-18-oic acid
		(13S)-pimara-715-dien-18-oic acid
Metabolite191	305.0696816_67.85483903	cis-Dihydroquercetin
		57345-Pentahydroxyflavanone
		Pratenol B
Metabolite192	305.2115078_38.84250061	17beta-hydroxy-5alpha-androstan-13-dione
		17beta-Hydroxy-5alpha-androstan-36-dione ~~;6-Ketodihydrotestosterone
		10-Acetoxy-8-heptadecene-46-diyn-3-ol
Metabolite193	307.2627952_24.38158879	5Z8Z14Z-eicosatrienoic acid
		2alpha-Methyl-5alpha-androstane-3beta17b ~~eta-diol
		18-methyl-8Z11Z14Z-nodecatrienoic acid
		17alpha-Methyl-5alpha-androstane-3alpha1 ~~7beta-diol
		(8Z11Z14Z)-Icosatrienoic acid;Dihomo-gam ~~ma-linolenic acid;(ZZZ)-81114-Eicosatrie ~~noic acid;(ZZZ)-81114-Icosatrienoic acid ~~;(ZZZ)-81114-Eicosatrienoate;(ZZZ)-81114 ~~-Icosatrienoate;81114-Eicosatrienoate;81 ~~114-Icosatrienoate

ID	MZ_Time	Name
Metabolite194	309.2266964_27.13280805	123-Tris(1-ethoxyethoxy)propane
Metabolite195	311.1464756_113.2350793	Mannopine
Metabolite196	311.1848731_23.91935054	Valdiate
		Botrydial
		methyl 8-2-(2-formyl-vinyl)-3-hydroxy-5-~~oxo-cyclopentyl-octanoate
		3-Hydroxy-68-dimethoxy-7(11)-eremophilen~~-128-olide
Metabolite197	314.2323616_25.18022611	3-(4Z)-dec-4-enoyloxy-4-(trimethylazaniu~~myl)butanoate
		3-dec-4-enoyloxy-4-(trimethylammonio)but~~yrate
		3-(dec-9-enoyloxy)-4-(trimethylazaniumyl~~)butanoate
		9-Decenoylcarnitine
Metabolite198	317.0834007_115.7389866	cis-4-(7-Hydroxtpyren-8-yl)-2-oxobut-3-e~~noate
		45-Chrysenedicarboxylate
		cis-4-(8-Hydroxypyren-7-yl)-2-oxobut-3-e~~noate
		Cysteinyldopa;5-S-Cysteinyl-DOPA
		2-(4-Chlorophenyl)-3-phenyl-3-(2-pyridin~~yl)acrylonitrile
Metabolite199	320.0752775_49.2637843	N-Gluconyl ethanolamine phosphate
Metabolite200	323.0559865_188.6266868	77-Dihydroxy-68-bicoumarin
Metabolite201	323.1619415_44.80944076	Mequitazine
Metabolite202	324.2890745_23.24693604	N-(9Z12Z-octadecadienoyl)-ethanolamine
		Linoleoyl ethanolamide
Metabolite203	324.3264413_23.46574137	N-(14-Methylhexadecanoyl)pyrrolidine
Metabolite204	325.0356652_33.70423646	Dorzolamide
		Chlorobenzilate;Ethyl-44-dichlorobenzila~~te;Ethyl 2-hydroxy-22-bis(4-chlorophenyl~~)acetate
		5-O-(1-Carboxyvinyl)-3-phosphoshikimate;~~O5-(1-Carboxyvinyl)-3-phosphoshikimate
Metabolite205	325.0362277_183.2206842	Dorzolamide
		5-O-(1-Carboxyvinyl)-3-phosphoshikimate;~~O5-(1-Carboxyvinyl)-3-phosphoshikimate
		Chlorobenzilate;Ethyl-44-dichlorobenzila~~te;Ethyl 2-hydroxy-22-bis(4-chlorophenyl~~)acetate
Metabolite206	325.2002549_271.6737314	Lactapiperanol D
		12-oxo-1418-dihydroxy-9Z13E15Z-octadecat~~rienoic acid
		1418-dihydroxy-12-oxo-9E13Z15E-octadecat~~rienoic acid
		23-dinor-9S15S-dihydroxy-11-oxo-5Z13E-pr~~ostadienoic acid
		Cibaric acid

ID	MZ_Time	Name
Metabolite207	325.2373418_270.0463006	1-Acetoxy-2-hydroxy-16-heptadecyn-4-one
		Dihydromocolin L acid
		Decylubiquinol;6-Decylubiquinol;2-Decyl- ~~56-dimethoxy-3-methyl-14-benzenediol
		2-hydroxy-4-oxoheptadec-16-yn-1-yl aceta ~~te
		methyl 15-hydroperoxy-9Z12Z16E-octadecat ~~rienoate
Metabolite208	325.2739218_24.83092993	(Z)-15-Oxo-11-eicosenoic acid
		(13R14R)-7-Labdene-131415-triol
		14-hydroxy-11Z17Z-eicosadienoic acid
		(13R14R)-8-Labdene-131415-triol
		11R-hydroxy-12E14Z-eicosadienoic acid
Metabolite209	326.3052063_225.9404628	N-Oleoylethanolamine
		N-(9Z-octadecenoyl)-ethanolamine
		Oleoylethanolamide;OEA
Metabolite210	327.2529148_282.4535347	1-heptadecene-23R-dicarboxylic acid
		33-Difluoro-17-methyl-5alpha-androstan-1 ~~7beta-ol
		Avocadyne 1-acetate
		1-Acetoxy-2-hydroxy-16-heptadecen-4-one
		Avocadyne 4-acetate
Metabolite211	328.3204155_23.67289039	NN-dimethylsphing-4-enine
		N-(9Z-octadecenoyl)-ethanolamine(d2)
		N-(Octadecanoyl)-ethanolamine
		NN-Dimethylsphing-4-enine
		NN-Dimethylsphingosine
Metabolite212	329.2492703_24.23880574	(4Z7Z10Z13Z16Z19Z)-Docosahexaenoic acid; ~~4710131619-Docosahexaenoic acid;Docosahe ~~xaenoic acid;Docosahexaenoate
		101316-Docosatriynoic acid
		4Z7Z10Z13Z16Z19Z-docosahexaenoic acid
		3915-Docosatriynoic acid
		Retinol acetate
Metabolite213	333.2025695_53.23398441	7beta12alpha-Dihydroxykaurenolide
		Gibberellin A12
		Marrubiin
		Gibberellin A53 aldehyde
		4-Deoxycohumulone
Metabolite214	334.0515155_77.97921766	Carpropamid
Metabolite215	337.273374_23.656561	3-Methyl-5-pentyl-2-furanundecanoic acid
		Isolinderanolide
		5beta-Pregne-3alpha17alpha20alpha-trio ~~l
		Pregnetriol
		2alpha-(Hydroxymethyl)-17-methyl-5alpha- ~~androstane-3beta17beta-diol
Metabolite216	339.0513248_61.08613749	Chloropropylate
		UK-47265
		Versicolorin A

ID	MZ_Time	Name
Metabolite217	341.2329607_274.1815104	3alpha-Hydroxy-35-dihydromocolin L aci ~~d
Metabolite218	343.0468905_75.60017496	Triazolam
Metabolite219	343.267157_25.87009427	5Z8Z11Z14Z17Z20Z-tricosahexaenoic acid
Metabolite220	349.1827795_49.88852912	(1S2S4S)-18-Epoxy-p-menthane-27-diol 2-O ~~-b-D-glucoside
		cis-10-Hydroxylilyl oxide 7-glucoside
		Schizonepetoside E
		(1S2S4R)-p-Menth-8-ene-1210-triol 2-gluc ~~oside
		Nepetariaside
Metabolite221	351.0141535_57.38392432	Apigenin 7-sulfate
Metabolite222	352.1024216_46.39868252	Indole-3-acetic-acid-O-glucuronide
Metabolite223	354.2997206_23.31851269	N-(9Z-octadecenoyl)-alanine
		N-hexadecanoyl-proline
Metabolite224	355.2839609_270.5369581	1-(9Z12Z-octadecadienoyl)-rac-glycerol
		MG(18:2(9Z12Z)0:00:0)
		Methyl acetyl ricinoleate
		1-methoxy-9S11R15S-trihydroxy-5Z13E-pros ~~tadiene
		MG(0:018:2(9Z12Z)0:0)
Metabolite225	356.0126967_188.9832074	2-Amino-78-dihydro-4-hydroxy-6-(diphosph ~~ooxymethyl)pteridine;2-Amino-4-hydroxy-6 ~~-hydroxymethyl-78-dihydropteridine dipho ~~sphate;78-Dihydropterin pyrophosphate
		3-Iodothyromine
		MC-5127
		Thiamphenicol
Metabolite226	359.037607_41.92676819	Triflumuron;Trifluron
Metabolite227	361.2005237_25.74329187	Aldosterone;11beta21-Dihydroxy-320-dioxo ~~-4-pregnen-18-al
		19-Oic-deoxycorticosterone
		7-Methylrosmanol
		11beta1721-trihydroxypreg-14-diene-320 ~~-dione
		11beta-Hydroxy-320-dioxopregn-4-en-21-oi ~~c acid
Metabolite228	362.1159299_25.41855461	3-Hydroxyomeprazole
		Omeprazole sulfone
		5-hydroxyesomeprazole
		Bezafibrate
		5-Hydroxyomeprazole
Metabolite229	370.0508529_70.51747626	Amidosulfuron
Metabolite230	370.2954109_24.37763721	trans-2-Tetradecenoylcarnitine
		3-(5Z)-tetradec-5-enoyloxy-4-(trimethyla ~~zaniumyl)butanoate
		cis-5-Tetradecenoylcarnitine
Metabolite231	373.314117_23.98063128	1-Phenyl-13-nodecanedione
		5-(1013-Nodecadienyl)-13-benzenediol

ID	MZ_Time	Name
Metabolite232	375.2147769_41.02995809	11beta1721-trihydroxy-6-methylpreg-14-~~diene-320-dione
		8-oxo-7S17S-dihydroxy-4Z9E11E13Z15E19Z-d~~ocosahexaenoic acid
		1112-Dimethylrosmanol
		11beta-Hydroxy-320-dioxopregn-4-en-21-oi~~c acid
		Methylprednisolone
Metabolite233	380.2555991_29.37400124	Sphingosine 1-phosphate
		Aurachin C
		Sphingosine 1-phosphate;Sphing-4-enine 1~~-phosphate;S1P
		Aurachin B
		Sphing-4-enine-1-phosphate
Metabolite234	383.330962_24.7926599	5alpha-cholesta-824-dien-3-one
		(4E6Z8Z)-(1R)-4-methyl-910-seco-4(5)6824~~-cholestatetraen-1-ol
		7-Dehydrodesmosterol;Cholesta-5724-trien~~e-3beta-ol
		cholest-5-en-23-yn-3beta-ol
		Cholesta-14-dien-3-one
Metabolite235	384.3098059_24.07826702	N-(9Z-octadecenoyl)-threonine
		2-(5Z8Z11Z14Z-eicosatetraenoyl)-sn-glyce~~rol-d5
Metabolite236	384.3197264_242.3193768	2-(5Z8Z11Z14Z-eicosatetraenoyl)-sn-glyce~~rol-d5
Metabolite237	388.2543973_276.8151704	N-(9Z12Z-octadecadienoyl)-taurine
Metabolite238	388.3062948_24.42117584	3-(2-hydroxytetradecanoyl)oxy-4-(trimeth~~ylazaniumyl)butanoate
		3-(3-hydroxytetradecanoyl)oxy-4-(trimeth~~ylazaniumyl)butanoate
		2-Hydroxymyristoylcarnitine

One identified metabolites usually have multiple matches. For a metabolite, each row under column "Name" represents a match unless the row starts with "∼ ∼" which means the name expands to the next row.

Table 3: **Nodes for Control Subjects**

Node	Cluster	Name	centrality
X10	1	S-Aa	0.995
X11	1	Blautia	0.998
X12	1	Veillonella	0.995
X13	1	Roseburia	0.997
X14	1	Varibaculum	0.997
X15	1	Fusobacterium	0.945
X16	1	Escherichia/Shigella	0.997
X17	1	Fusicatenibacter	0.879
X18	1	ChristensenellaceaeR-Group	0.986
X2	1	Ezakiella	0.995
X20	1	Lawsonella	0.965
X21	1	LachnospiraceaeNKAgroup	0.987
X23	1	Dorea	0.998
X24	1	Tyzzerella	0.889
X26	1	Mogibacterium	0.987
X28	1	Ruminococcus	0.637
X29	1	Coprococcus	0.657
X3	1	Campylobacter	0.995
X30	1	LachnospiraceaeUCG-	0.971
X31	1	Negativibacillus	0.998
X33	1	Lachnoclostridium	0.995
X36	1	Christensenellaceae	0.996
X37	1	LachnospiraceaeNDgroup	0.997
X38	1	Catenibacterium	0.898
X39	1	ClostridialesvadinBBgroup	0.995
X4	1	Faecalibacterium	0.995
X40	1	Paraprevotella	0.995
X41	1	Mobiluncus	0.903
X42	1	FamilyXI	0.997
X43	1	Rikenella	0.995
X44	1	Jonquetella	0.994
X45	1	Flavonifractor	0.903
X46	1	Muribaculaceae	0.995
X48	1	Intestinimonas	0.996
X49	1	GCA-	0.998
X5	1	Peptoniphilus	0.983
X50	1	UC–E	0.957
X51	1	Barnesiella	0.536
X58	1	Romboutsia	0.986
X60	1	Brevibacterium	0.928
X61	1	Gardnerella	0.939
X63	1	Anaeroglobus	0.981
X66	1	Eisenbergiella	0.987
X68	1	Parvimonas	0.992
X7	1	Parasutterella	0.996
X73	1	Anaerofilum	0.987
X75	1	DTU	1
X76	1	Streptobacillus	0.996
X77	1	Sellimonas	0.806
X78	1	Helcococcus	0.21

Node	Cluster	Name	centrality
X79	1	Arcanobacterium	0.995
X8	1	Alistipes	0.997
X81	1	Methanobrevibacter	0.999
X82	1	Izimaplasmatales	0.991
X83	1	Coprobacter	0.868
X84	1	Faecalitalea	0.978
X87	1	Victivallis	0.997
X88	1	Dermabacter	0.142
X9	1	Phascolarctobacterium	0.996
X90	1	Desulfovibrionaceae	0.995
X91	1	Bacteroidia	0.89
X92	1	Turicibacter	0.99
X93	1	Puniceicoccaceae	0.996
Y18	1	il10_stool	0
Y24	1	il8_stool	0
Z1026	1	250.1104715_76.2262946	0
Z1116	1	268.7733419_53.70521998	0.765
Z1357	1	704.9154417_59.82256431	0
Z1393	1	114.8930105_48.86349712	0.79
Z1431	1	163.0027707_259.2928112	0
Z1479	1	203.1394105_38.39122048	0
Z1600	1	101.0789783_31.12824974	0.711
Z1689	1	120.9649122_25.73386363	0.879
Z1703	1	225.0064645_237.6846613	0
Z1706	1	272.997274_161.5683001	0
Z179	1	122.5592133_70.64947873	0.653
Z1813	1	230.1145763_22.43679091	0
Z2016	1	296.2580789_20.40639836	0.598
Z2064	1	324.3264413_23.46574137	0
Z2120	1	278.9103495_223.521956	0
Z2210	1	368.6929478_53.05598228	0
Z2236	1	193.0275845_67.29696892	0
Z2274	1	93.02403583_235.9278593	0
Z2280	1	162.0351851_62.60806268	0
Z2297	1	166.9786646_221.7283288	0
Z2323	1	183.9450208_231.976564	0
Z2348	1	136.0554926_158.5345311	0.762
Z2386	1	168.9489231_44.81085701	0.678
Z2389	1	899.2612722_90.3761387	0.787
Z2396	1	221.9938015_276.896644	0
Z2409	1	340.8628965_250.9674069	0
Z2453	1	292.1147454_93.00318839	0
Z2519	1	237.0873371_43.84481292	0.623
Z2550	1	280.2634847_25.19325191	0.854
Z2652	1	343.0468905_75.60017496	0
Z2709	1	990.6605452_31.61099857	0
Z2768	1	126.9208298_46.45055576	0.734
Z2833	1	340.2121164_24.64036356	0
Z2899	1	398.9756106_248.961835	0
Z2986	1	414.0406892_232.9132528	0.636
Z3061	1	131.0339083_66.24304779	0
Z3080	1	281.9932505_61.20245473	0

Node	Cluster	Name	centrality
Z3105	1	445.9937969_210.7849539	0
Z3146	1	100.0756415_33.22355974	0.706
Z3148	1	887.5643519_33.2466793	0
Z3157	1	912.7728297_57.55151977	0
Z3165	1	538.7713275_51.56546186	0.651
Z3215	1	279.1590198_263.8489868	0.679
Z3222	1	324.2355902_24.75914536	0
Z3263	1	120.9650287_290.5785806	0
Z333	1	405.0473968_102.6649708	0.798
Z3340	1	123.0553669_273.0350179	0
Z3411	1	186.9227892_217.4884614	0
Z3462	1	264.1959355_242.2537927	0
Z3495	1	147.0441826_250.7399794	0.834
Z3585	1	149.0636146_67.62618086	0
Z3594	1	986.4062282_48.71458208	0
Z3615	1	130.0498701_77.00001118	0.862
Z3656	1	94.52080231_247.0867375	0
Z3691	1	378.2396085_29.88098184	0
Z3708	1	478.7544361_46.73237716	0
Z3753	1	344.0141539_282.1473699	0
Z3757	1	776.5911355_49.07582222	0.787
Z3799	1	912.2327324_51.59295249	0
Z3848	1	988.4046918_48.76131449	0
Z3867	1	100.1121195_267.3263044	0.883
Z3870	1	210.1489822_268.9105086	0
Z3894	1	419.7915953_53.7643684	0
Z3921	1	314.2323616_25.18022611	0.734
Z3929	1	592.538197_48.92282976	0
Z3982	1	380.2555991_29.37400124	0
Z3983	1	416.8018319_47.79615456	0
Z4053	1	525.0169181_233.4096206	0
Z4061	1	266.9382433_273.0953446	0
Z4091	1	210.1124677_244.9429312	0
Z4104	1	410.6764515_49.85740218	0
Z4133	1	123.9279629_45.77709142	0.63
Z4247	1	367.2674171_24.27414537	0.753
Z4262	1	530.7690268_49.49463226	0
Z4265	1	382.9265802_270.0240707	0
Z4290	1	299.147916_23.69601636	0
Z4329	1	184.0686197_29.18306242	0
Z4358	1	354.2482441_26.54116245	0
Z4373	1	324.2890745_23.24693604	0
Z4377	1	243.1591096_283.5541932	0
Z4394	1	942.3315593_48.89904668	0
Z4414	1	120.0444951_275.9107179	0
Z4487	1	356.2637783_26.74976422	0
Z4496	1	215.179157_146.5877319	0
Z4535	1	792.4253042_50.6271348	0
Z4541	1	780.3391151_50.87513542	0
Z4560	1	319.4682189_218.6856706	0

Node	Cluster	Name	centrality
Z4655	1	283.175178_278.9540313	0.889
Z4712	1	492.7317082_46.7595242	0
Z4722	1	349.1827795_49.88852912	0
Z4745	1	192.0243549_65.5576747	0
Z486	1	359.037607_41.92676819	0.784
Z4934	1	263.1640202_245.6969479	0
Z4981	1	333.2025695_53.23398441	0
Z4986	1	198.482996_289.607927	0.745
Z748	1	273.1846629_247.9658111	0
Z774	1	240.0746908_46.54104939	0.777
Z880	1	133.5357657_63.37980561	0
Z933	1	250.1111657_87.46153534	0
Z935	1	308.8805468_44.41939858	0.731
Y13	2	tnfa_plasma	0
Y17	2	il1b_stool	0
Y2	2	LBP_plasma	0
Y25	2	tnfa_stool	0
Y6	2	il10_plasma	0
Z1031	2	1242.410464_77.39366989	0.013
Z109	2	172.0186099_291.5802625	0
Z1154	2	261.0454749_61.001452	0
Z1292	2	573.1144304_275.4970137	0.023
Z1649	2	463.9682416_236.7780081	0
Z1678	2	447.1286969_63.49841042	0.013
Z1864	2	729.5759688_26.39328552	0
Z1913	2	323.0559865_188.6266868	0.006
Z229	2	572.9120113_275.6724415	0
Z2302	2	217.1193567_23.55714097	0
Z2432	2	161.1324143_25.00469172	0.021
Z2477	2	529.952784_236.7352295	0
Z2882	2	642.1072271_151.6957397	0.013
Z2978	2	239.0248209_170.8886	0
Z30	2	267.0587683_153.8231895	0
Z3337	2	340.0415441_66.54011089	0
Z3374	2	622.9680298_56.59629014	0.022
Z3505	2	458.8552407_213.5329444	0
Z3586	2	293.0343078_56.07587177	0.013
Z37	2	399.274687_238.8212711	0
X53	3	Sarcina	0.27
X55	3	Butyricimonas	0.016
X57	3	LachnospiraceaeACgroup	0.009
X59	3	Peptococcaceae	0.049
X62	3	Marvinbryantia	0.021
X64	3	Collinsella	0.009
X65	3	Veillonellaceae	0.28
X67	3	UBA	0.008
X71	3	Desulfovibrio	0.009
X72	3	Clostridiales	0.009
X85	3	Solobacterium	0.007
X86	3	Klebsiella	0.009

Node	Cluster	Name	centrality
X89	3	MollicutesRF	0.008
X94	3	Eubacterium	0.009
Y1	3	crp_plasma	0.001
Y16	3	ifng_stool	0.026
Y20	3	il13_stool	0.025
Y21	3	il2_stool	0.006
Y5	3	il1b_plasma	0.026
Y8	3	il13_plasma	0.013
Y9	3	il2_plasma	0
Z1024	3	631.6505326_47.91791433	0
Z1108	3	193.0683198_68.8963676	0.002
Z1112	3	267.1741406_271.5048621	0
Z112	3	388.342105_202.1368686	0
Z114	3	375.2147769_41.02995809	0
Z1171	3	310.2375039_22.90641697	0.011
Z1187	3	625.3953802_34.35925871	0
Z1268	3	573.781483_49.91472553	0
Z1345	3	248.1643711_199.634382	0
Z1351	3	167.0872736_53.86261152	0.002
Z1453	3	267.1719106_24.38465976	0
Z1556	3	489.820671_47.39086302	0
Z1629	3	486.5523581_46.43214499	0
Z1660	3	784.2802005_46.2095096	0
Z182	3	373.3217188_16.6549138	0.019
Z1828	3	513.7801101_49.36797531	0
Z1844	3	565.407932_22.26285656	0
Z1855	3	706.3544326_47.8789961	0
Z1950	3	238.9695864_74.8579365	0.003
Z1986	3	553.7238317_45.82948904	0
Z2008	3	567.7463693_47.69934757	0
Z2017	3	134.1175877_237.0782071	0.01
Z2031	3	568.167864_76.16009421	0.003
Z2040	3	429.8185086_45.98467468	0
Z2051	3	296.2296861_25.01734028	0.003
Z2118	3	640.4116631_46.71383402	0
Z2157	3	245.9476038_61.21355299	0
Z2164	3	632.4225745_48.22673156	0
Z2172	3	992.1015451_53.88251779	0
Z2176	3	665.4610862_23.27106959	0
Z2185	3	412.6215857_46.01185503	0
Z2202	3	770.303568_53.7245422	0
Z2251	3	257.1469329_57.59100644	0
Z2328	3	633.6493091_48.02008967	0
Z2406	3	549.409083_24.225831	0
Z2411	3	373.7622666_23.5216531	0.003
Z2412	3	276.0428459_60.58794386	0
Z2415	3	168.0813779_116.8544098	0
Z2445	3	946.1708173_46.70700997	0
Z2448	3	620.4423295_53.98930776	0
Z2468	3	666.9517439_62.02424307	0
Z2474	3	325.0362277_183.2206842	0.001

Node	Cluster	Name	centrality
Z3709	2	351.0141535_57.38392432	0.006
Z3759	2	263.0877348_86.65191513	0.006
Z4423	2	339.0513248_61.08613749	0
Z4490	2	827.9815367_59.66499464	0
Z4521	2	247.0286384_56.42924568	0
Z4533	2	200.043773_173.59216	0
Z4748	2	1169.87602_79.19535953	0
Z4776	2	106.5305737_221.7642466	0
Z4915	2	1043.701414_32.13886234	0
Z4979	2	415.3212036_24.0310311	0
Z4992	2	269.9944305_61.1314616	0
Z675	2	374.9404227_240.7293403	0
Z679	2	209.0159941_42.98294885	0.013
Z733	2	741.1960989_21.48020475	0.023
Z90	2	136.0010736_160.7714981	0
X19	3	Peptostreptococcus	0.009
X22	3	Sutterella	0.015
X25	3	Lachnospira	0.009
X32	3	Pyramidobacter	0.009
X34	3	Negativicoccus	0.021
X35	3	Mycoplasma	0.009
X47	3	Gemella	0.256
X52	3	Hungatella	0.009
Z2486	3	557.9442946_26.10071328	0
Z2487	3	284.0806206_101.5464744	0
Z2509	3	240.7657039_53.48793971	0
Z2527	3	426.9130106_45.15832343	0
Z2534	3	341.8631547_45.22397781	0
Z2557	3	134.0351129_44.79168398	0
Z2571	3	160.1154535_273.6074586	0
Z2572	3	629.6528806_45.84530522	0
Z2606	3	472.5758073_53.12604395	0
Z2638	3	325.2739218_24.83092993	0.004
Z2685	3	690.3809507_52.31292661	0
Z2716	3	776.556393_29.99264438	0
Z2724	3	414.6178921_48.6222331	0
Z2731	3	807.1891888_114.3291691	0
Z2744	3	446.3708317_22.84898132	0
Z2760	3	238.5112019_230.8993249	0
Z2769	3	638.4117542_45.43147663	0
Z2796	3	111.0804055_17.22343399	0
Z2803	3	728.408532_46.05562221	0
Z2807	3	480.7879808_50.27028212	0
Z281	3	553.0738976_74.44593109	0.001
Z2830	3	118.0541193_26.23313341	0
Z2930	3	515.644901_47.57453209	0
Z2956	3	332.9213099_43.66445022	0
Z2997	3	303.2317902_24.22334679	0.01
Z3018	3	406.8550282_45.6560953	0
Z3045	3	407.8561108_47.61232771	0
Z3097	3	145.1012001_273.3073104	0
Z3102	3	1044.706568_30.61476831	0

Node	Cluster	Name	centrality
Z3111	3	340.6854165_46.21624468	0
Z3185	3	499.7576548_47.3678274	0
Z3211	3	415.8875122_45.5099193	0
Z3235	3	904.393269_49.59433866	0
Z3260	3	142.0724301_59.63908685	0
Z3261	3	477.8534446_44.67341584	0
Z3268	3	333.9233712_45.54005851	0
Z3271	3	163.1329087_280.7491753	0.01
Z3302	3	208.1189012_16.54244465	0.003
Z3360	3	493.8148364_45.89348981	0
Z3385	3	257.1745871_236.293913	0
Z3415	3	280.1542979_29.28158682	0
Z3461	3	990.1012949_53.3565443	0
Z3514	3	593.7474745_47.48772859	0
Z3525	3	873.6422691_33.06718546	0.004
Z3548	3	503.0032234_59.67490373	0
Z3592	3	507.3639293_29.22026011	0
Z3601	3	501.7547534_45.43111399	0
Z3603	3	475.0032067_59.4397722	0
Z3614	3	766.3086875_53.50034593	0
Z3649	3	733.558769_28.42181356	0.004
Z3653	3	732.5523428_26.52216379	0.004
Z3701	3	208.0556603_58.25423421	0
Z3702	3	541.3689066_32.56723176	0
Z3976	3	618.4438821_52.31875966	0
Z4034	3	260.9878139_45.63944435	0
Z4037	3	420.3187287_225.9529405	0
Z4045	3	678.4004629_51.35188375	0
Z4139	3	482.7863309_46.05655351	0
Z4154	3	840.2416273_55.02610457	0
Z4186	3	216.1596843_276.6806558	0
Z4221	3	880.2712996_46.15083795	0
Z4226	3	474.5736256_51.40654031	0
Z4276	3	311.1848731_23.91935054	0.002
Z4302	3	408.8572312_47.94473265	0
Z4305	3	583.7178219_48.33838125	0
Z4374	3	240.8387272_45.76118125	0.004
Z4390	3	215.1388438_55.86631735	0.018
Z4432	3	113.975639_211.0282257	0
Z4459	3	384.3197264_242.3193768	0
Z4465	3	928.3579065_49.58115933	0
Z4553	3	109.0633222_45.03556619	0
Z4651	3	354.2997206_23.31851269	0.01
Z4660	3	396.2800277_25.54244168	0
Z4684	3	417.8844063_45.68398018	0
Z4694	3	238.2246723_278.4957089	0
Z4700	3	431.3870614_23.18176184	0
Z4703	3	135.1095531_40.25772856	0
Z4735	3	430.2440777_40.55492873	0
Z4740	3	151.0753367_265.5548362	0

Node	Cluster	Name	centrality
Z4808	3	716.5304224_44.42985116	0.004
Z4840	3	118.0604132_262.0736413	0
Z4852	3	158.0679212_45.03549817	0
Z4873	3	141.0714947_59.77032705	0
Z580	3	524.7939864_52.44905655	0.003
Z687	3	238.0038882_42.09741619	0.003
Z696	3	145.1011214_25.46504197	0.004
Z736	3	429.337853_23.02364415	0.003
Z738	3	433.9040187_55.63054664	0.003
Z787	3	484.556336_46.27038779	0
Z798	3	214.0668126_69.79801886	0.002
Z949	3	704.5237752_29.99151667	0.019
Z988	3	786.2764336_46.27265151	0

Table 4: **Nodes for Patients**

Node	Cluster	Name	centrality
Y18	1	il10_stool	0
Y19	1	il12p70_stool	0
Y22	1	il4_stool	0
Y23	1	il6_stool	0
Y24	1	il8_stool	0
Y25	1	tnfa_stool	0
Z110	1	282.2423582_18.33577261	0
Z1106	1	268.1394681_29.98248278	0
Z1187	1	236.1646733_147.1297389	0
Z1210	1	268.2271515_158.0892218	0
Z1263	1	222.1431251_274.5401817	0
Z1266	1	1006.07866_47.08601195	0
Z129	1	154.074217_57.5568992	0
Z1346	1	147.0145463_76.86325559	0
Z1363	1	579.6811942_50.72314898	0
Z1454	1	653.4395877_23.63294367	0
Z1486	1	326.3052063_225.9404628	0
Z1615	1	368.1532462_61.9436115	0
Z1628	1	262.0490448_60.05490098	0
Z1641	1	324.9365741_216.5040175	0
Z165	1	380.0064157_282.5842226	0
Z1667	1	731.2610899_77.21260086	0
Z1711	1	134.0945634_107.7805766	0
Z1805	1	477.1500708_128.5590838	0
Z1871	1	414.3211854_24.49147535	0
Z2002	1	786.2764336_46.27265151	0
Z207	1	212.0428642_98.90626461	0
Z2108	1	368.8881172_53.90887289	0
Z2111	1	918.1705514_53.15073637	0
Z212	1	268.1482513_35.70628463	0
Z2205	1	295.1291332_40.71645416	0
Z2251	1	202.9974299_181.1273686	0
Z234	1	564.3593971_29.97669546	0
Z2349	1	119.0853706_25.89055982	0
Z2364	1	100.0756415_33.22355974	0
Z2393	1	594.1594056_264.4382767	0
Z2432	1	484.8055406_50.73121774	0
Z2489	1	214.4566618_213.9458277	0
Z2499	1	576.5134628_48.89531542	0
Z2619	1	272.997274_161.5683001	0
Z2677	1	490.2897653_32.88695183	0
Z2775	1	299.22163_281.1824008	0
Z2777	1	188.119738_220.0672542	0
Z2786	1	488.551558_48.18763674	0
Z2919	1	271.1903216_280.4492261	0
Z3044	1	154.0585946_60.66412383	0
Z3048	1	566.478314_48.09512058	0
Z3119	1	900.6666162_33.38982178	0
Z3123	1	538.1611687_19.96827538	0
Z3135	1	388.3062948_24.42117584	0

Node	Cluster	Name	centrality
Z3143	1	151.9906231_23.55224633	0
Z3234	1	439.1669283_79.42330438	0
Z3247	1	352.9143233_53.69540389	0
Z3261	1	412.8605163_50.68434597	0
Z3291	1	145.0971581_70.03299618	0
Z3305	1	302.9273526_229.1777775	0
Z3348	1	542.7643567_51.31815549	0
Z3567	1	616.0729152_145.6277228	0
Z3615	1	199.1476875_24.4268888	0
Z3694	1	438.8555868_55.12338739	0
Z377	1	203.0856158_274.4400499	0
Z3774	1	124.0758303_268.2042133	0
Z3815	1	417.7948835_51.81385442	0
Z3843	1	148.0508016_282.5366563	0
Z3853	1	607.8893913_61.60538741	0
Z3895	1	181.0144451_289.3266809	0
Z3945	1	149.0321471_169.231031	0
Z3961	1	238.2246723_278.4957089	0
Z3992	1	669.6786989_47.04748179	0
Z4	1	89.50995128_257.3324268	0
Z4046	1	155.0813707_44.33506394	0
Z4053	1	567.8917373_59.86922823	0
Z4056	1	307.2627952_24.38158879	0
Z4103	1	456.6025906_50.60915284	0
Z4111	1	424.069395_169.9539537	0
Z4158	1	277.1798116_273.6542266	0
Z4164	1	126.0662632_269.871915	0
Z419	1	271.1905111_149.8910105	0
Z4190	1	454.3897426_23.19516405	0
Z4193	1	268.1989265_282.8471966	0
Z4237	1	268.1473339_262.9479803	0
Z4287	1	176.9717686_29.80937561	0
Z4291	1	180.0960584_147.7175679	0
Z4300	1	301.1800287_278.6096092	0
Z4310	1	629.6528806_45.84530522	0
Z4330	1	317.0834007_115.7389866	0
Z4338	1	197.1900485_275.2543637	0
Z4366	1	167.1067386_277.1221859	0
Z4448	1	142.9867115_291.2005645	0
Z4505	1	176.0406668_61.44865445	0
Z4636	1	252.997131_19.18085603	0
Z4641	1	213.1486442_272.9265085	0
Z4647	1	281.1748318_275.226904	0
Z4698	1	348.7169549_45.57827424	0
Z4719	1	253.2161551_280.4516919	0
Z4838	1	218.9750503_243.2332564	0
Z4850	1	111.5190997_292.4971352	0
Z4946	1	166.1227113_142.0710616	0
Z5000	1	344.2280123_276.8687271	0
Z582	1	315.5679318_166.0358706	0
Z705	1	127.5174294_160.0218462	0
Z72	1	339.4785151_231.9354714	0

Node	Cluster	Name	centrality
Z808	1	608.3883523_30.34834924	0
Z839	1	197.066722_33.02317231	0
Z893	1	108.0443778_50.08327836	0
Z899	1	154.0494112_49.05688262	0
X1	2	Prevotella	0.754
X100	2	Sellimonas	0.971
X111	2	CandidatusMethanogranum	0.701
X112	2	Faecalitalea	0.748
X113	2	Solobacterium	0.965
X115	2	Klebsiella	0.814
X12	2	Acidaminococcus	0.968
X121	2	Bacteroidia	0.98
X123	2	Puniceicoccaceae	0.913
X124	2	Eubacterium	0.881
X125	2	Bacteroidetes	0.944
X13	2	S-Aa	0.951
X15	2	Parabacteroides	0.959
X16	2	Blautia	0.974
X17	2	Veillonella	0.969
X2	2	Ezakiella	0.965
X21	2	Varibaculum	0.965
X22	2	Megasphaera	0.851
X24	2	Murdochiella	0.986
X25	2	Escherichia/Shigella	0.986
X27	2	RuminococcaceaeUCG-	0.99
X3	2	Bacteroides	0.375
X32	2	Peptostreptococcus	0.981
X33	2	Lawsonella	0.969
X37	2	Tyzzerella	0.838
X39	2	Mogibacterium	0.967
X4	2	Campylobacter	0.679
X41	2	Bilophila	0.96
X42	2	LachnospiraceaeUCG-	0.742
X44	2	Anaerostipes	0.991
X45	2	Bacteroidales	0.851
X46	2	Lachnoclostridium	0.965
X47	2	Negativicoccus	0.84
X48	2	Christensenellaceae	0.436
X49	2	LachnospiraceaeNDgroup	0.787
X5	2	Akkermansia	1
X51	2	Catenibacterium	0.888
X53	2	ErysipelotrichaceaeUCG-	0.885
X55	2	Oscillibacter	0.718
X56	2	Paraprevotella	0.547
X57	2	Streptococcus	0.967
X6	2	Faecalibacterium	0.943
X61	2	Jonquetella	0.78
X64	2	Muribaculaceae	0.979
X65	2	Gallicola	0.959
X66	2	Gemella	0.969

Node	Cluster	Name	centrality
X67	2	Intestinimonas	0.991
X68	2	GCA-	0.965
X69	2	UC–E	0.97
X7	2	Peptoniphilus	0.986
X70	2	Barnesiella	0.962
X72	2	Hungatella	0.618
X73	2	Megamonas	0.995
X78	2	Haemophilus	0.962
X8	2	Anaerococcus	0.285
X80	2	Actinomyces	0.988
X82	2	Succinivibrio	0.997
X96	2	W	0.996
Y1	2	crp_plasma	0.252
Y15	2	LBP_stool	0.099
Z1102	2	324.9940115_29.19164325	0.453
Z1123	2	302.160363_34.72935043	0.633
Z1190	2	737.8601593_60.01423308	0
Z1213	2	814.6893088_30.6815438	0.546
Z125	2	178.5423687_191.6419107	0
Z1270	2	201.0907649_270.1012906	0.682
Z1272	2	325.1341183_56.24113111	0
Z1275	2	417.9692036_60.93149062	0
Z1276	2	284.1275894_25.01886544	0
Z1685	2	151.9373465_57.88557647	0
Z173	2	92.50337592_28.16350136	0
Z175	2	320.0221445_161.4934113	0
Z1804	2	597.3598289_26.64811277	0.436
Z1822	2	193.0683198_68.8963676	0.724
Z1878	2	552.6864865_46.12164471	0
Z1938	2	383.330962_24.7926599	0.705
Z1968	2	126.0298108_53.4239191	0
Z2053	2	578.6523115_45.23231124	0.79
Z2073	2	371.3034236_27.48195522	0.548
Z2082	2	358.9337791_48.7685075	0
Z2084	2	265.1181341_28.9415658	0.556
Z2109	2	797.0010461_59.61048236	0
Z2389	2	399.9070955_43.95211502	0
Z2450	2	147.9995144_216.3837857	0
Z2504	2	324.3264413_23.46574137	0
Z2524	2	478.7796452_54.21054046	0
Z2571	2	284.1940548_148.4240747	0
Z2608	2	202.1188087_44.48899796	0
Z269	2	278.5237748_164.1880968	0
Z2717	2	325.2002549_271.6737314	0
Z2738	2	989.6571162_33.29909158	0
Z2874	2	384.3098059_24.07826702	0.733
Z2924	2	325.2373418_270.0463006	0
Z2939	2	200.1017934_30.08666059	0
Z3022	2	148.0425503_41.63051475	0.752
Z3036	2	286.2007906_29.40836124	0.64
Z3074	2	147.0252009_169.8672982	0
Z3091	2	397.3136957_23.53984429	0.641

Node	Cluster	Name	centrality
Z3161	2	211.0402194_55.29877303	0
Z3239	2	578.7231807_51.8551086	0
Z3250	2	96.02465234_254.532485	0
Z3271	2	485.7838134_49.15489884	0.585
Z3316	2	356.0126967_188.9832074	0
Z3322	2	1046.35793_48.79401578	0
Z3323	2	273.0392843_241.8811386	0
Z3337	2	371.2982227_24.35719709	0.695
Z3351	2	880.5166028_47.66201568	0
Z3385	2	471.9916463_260.0828329	0
Z3390	2	370.2954109_24.37763721	0.725
Z341	2	315.0250909_67.68539767	0.254
Z3472	2	104.1070002_47.33711003	0.777
Z3611	2	294.8431548_45.28536473	0
Z3623	2	260.1140991_119.4960468	0
Z3638	2	894.8771997_59.53728783	0
Z3658	2	158.8748463_50.04674556	0
Z3663	2	131.0016197_249.2819198	0
Z3671	2	527.2962549_27.32976934	0.704
Z3734	2	354.2997206_23.31851269	0.489
Z3753	2	396.310299_24.00422718	0.613
Z3762	2	329.2492703_24.23880574	0.536
Z3785	2	355.2839609_270.5369581	0
Z3821	2	384.3197264_242.3193768	0
Z3830	2	346.8871293_54.0854066	0
Z3851	2	882.3777736_48.37267021	0
Z3858	2	569.3435138_29.28223645	0.716
Z3882	2	553.7238317_45.82948904	0.649
Z3897	2	194.117691_271.6399092	0.75
Z3917	2	296.2950618_22.96089384	0
Z4068	2	245.1857664_29.38673179	0.663
Z4071	2	399.3282549_25.35692796	0.648
Z4081	2	637.4296801_33.7003165	0
Z4089	2	984.3142268_49.70533839	0
Z4172	2	228.1593905_263.2521089	0.703
Z4197	2	318.2539852_24.57418925	0.778
Z4220	2	568.3388417_29.45742071	0.715
Z4229	2	398.3271188_23.5363148	0.625
Z4247	2	214.2166348_273.5124209	0
Z4262	2	569.8947294_59.49680977	0.706
Z4281	2	642.4522657_47.97155862	0
Z4292	2	205.1258189_35.93039371	0.261
Z4299	2	151.0753367_265.5548362	0
Z4302	2	824.5075499_47.92084328	0
Z442	2	287.146735_24.74468108	0
Z4589	2	492.7317082_46.7595242	0
Z4726	2	649.8945313_59.31347217	0.644
Z4741	2	506.0323493_188.3489368	0.695
Z4749	2	343.267157_25.87009427	0.679
Z4802	2	986.4062282_48.71458208	0
Z4815	2	492.3090788_32.82547233	0
Z4898	2	160.0758354_272.5560522	0

Node	Cluster	Name	centrality
Z4910	2	716.638444_50.1341068	0
Z4920	2	140.0536904_226.3703561	0.501
Z4997	2	516.5826703_50.14288978	0.762
Z728	2	286.1437304_24.51808299	0
Z74	2	266.1598092_49.8457619	0.735
Z892	2	472.3414243_23.45360534	0.656
Z99	2	480.0501812_92.0806803	0.711
X40	3	Lachnospiraceae	0.047
Y11	3	il6_plasma	0.638
Y13	3	tnfa_plasma	0.678
Y14	3	crp_stool	0.769
Y16	3	ifng_stool	0.804
Y20	3	il13_stool	0.81
Y21	3	il2_stool	0.78
Z1002	3	1242.410464_77.39366989	0.04
Z1062	3	241.0491872_148.2790569	0
Z1069	3	269.1748072_282.0032101	0
Z1101	3	160.1331467_36.54004876	0.06
Z1125	3	558.4619306_22.43594534	0
Z1282	3	172.0796713_64.71627178	0.058
Z1344	3	226.1799329_23.81498378	0
Z1374	3	113.0960976_36.23331657	0.061
Z1409	3	355.887118_54.44473324	0
Z1478	3	163.0977438_64.65031799	0
Z1482	3	464.3141503_26.64856704	0
Z1510	3	142.0774669_23.1165718	0.055
Z1603	3	209.059471_223.1899111	0.063
Z1604	3	192.1054301_145.118138	0
Z1625	3	102.0662019_25.43606796	0
Z1651	3	361.32195_277.9430949	0
Z1686	3	285.1190242_140.0449253	0
Z1724	3	280.199389_119.568085	0
Z1754	3	234.9275323_17.75469821	0.061
Z1760	3	901.6693921_33.37918824	0
Z1802	3	143.1067056_216.2861138	0
Z1872	3	1144.780138_61.70926681	0.072
Z1910	3	253.2161429_223.4999538	0
Z1919	3	124.209505_33.01028637	0
Z2037	3	172.096794_157.1050358	0
Z2132	3	305.2115078_38.84250061	0
Z2228	3	240.9530126_169.3224385	0
Z2231	3	187.0412093_203.2498126	0
Z2316	3	1222.276958_87.97867276	0
Z2463	3	128.493985_209.4085933	0
Z260	3	143.1260048_20.89179786	0.063
Z2662	3	102.0717588_220.6985639	0
Z2668	3	119.0011052_221.6903775	0
Z2686	3	123.0553669_273.0350179	0
Z2687	3	415.0169337_183.4257507	0
Z2807	3	956.1941938_46.41226154	0
Z2832	3	171.1492327_279.4465714	0.059
Z2905	3	630.7910635_58.29911412	0.039

Node	Cluster	Name	centrality
Z2994	3	169.0969903_37.77340052	0.058
Z3055	3	264.2403542_277.8971519	0
Z3058	3	173.1325899_278.73048	0
Z3064	3	448.8286529_50.73225461	0
Z3130	3	605.5707703_50.04378709	0
Z3132	3	293.8487572_44.37434733	0.061
Z3150	3	397.2010289_23.39363222	0
Z3162	3	884.3084081_45.67719151	0
Z3213	3	130.1226825_266.4769854	0
Z3298	3	102.0657847_202.2483921	0
Z3327	3	475.3792258_24.28820821	0
Z3427	3	549.3055773_23.98311694	0
Z3484	3	281.1381942_23.71856619	0
Z3486	3	191.1795459_275.5768916	0
Z3561	3	246.5437312_168.7210072	0.055
Z3568	3	257.9857958_45.44407649	0.053
Z3737	3	147.0241535_129.9190303	0.063
Z3759	3	150.0914201_261.9530434	0
Z3839	3	137.0551097_170.4936464	0.037
Z3848	3	264.1188011_69.52878496	0.054
Z3854	3	149.0961937_279.6069524	0
Z398	3	262.1652371_36.22342058	0.06
Z4088	3	548.3012657_24.28626579	0
Z412	3	552.076813_68.03506987	0
Z4167	3	105.0697997_25.42452132	0.056
Z4218	3	390.9774607_19.01456109	0
Z425	3	590.1446337_146.9788785	0
Z4276	3	320.8773485_46.08997922	0
Z4324	3	236.1724812_172.760009	0
Z4325	3	230.0956496_64.16252146	0
Z4326	3	145.0439438_237.2508188	0
Z4327	3	613.8053155_46.36012258	0
Z4348	3	201.1635832_23.32668369	0
Z437	3	453.1678819_26.75108274	0
Z4453	3	110.0349469_277.5951096	0
Z4658	3	531.2748433_24.58405024	0
Z4695	3	115.0389974_130.0844245	0
Z4713	3	353.9004298_55.89421825	0.054
Z4783	3	251.0088217_283.7225851	0
Z4854	3	388.2543973_276.8151704	0
Z488	3	1036.014591_103.2180223	0.059
Z49	3	427.374601_28.99077612	0.062
Z4930	3	390.9760769_63.73039673	0.054
Z509	3	216.4758596_215.8310745	0
Z519	3	798.2225486_101.4633623	0.056
Z590	3	506.1301544_101.3032385	0.05
Z629	3	235.2055533_24.36889468	0
Z673	3	973.2923292_50.98239474	0.048
Z714	3	296.7269819_55.49108254	0.052
Z75	3	233.0871787_63.28205961	0.059
Z752	3	228.9729833_52.1354952	0
Z759	3	149.1286603_20.06305135	0.06

Node	Cluster	Name	centrality
Z784	3	182.0402824_43.85081861	0.058
Z885	3	161.136551_37.00316326	0.062
Z962	3	311.1464756_113.2350793	0
Z970	3	435.2727659_22.81793404	0
X10	4	Alistipes	0.149
X105	4	Methanobrevibacter	0.113
X11	4	Phascolarctobacterium	0.047
X114	4	CandidatusSoleaferrea	0.016
X116	4	Victivallis	0.04
X119	4	Slackia	0.047
X14	4	Dialister	0.11
X20	4	Agathobacter	0.126
X23	4	Fusobacterium	0.047
X26	4	Corynebacterium	0.048
X29	4	Subdoligranulum	0.044
X30	4	Fusicatenibacter	0.143
X34	4	LachnospiraceaeNKAgroup	0.051
X36	4	Dorea	0.043
X38	4	Lachnospira	0.246
X43	4	Negativibacillus	0.047
X52	4	Gastranaerophilales	0.056
X58	4	Mobiluncus	0.015
X59	4	FamilyXI	0.044
X62	4	Bifidobacterium	0.047
X63	4	Flavonifractor	0.033
X74	4	Sarcina	0.044
X75	4	CAG-	0.088
X76	4	Moryella	0.047
X77	4	RikenellaceaeRCgutgroup	0.039
X81	4	Lactobacillus	0.012
X84	4	Butyricimonas	0.04
X85	4	RuminococcaceaeNKAgroup	0.04
X86	4	LachnospiraceaeACgroup	0.04
X87	4	Gardnerella	0.043
X89	4	Anaeroglobus	0.043
X9	4	Parasutterella	0.158
X90	4	Eisenbergiella	0.032
X92	4	Erysipelatoclostridium	0.036
X93	4	Desulfovibrio	0.04
X97	4	Allisonella	0.038
X98	4	DTU	0.013
Y12	4	il8_plasma	0.034
Y5	4	il1b_plasma	0.021
Z1020	4	570.4390168_22.36275247	0.014
Z1036	4	253.2157075_24.52115516	0
Z1078	4	161.0378718_154.992945	0
Z1150	4	250.1111657_87.46153534	0
Z1298	4	90.04635781_38.48415153	0
Z1343	4	257.1745871_236.293913	0
Z1353	4	527.1835705_114.8119424	0
Z1358	4	259.9573465_210.0967541	0.019

Node	Cluster	Name	centrality
Z1439	4	282.2511006_230.830527	0
Z1536	4	433.3310605_24.379677	0.023
Z1570	4	370.0508529_70.51747626	0
Z1583	4	597.5089062_22.64200499	0.025
Z1702	4	281.2110167_225.4472108	0
Z1727	4	222.0059001_47.27084613	0
Z1803	4	980.2910866_47.82416146	0
Z1860	4	96.06377531_111.0426366	0
Z189	4	375.2147769_41.02995809	0
Z1971	4	453.8394203_47.2140668	0
Z2000	4	354.0773471_66.88219305	0
Z2009	4	980.2805744_50.21452485	0
Z2015	4	412.7639799_47.54683679	0
Z2027	4	509.7158276_48.3664433	0
Z2031	4	494.7282845_49.75481106	0
Z2035	4	1100.755038_58.93991683	0
Z2047	4	161.0376054_60.0417764	0
Z2059	4	179.0694419_192.4843435	0.082
Z2074	4	172.1696336_23.56156206	0.028
Z2135	4	203.143031_253.9576079	0
Z222	4	353.0272449_46.50104729	0
Z2264	4	221.0767318_89.74719913	0
Z2283	4	145.0349956_18.67917617	0.032
Z2289	4	457.8783206_47.22264863	0
Z2379	4	361.2005237_25.74329187	0
Z2431	4	480.0785155_69.71776839	0.021
Z2478	4	931.3108533_115.8060022	0
Z2568	4	648.1814296_110.4309332	0
Z2614	4	484.330857_30.9831963	0
Z2618	4	150.0766456_58.60377347	0.014
Z2675	4	747.5737092_26.94706355	0
Z2714	4	705.8858281_59.6784907	0.02
Z2720	4	195.9683681_235.4212956	0
Z2791	4	263.073591_60.34878772	0
Z2798	4	120.9662404_58.75926633	0.015
Z2810	4	149.0950297_45.23961258	0
Z2840	4	1136.179743_50.47850341	0
Z2870	4	352.1024216_46.39868252	0
Z2916	4	421.95591_57.66165548	0
Z2917	4	160.0344389_59.51557066	0
Z2961	4	183.1380953_268.7191545	0
Z2968	4	392.2880853_285.6734052	0.034
Z2999	4	670.6893838_45.79481853	0
Z3024	4	132.0036499_292.8343824	0
Z3077	4	257.9773173_217.0013601	0
Z3082	4	353.0556935_30.88930502	0
Z3110	4	151.086473_19.77301555	0.031
Z3189	4	233.9667694_288.4688297	0
Z3197	4	299.1385157_23.12535687	0.289

Node	Cluster	Name	centrality
Z3210	4	874.433001_48.22773002	0
Z3278	4	127.0614116_17.85277005	0
Z3389	4	1152.155543_50.74968925	0
Z340	4	536.4962811_50.11057948	0.029
Z3485	4	181.0284234_218.3154496	0
Z3519	4	132.9775407_21.53193324	0
Z353	4	618.0435786_241.3650585	0
Z3542	4	286.3099289_23.43766505	0.032
Z3547	4	583.7178219_48.33838125	0.016
Z3608	4	528.30799_26.92641158	0
Z3661	4	145.049581_37.19921588	0.274
Z3680	4	1100.235363_49.7431831	0
Z3718	4	283.175178_278.9540313	0.022
Z3727	4	273.1846629_247.9658111	0
Z3741	4	771.5732586_26.21215684	0
Z3761	4	824.558252_40.4771494	0
Z3786	4	207.8593857_55.46938594	0.03
Z3807	4	121.077893_38.26749032	0.134
Z3973	4	397.2939916_23.58638941	0
Z4041	4	298.143644_31.59066217	0.013
Z4275	4	141.0139568_242.5067545	0
Z4288	4	386.3257974_24.04529562	0
Z4290	4	130.9664179_39.18501884	0
Z4333	4	229.937911_209.5747208	0
Z4334	4	878.4301812_48.32639771	0
Z45	4	226.2166129_215.0728656	0
Z4526	4	755.54237_25.68319519	0
Z4629	4	122.0694675_69.24621509	0.014
Z4685	4	386.3494655_23.24983513	0.026
Z4730	4	744.5493093_28.67674597	0
Z4757	4	134.0811916_68.16763006	0.024
Z4759	4	734.5635054_29.29315382	0
Z4813	4	814.6211776_30.05374434	0
Z4922	4	770.5676662_26.16126084	0
Z4986	4	189.1638055_255.1194136	0
Z548	4	445.839986_49.9749697	0.011
Z558	4	160.0253384_69.57499715	0
Z666	4	566.4088334_23.97301826	0.058
Z683	4	126.0773061_20.03507824	0
Z691	4	270.9969029_61.15352408	0
Z704	4	536.3331226_31.09239033	0.013
Z71	4	146.1059191_54.29342556	0.012
Z750	4	220.1010666_64.31336935	0.029
Z804	4	179.024791_166.4983042	0
Z879	4	159.5379531_168.0881695	0
Z972	4	739.881265_59.73890402	0.037