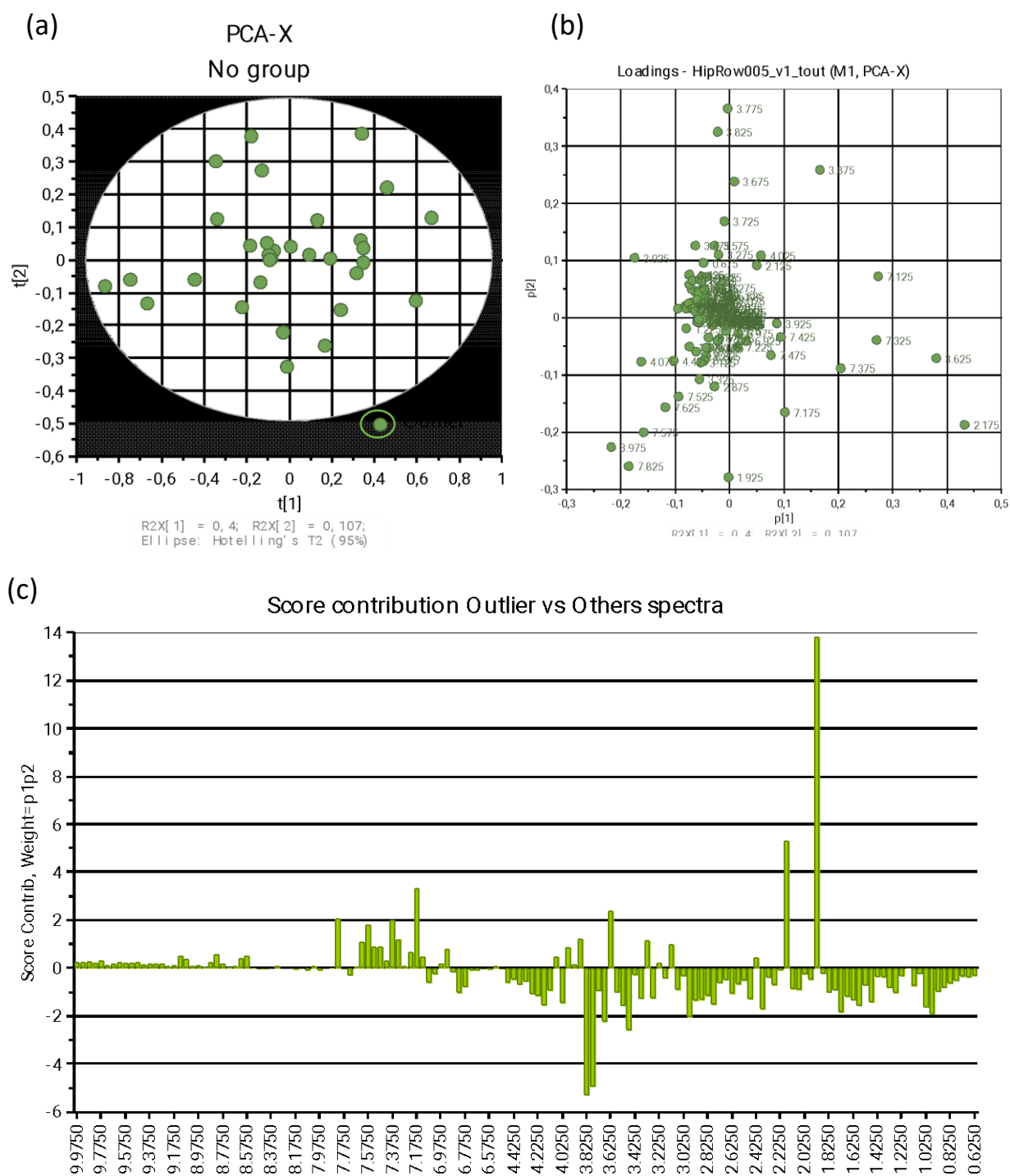


Figure S1. Overall PCA for all urine samples (a) score plot; (b) loading plot and (c) contribution plot



Valine
 $p = 0.0487$

Creatinine
 $p = 0.0371$

Citrate 1
 $p = 0.0032$

Citrate 2
 $p = 0.0122$

Figure 1 consists of five dot plots arranged horizontally, each representing a different urinary metabolite: Urea, Creatinine, Formate, Hippuric acid, and Methylguanidine. Each plot compares the distribution of concentrations in Women and Men. The y-axis for each plot represents the concentration of the metabolite. Individual data points are shown as black dots. A horizontal line indicates the mean, and vertical error bars represent the standard deviation. The p-value for each comparison is displayed above the plot.

Metabolite	Y-axis Range	Women Mean (approx.)	Men Mean (approx.)	p-value
Urea	0 - 2000	~800	~1200	0.0027
Creatinine	0 - 600	~150	~220	0.0269
Formate	0 - 5	~1.8	~3.0	0.0007
Hippuric acid	0 - 25	~4.0	~9.5	0.0136
Methylguanidine	0 - 8	~1.5	~3.5	0.0055

A06AD11	B01AA03	M02AC											
A02BC02	A03FA01	A04AA01	A12AX		B01AB05	B03AA01	H02AB02	nutritional drink	N02AA05	N02AA05	N02AA55	N02BE01	
A12AX	J01MA12	R05CB15	R05FA02										
A06AD65	A12AX	C01DA02	D07BA04	N02AJ06	N05CH01	S01XA20	B03AA01	M05BA08	N02BE01				
A02BC02	A12AX	B01AB05	B03AA01	C09CA01	M01AE01	N02AA05	N02AA05	N02AA05	N02AA55	N02BE01	N02BE01	N02BE01	
B01AB05	C08CA01	J01DB01	J01DC02	N02AA05	N02AA05	N02AE01	N02BE01						
A10AD05	B01AB05	C03CA01	C03DA01	N01DB01	N02AA05	N02AA55	N02BE01	N02BE01	N02BE01	N05AH04	N05AH04	N05AH04	
B01AB05	B03BB01	G04BD12	H02AB06	N02AA05	N02AA55	N02AE01	N02BE01	R02AB30	R05CB01	R05CB15	energy drink		
B01AB05	A12AX	B03AA01	G04CB02	J01DC02	N02AA05	N02AA55	N02BE01	N05CH01					
A02BC03	A10AB05	A10AE04	A10BA02	A12AA04	B01AB05	C01DA08	C08CA01	C09CA06	N02AA05	N02BE01			
A02BC02	A10AB05	A12AX	B03AA01	C07AB07	H02AB06	N02AA05	N02AA55	N02BE01	R03AC02	R03AK07			
A04AA02	multivitamin	A12AX	B01AB05	C07AB02	J01XE01	M05BA08	N02AA05	N02BE01					
A04AA01	multivitamin	B01AA03	H02AB09	G04BD12	J01EA01	M05BA08	N02AA05	N02AA05	N02BE01				
A04AA02	H02AB02	J05AB11	N02AA05	N05AD06	N02BE01								
A02BC02	A06AD65	A12AX	B01AA03	C03CA01	C07AB07	C09CA01	M05BA08	C10AA07	N02AA55	N02AA05			
A02BC02	A03FA01	multivitamin	A12AX	B01AB05	B03AA01	M05BA08	N02AA05	N02AA55	N02BE01				
A02BA02	A06AC01	A04AA01	A06AD65	B01AA03	B01AB05	C10AA05	H02AB02	C03CA01	M05BA08	N02AA05			
A03DA02	A04AA02	A10AB05	A10AE05	A10BA02	A10BH01	d3 vitamin	multivitamin	A12AX	B01AB05	B03AA01	C09AA04		
B01AA03	A04AA02	A12AX	B03AA01	C07AB02	C08CA01	M05BA08	N02AA05	N02AA55	N02BE01	N02BE01			
A06AD65	A12AX	B01AA03	B03AA07	C07AB07	C09CA01	G04CB02	multivitamin	J01CR02	N02AA05	N02AA55	N02BE01	N02BE01	
M05BA04	A12AX	N02AA55	N06AX11	N05CD07									
A02BC05	A06AD11	multivitamin	A12AX	B01AC30	B03AA01	B03BA03	C01DA08	C07AB02	C08CA01	M05BA08	N02BE01		
N02AA55	M05BA08	N06AX11	N05AD09	N02BE01	N02AA55	N02AA05	H02AB02	B03AA01	A12AX	A04AA02			
N02AA55	N02AA05												
A06AD65	multivitamin	A12AX	B01AF01	B03AA01	C07AB07	G03CA03	M05BA08	N02AA05	N02AA55	N05CH01			
B01AB05													
B01AB05	B01ACD6	C03DA01	C07AB07	CAD9AA05	C10AA05	M05BA04	M05BX04	N02AA05	N02AA55			N02BE01	
A12BA01	J01CA08	J01EA01	N02BE01	N05BA01	N05BA01	N05CF01							
A06AB08	A06AD65	multivitamin	A12AX	B01AB05	B02AA02	C03CA01	J01DC02	M05BA04	N02AA05	N02AA55	N02BE01		
multivitamin	B01AB05	N05BA01	M01AB05	A11DA01	A04AA01								
A06AD11	A06AD15	lactobacillus GG	multivitamin	A12AA04	B01AA03	A12BA01	B03BA03	J01DC02	N02AA05	N02AA55	N02BE01		
B01AB05	B03BB01	L04AX03	oxynorm										
A02BC02	multivitamin	A12AA04	A12BA01	B01AE01	multivitamin	C01AA05	C01DA08	C07AB07	N02AA05	N02AA55	N02BE01		

Table S2 . List of diseases among all participants and according to frailty status. Data are expressed as number of patients and frequency (%).

Diseases (frequency (%))	All (n=33)	non-frail (n=5)	pre-fail (n=18)	frail (n=10)
Hypertension	23 (70)	2 (40)	14 (78)	7 (70)
Diabetes	7 (21)	1 (20)	4 (22)	2 (20)
Cardiovascular diseases*	31 (94)	5 (100)	17 (94)	9 (90)
Musculoskeletal diseases**	29 (88)	5 (100)	17 (94)	7 (70)
Chronic urinary infection or other renal decease	4 (12)	0 (0)	2 (11)	2 (20)
Problems with voiding e.g.. incontinence	17 (52)	1 (20)	12 (67)	4 (40)
Osteoporosis	7 (21)	0 (0)	4 (22)	3 (30)

*including coronary hearth disease. angina pectoris. history of myocardial infarction. heart failure;

**Musculoskeletal including arthritis. rheumatoid arthritis.

Table S3. Supplementary documents concerning the Variable Importance in Projection (VIP) score for each outcome.

VIP for PLS-DA regarding mortality		
Primary ID (chemical shift)	VIP	Targeted metabolites
3.27500033" "	3.876950026	
2.17500019" "	3.56086993 2	Paracetamol (Acetaminophen) + Acetaminophen glucuronide
7.12500048" "	2.99595999 7	Acetaminophen derivatives
4.07500029" "	2.932940006	
3.62500024" "	2.917439938	
2.87500024" "	2.859430075	
7.17500019" "	2.73318004 6	Acetaminophen derivatives
4.02500010" "	2.414190054	
7.37500048" "	2.206650019	
7.32500029" "	2.185909986	
3.97500038" "	2.166569948	
3.02500033" "	2.10048008	
1.92500031" "	1.85157001	Acetate
7.82500029" "	1.733360052	
2.12500024" "	1.541049957	
7.57500029" "	1.536720037	
3.87500024" "	1.351250052	
3.22500038" "	1.332299948	
7.52500057" "	1.330680013	
2.72500038" "	1.20430004 6	Dimethylamine
7.62500048" "	1.19855999 9	Hippuric acid
1.87500024" "	1.162320018	
3.57500029" "	1.149960041	
2.22500038" "	1.14151001	Acetone
4.42500019" "	1.111529946	
3.77500033" "	1.072299957	
3.72500038" "	1.05456996	
3.07500029" "	0.96401298	
3.17500019" "	0.955281973	
8.22500038" "	0.909794986	
2.67500019" "	0.898232996	
1.22500026" "	0.893936992	
1.17500019" "	0.809105992	
3.92500019" "	0.777442992	
1.67500031" "	0.766892016	
3.12500024" "	0.766375005	

2.47500038" "	0.759234011	
7.42500019" "	0.743125975	
3.82500029" "	0.738216996	
8.82500076" "	0.727976978	
2.27500033" "	0.722187996	
2.57500029" "	0.71172303	
2.52500033" "	0.702306986	
1.32500029" "	0.69817298 7	Lactate
7.47500038" "	0.687752008	
1.77500021" "	0.685276985	
3.32500029" "	0.678472996	
3.37500024" "	0.677133024	
4.12500048" "	0.675014973	
1.42500031" "	0.674727023	
2.37500024" "	0.664951026	
3.52500033" "	0.663039029	
1.37500024" "	0.641982019	
1.47500026" "	0.63547998 7	Alanine
2.42500019" "	0.625910997	
3.42500019" "	0.62570399	
2.07500029" "	0.619328022	
1.72500026" "	0.609368026	
2.62500024" "	0.588383019	
8.07500076" "	0.573998988	
8.57500076" "	0.57209003	
2.32500029" "	0.563531995	
1.97500026" "	0.556529999	
7.07500029" "	0.556261003	
4.17500019" "	0.549516976	
9.12500000" "	0.549178004	
7.67500019" "	0.52960598 5	Hippuric acid
4.47500038" "	0.529430985	
2.02500033" "	0.512973011	
1.12500024" "	0.504921973	
3.47500038" "	0.497173011	
1.82500029" "	0.493827999	
0.97500026" "	0.49331000 4	Valine
6.82500029" "	0.483013004	
6.87500048" "	0.479968011	
1.62500024" "	0.470990986	
1.52500021" "	0.470589012	
0.92500025" "	0.469552994	
1.57500029" "	0.467061996	

1.27500021" "	0.464507997	
6.97500038" "	0.460750997	
1.07500029" "	0.450549006	
7.87500048" "	0.448967993	
2.82500029" "	0.446545005	
2.92500019" "	0.440290987	
2.77500033" "	0.436857015	
4.37500048" "	0.429668009	
6.62500048" "	0.42809099	
4.22500038" "	0.427345991	
7.22500038" "	0.421555996	
8.27500057" "	0.421526998	
4.32500029" "	0.410066009	
8.12500000" "	0.408854991	
0.87500024" "	0.405831993	
7.97500038" "	0.39586699	
2.97500038" "	0.379444987	
4.27500010" "	0.37340501	
8.32500076" "	0.365776986	
8.17500019" "	0.344644994	
8.87500000" "	0.343387991	
8.62500000" "	0.339143008	
0.82500023" "	0.327154994	
1.02500021" "	0.323163986	
0.77500021" "	0.314696997	
7.92500019" "	0.312976003	
0.72500026" "	0.310793996	
7.72500038" "	0.303645015	
7.27500057" "	0.302733004	
6.67500019" "	0.291162997	
8.37500000" "	0.286697	
7.77500057" "	0.283562988	
6.77500057" "	0.275002003	
7.02500057" "	0.270597011	
8.47500038" "	0.263000011	
6.92500019" "	0.262486994	
6.72500038" "	0.245100006	
3.67500019" "	0.233806998	
0.62500024"	0.228296995	
8.52500057" "	0.228003994	
0.67500025" "	0.215964004	
6.57500029" "	0.200363994	
8.42500019" "	0.175882995	
6.52500010" "	0.157995999	
8.02500057" "	0.104621999	
8.67500019" "	0.085220799	

9.07500076" "	0.082114503	
9.02500057" "	0.079643801	
9.92500019" "	0.073346503	
8.97500038" "	0.068037197	
9.97500038" "	0.065927498	
9.82500076" "	0.065760799	
9.87500000" "	0.064868197	
8.77500057" "	0.064815402	
9.52500057" "	0.063196503	
9.37500000" "	0.063153602	
9.62500000" "	0.060855899	
9.42500019" "	0.059576701	
9.17500019" "	0.058416001	
9.27500057" "	0.057606298	
9.77500057" "	0.056871999	
9.47500038" "	0.056492001	
9.32500076" "	0.055498101	
9.67500019" "	0.052842502	
9.57500076" "	0.051442001	
9.72500038" "	0.0470392	
8.92500019" "	0.044805601	
9.22500038" "	0.0435877	
8.72500038" "	0.042292599	
4.52500010" "	0.031485599	

VIP for PLS-DA regarding non-frail vs. pre-frail vs. frail

Primary ID (chemical shift)	VIP	Targeted metabolites
2.17500019" "	2.621119976	Paracetamol (Acetaminophen) + Acetaminophen glucuronide
3.02500033" "	2.617899895	
3.62500024" "	2.466789961	
3.87500024" "	2.466470003	
7.12500048" "	2.291450024	Acetaminophen derivates
7.17500019" "	2.124409914	Acetaminophen derivates
3.77500033" "	2.122129917	
2.12500024" "	2.034060001	
4.07500029" "	1.972609997	
3.17500019" "	1.931540012	
7.42500019" "	1.870519996	
7.52500057" "	1.812280059	

7.82500029" "	1.762500048	
2.32500029" "	1.721240044	
2.27500033" "	1.69216001	
7.32500029" "	1.684129953	
3.82500029" "	1.653949976	
4.02500010" "	1.633700013	
4.17500019" "	1.543280005	
3.97500038" "	1.519109964	
2.07500029" "	1.480399966	
3.67500019" "	1.415519953	
3.22500038" "	1.413550019	
3.52500033" "	1.365589976	
2.47500038" "	1.322620034	
7.57500029" "	1.312250018	
1.42500031" "	1.270120025	
1.97500026" "	1.263640046	
1.77500021" "	1.254109979	
3.12500024" "	1.239650011	
3.27500033" "	1.233690023	
7.62500048" "	1.213289976	
1.72500026" "	1.203529954	
4.32500029" "	1.20144999	
2.87500024" "	1.196760058	
4.22500038" "	1.196689963	
2.67500019" "	1.158910036	
1.62500024" "	1.158480048	
7.47500038" "	1.132200003	
3.57500029" "	1.110460043	
3.47500038" "	1.09691	
2.02500033" "	1.095469952	
7.37500048" "	1.086770058	
3.07500029" "	1.083220005	
1.87500024" "	1.079749942	
2.72500038" "	1.076120019	
4.27500010" "	1.041120052	
1.57500029" "	1.000499964	
2.42500019" "	0.994534016	
4.42500019" "	0.985616028	
3.92500019" "	0.984224021	
4.37500048" "	0.971475005	
0.87500024" "	0.96302402	
2.22500038" "	0.957993984	
4.47500038" "	0.943037987	
1.82500029" "	0.940477014	
7.92500019" "	0.920060992	
2.52500033" "	0.900605023	

2.92500019" "	0.891274989	
1.67500031" "	0.871165991	
8.82500076" "	0.839631975	
7.22500038" "	0.832316995	
2.57500029" "	0.825942993	
1.07500029" "	0.81397599	
4.12500048" "	0.807277024	
2.77500033" "	0.803331971	
2.37500024" "	0.796149015	
2.97500038" "	0.778917015	
1.17500019" "	0.750138998	
1.47500026" "	0.717920005	
1.92500031" "	0.710305989	
8.57500076" "	0.686053991	
0.72500026" "	0.650497019	
7.67500019" "	0.63865602	
2.62500024" "	0.614539981	
9.12500000" "	0.609982014	
7.02500057" "	0.59641403	
1.22500026" "	0.588941991	
8.47500038" "	0.572656989	
3.37500024" "	0.56212002	
7.27500057" "	0.560696006	
6.97500038" "	0.559583008	
6.92500019" "	0.559319019	
2.82500029" "	0.539941013	
0.97500026" "	0.530727983	
3.42500019" "	0.511327028	
7.77500057" "	0.508264005	
0.92500025" "	0.491261989	
8.62500000" "	0.471403003	
1.37500024" "	0.465869009	
6.62500048" "	0.463712007	
3.72500038" "	0.462334007	
7.07500029" "	0.46154201	
3.32500029" "	0.429926008	
1.32500029" "	0.42850399	
6.82500029" "	0.421849996	
0.67500025" "	0.420361996	
1.27500021" "	0.384627014	
0.82500023" "	0.381965011	
6.57500029" "	0.381561995	
1.02500021" "	0.375689	
1.52500021" "	0.368059993	
6.67500019" "	0.364618003	
1.12500024" "	0.360635996	

7.72500038" "	0.33949101	
8.87500000" "	0.329645008	
0.77500021" "	0.315535009	
8.07500076" "	0.309215993	
6.72500038" "	0.304587007	
0.62500024"	0.290042996	
6.52500010" "	0.248482004	
8.17500019" "	0.236695006	
8.32500076" "	0.224267006	
8.22500038" "	0.195954993	
8.27500057" "	0.191910997	
8.67500019" "	0.183440998	
7.97500038" "	0.177037999	
8.52500057" "	0.169108003	
9.07500076" "	0.168966994	
8.42500019" "	0.166018993	
8.37500000" "	0.163282007	
6.87500048" "	0.160127997	
6.77500057" "	0.154459998	
7.87500048" "	0.139191002	
8.12500000" "	0.13651	
8.77500057" "	0.136365995	
9.97500038" "	0.131915003	
9.02500057" "	0.130785003	
8.02500057" "	0.129278004	
9.92500019" "	0.129040003	
9.87500000" "	0.127765998	
9.82500076" "	0.127290994	
9.62500000" "	0.125210002	
9.17500019" "	0.124076001	
9.37500000" "	0.123880997	
8.72500038" "	0.123186	
9.67500019" "	0.12314	
9.52500057" "	0.121652	
9.32500076" "	0.121462002	
8.92500019" "	0.120945998	
9.47500038" "	0.119561002	
9.42500019" "	0.118308999	
9.77500057" "	0.116705999	
9.57500076" "	0.113314003	
9.22500038" "	0.112209998	
8.97500038" "	0.109160997	
9.27500057" "	0.095765002	
4.52500010" "	0.092202596	
9.72500038" "	0.087254703	

VIP for PLS-DA regarding non-frail vs. frail

Primary ID (chemical shift)	VIP	Targeted metabolites
3.62500024" "	3.454440117	
3.02500033" "	3.097249985	
2.17500019" "	2.919209957	Paracetamol (Acetaminophen) + Acetaminophen glucuronide
7.12500048" "	2.666670084	Acetaminophen derivatives
7.32500029" "	2.505949974	
3.57500029" "	2.278759956	
4.07500029" "	2.217700005	
3.87500024" "	2.185780048	
7.42500019" "	2.125240088	
3.27500033" "	2.102649927	
3.97500038" "	1.812489986	
4.42500019" "	1.651720047	
3.92500019" "	1.627429962	
2.87500024" "	1.615700006	
7.37500048" "	1.57573998	
7.82500029" "	1.514790058	
4.02500010" "	1.505769968	
7.57500029" "	1.479060054	
7.27500057" "	1.459339976	
3.52500033" "	1.458119988	
3.67500019" "	1.395799994	
7.47500038" "	1.374060035	
7.22500038" "	1.368549943	
3.72500038" "	1.365759969	
3.22500038" "	1.340330005	
4.32500029" "	1.295719981	
1.87500024" "	1.27128005	
2.32500029" "	1.167850018	
1.92500031" "	1.150570035	
8.82500076" "	1.106809974	
2.12500024" "	1.083619952	
0.92500025" "	1.076050043	
1.47500026" "	1.071099997	
1.32500029" "	1.041120052	
1.42500031" "	1.038969994	
7.02500057" "	1.037529945	
3.07500029" "	1.021450043	
2.47500038" "	1.013219953	

1.17500019" "	0.998085976	
1.52500021" "	0.995872021	
7.62500048" "	0.97261697 1	Hippuric acid
1.57500029" "	0.964936018	
3.12500024" "	0.945870996	
2.27500033" "	0.940083981	
2.67500019" "	0.920063019	
2.57500029" "	0.910143971	
3.77500033" "	0.896764994	
3.32500029" "	0.895362973	
2.02500033" "	0.891874015	
7.17500019" "	0.87661701 4	Acetaminophen derivatives
3.17500019" "	0.872853994	
2.62500024" "	0.853223026	
2.42500019" "	0.848438978	
2.72500038" "	0.846161008	
0.97500026" "	0.842419982	
1.62500024" "	0.831054986	
7.92500019" "	0.800468981	
1.22500026" "	0.784087002	
9.12500000" "	0.744544029	
4.37500048" "	0.733959973	
3.42500019" "	0.729426026	
0.72500026" "	0.721149981	
4.27500010" "	0.710471988	
2.52500033" "	0.709295988	
2.92500019" "	0.700329006	
8.47500038" "	0.656902015	
4.47500038" "	0.65635401	
4.22500038" "	0.654479027	
4.12500048" "	0.650339007	
7.52500057" "	0.640393972	
1.27500021" "	0.632025003	
1.82500029" "	0.629858971	
1.37500024" "	0.628601015	
2.22500038" "	0.617352009	
8.02500057" "	0.610783994	
4.17500019" "	0.609121025	
1.12500024" "	0.608013988	
8.07500076" "	0.589842021	
6.97500038" "	0.588469028	
0.87500024" "	0.580259979	
1.07500029" "	0.548677981	
7.07500029" "	0.546272993	
1.67500031" "	0.544571996	

3.37500024" "	0.526149988	
1.72500026" "	0.475430995	
1.77500021" "	0.474720001	
2.82500029" "	0.471480012	
2.37500024" "	0.471421003	
2.97500038" "	0.464751989	
3.47500038" "	0.460727006	
3.82500029" "	0.457672	
1.02500021" "	0.45728901	
7.67500019" "	0.43838301 3	Hippuric acid
2.77500033" "	0.430925995	
0.82500023" "	0.416177005	
2.07500029" "	0.414418012	
8.57500076" "	0.399253994	
8.87500000" "	0.382472992	
8.17500019" "	0.374899	
7.77500057" "	0.352337003	
6.92500019" "	0.351927012	
8.62500000" "	0.344518989	
8.12500000" "	0.342314005	
1.97500026" "	0.336214989	
6.62500048" "	0.332626998	
0.62500024" "	0.331806988	
8.27500057" "	0.329948008	
0.77500021" "	0.323285013	
6.77500057" "	0.313609987	
8.22500038" "	0.312730014	
0.67500025" "	0.289485991	
6.87500048" "	0.289072007	
8.37500000" "	0.268164992	
6.82500029" "	0.260825008	
7.72500038" "	0.258183002	
6.52500010" "	0.239063993	
6.57500029" "	0.223114997	
8.52500057" "	0.214689001	
7.87500048" "	0.210011005	
6.72500038" "	0.190148994	
8.42500019" "	0.147286996	
6.67500019" "	0.139761001	
7.97500038" "	0.120927997	
8.77500057" "	0.120274998	
8.32500076" "	0.114081003	
8.72500038" "	0.090801403	
4.52500010" "	0.080738999	
9.72500038" "	0.080002204	
9.27500057" "	0.065201998	

8.67500019" "	0.048496801	
9.47500038" "	0.047562402	
9.77500057" "	0.047542401	
9.02500057" "	0.045168102	
9.57500076" "	0.037988201	
9.32500076" "	0.037558001	
9.22500038" "	0.037190098	
9.67500019" "	0.034524601	
9.07500076" "	0.033525299	
9.52500057" "	0.033387899	
8.92500019" "	0.0324503	
9.17500019" "	0.0316412	
9.37500000" "	0.0311174	
9.87500000" "	0.030564001	
9.62500000" "	0.029415799	
9.92500019" "	0.0270292	
9.82500076" "	0.026491901	
9.42500019" "	0.025451699	
8.97500038" "	0.0253853	
9.97500038" "	0.016777501	

VIP for PLS-DA regarding total FIM

Primary ID (chemical shift)	VIP	Targeted metabolites
2.17500019" "	3.507910013	Paracetamol (Acetaminophen) + Acetaminophen glucuronide
3.62500024" "	2.895889997	
1.92500031" "	2.57359004	
7.82500029" "	2.220020056	
7.12500048" "	2.147399902	Acetaminophen derivatives
7.32500029" "	2.137599945	
3.97500038" "	2.033760071	
3.27500033" "	2.015810013	
3.47500038" "	1.959319949	
3.02500033" "	1.807489991	
7.37500048" "	1.686609983	
7.57500029" "	1.655910015	
7.52500057" "	1.630929947	
1.42500031" "	1.552189946	
3.77500033" "	1.497400045	
3.57500029" "	1.406389952	
7.62500048" "	1.404539943	
0.87500024" "	1.396939993	

2.47500038" "	1.395370007	
3.92500019" "	1.387320042	
7.27500057" "	1.365689993	
3.42500019" "	1.359899998	
4.07500029" "	1.35698998	
3.72500038" "	1.332020044	
1.27500021" "	1.329550028	
2.57500029" "	1.326920033	
4.02500010" "	1.31408	
7.42500019" "	1.292050004	
4.42500019" "	1.28204	
2.22500038" "	1.272699952	
7.22500038" "	1.25030005	
3.87500024" "	1.228559971	
2.67500019" "	1.223109961	
3.12500024" "	1.22021997	
2.32500029" "	1.212139964	
7.47500038" "	1.193510056	
2.72500038" "	1.169039965	
4.17500019" "	1.159190059	
3.52500033" "	1.143460035	
3.67500019" "	1.107609987	
1.17500019" "	1.103770018	
3.37500024" "	1.091519952	
2.52500033" "	1.063269973	
4.27500010" "	1.048629999	
1.22500026" "	1.045660019	
3.22500038" "	1.038300037	
1.32500029" "	1.036730051	
1.87500024" "	1.034340024	
3.82500029" "	1.017740011	
2.27500033" "	1.009140015	
2.07500029" "	0.98634702	
8.82500076" "	0.984538972	
1.47500026" "	0.932119012	
1.72500026" "	0.922908008	
0.92500025" "	0.922538996	
6.92500019" "	0.911436021	
4.12500048" "	0.862652004	
1.67500031" "	0.857032001	
1.07500029" "	0.852024972	
1.62500024" "	0.850190997	
1.02500021" "	0.848508	
2.12500024" "	0.83664	
0.97500026" "	0.82872802	
7.17500019" "	0.81079697	6 Acetaminophen derivatives
	6	

1.77500021" "	0.779514015	
1.57500029" "	0.757265985	
3.32500029" "	0.74387598	
8.07500076" "	0.737294972	
4.32500029" "	0.734041989	
2.97500038" "	0.718600988	
3.17500019" "	0.714731991	
7.72500038" "	0.712873995	
2.37500024" "	0.702413023	
9.12500000" "	0.698108971	
7.02500057" "	0.685755014	
1.97500026" "	0.685643971	
1.82500029" "	0.68244499	
4.37500048" "	0.68206799	
4.22500038" "	0.678451002	
2.92500019" "	0.675050974	
3.07500029" "	0.672038019	
7.92500019" "	0.671432972	
8.47500038" "	0.643477976	
2.02500033" "	0.633783996	
8.57500076" "	0.632566988	
6.87500048" "	0.630869985	
4.47500038" "	0.628924012	
1.37500024" "	0.625042975	
1.52500021" "	0.601720989	
7.67500019" "	0.594356	
2.82500029" "	0.574029982	
1.12500024" "	0.544685006	
2.42500019" "	0.533536971	
2.77500033" "	0.532441974	
2.62500024" "	0.512243986	
0.72500026" "	0.508642972	
8.62500000" "	0.423851013	
0.82500023" "	0.397287011	
8.32500076" "	0.365197003	
6.57500029" "	0.364463001	
8.22500038" "	0.356682986	
8.27500057" "	0.342691004	
0.77500021" "	0.334650993	
7.07500029" "	0.329358011	
2.87500024" "	0.325926006	
6.97500038" "	0.323323011	
8.87500000" "	0.313636005	
0.67500025" "	0.306818008	
0.62500024"	0.280856997	
6.82500029" "	0.243205994	

8.37500000" "	0.204136997	
6.77500057" "	0.192056	
7.87500048" "	0.189191997	
6.52500010" "	0.186387002	
7.97500038" "	0.183009997	
7.77500057" "	0.171222001	
6.67500019" "	0.163661003	
8.42500019" "	0.150803998	
8.52500057" "	0.141563997	
6.72500038" "	0.123822004	
6.62500048" "	0.102707997	
8.67500019" "	0.080725901	
8.97500038" "	0.0647965	
9.82500076" "	0.057742	
8.77500057" "	0.0577267	
9.22500038" "	0.056444898	
8.02500057" "	0.0549049	
9.07500076" "	0.0523431	
9.27500057" "	0.051940601	
9.92500019" "	0.050994098	
9.02500057" "	0.050936699	
8.17500019" "	0.049567401	
9.52500057" "	0.048691101	
9.97500038" "	0.048231501	
9.87500000" "	0.048103701	
9.77500057" "	0.045664798	
9.42500019" "	0.043876499	
9.62500000" "	0.0438172	
9.47500038" "	0.043655101	
8.92500019" "	0.043543	
9.32500076" "	0.043239001	
8.12500000" "	0.043184999	
9.17500019" "	0.041376401	
9.37500000" "	0.040614299	
9.57500076" "	0.040134799	
8.72500038" "	0.038870499	
9.67500019" "	0.038605802	
9.72500038" "	0.030107301	
4.52500010" "	0.0256663	

VIP for PLS-DA regarding motor component of FIM

Primary ID (chemical shift)	VIP	Targeted metabolites
2.17500019 " "	3.54028010 4	Paracetamol (Acetaminophen) + Acetaminophen glucuronide
3.62500024 " "	3.164220095	
7.12500048 " "	2.70602989 2	Acetaminophen derivatives
3.27500033 " "	2.573440075	
4.07500029 " "	2.467999935	
3.97500038 " "	2.323559999	
3.02500033 " "	2.307369947	
7.82500029 " "	2.286619902	
7.32500029 " "	2.238549948	
1.92500031 " "	1.94774997 2	Acetate
3.57500029 " "	1.89581000 8	Glycine
2.67500019 " "	1.870460033	
7.57500029 " "	1.669399977	
7.37500048 " "	1.669059992	
7.52500057 " "	1.64388001	
8.82500076 " "	1.463950038	
0.87500024 " "	1.456159949	
3.87500024 " "	1.446959972	
7.62500048 " "	1.441059947	
4.42500019 " "	1.38530004	
3.32500029 " "	1.357059956	
7.17500019 " "	1.34720003 6	Acetaminophen derivatives
2.12500024 " "	1.308109999	
2.57500029 " "	1.302189946	
3.77500033 " "	1.301290035	
8.07500076 " "	1.272570014	
4.02500010 " "	1.263440013	
2.52500033 " "	1.250480056	
3.22500038 " "	1.201089978	
3.72500038 " "	1.161170006	
1.27500021 " "	1.142920017	
3.92500019 " "	1.118489981	
2.87500024 " "	1.070240021	
1.42500031 " "	1.070160031	
3.52500033 " "	1.055189967	
2.47500038 " "	1.046519995	
3.82500029 " "	1.023939967	
9.12500000 " "	1.000180006	
7.02500057 " "	0.992079973	
3.12500024 " "	0.965856016	

6.97500038" "	0.924398005	
3.67500019" "	0.916547	
4.32500029" "	0.907444	
2.32500029" "	0.896317005	
7.42500019" "	0.84702599	
3.07500029" "	0.837459028	
1.32500029" "	0.831602991	
1.22500026" "	0.829024971	
3.17500019" "	0.827152014	
2.82500029" "	0.810347021	
4.27500010" "	0.795050979	
1.02500021" "	0.794301987	
1.07500029" "	0.786082983	
7.07500029" "	0.778559983	
3.37500024" "	0.768333018	
4.47500038" "	0.755715013	
1.17500019" "	0.749069989	
3.42500019" "	0.744826019	
0.92500025" "	0.737303019	
7.47500038" "	0.725162029	
7.97500038" "	0.722177982	
8.57500076" "	0.716573	
4.17500019" "	0.698027015	
1.47500026" "	0.697835028	
2.42500019" "	0.686851978	
0.72500026" "	0.680082023	
2.77500033" "	0.679543018	
2.22500038" "	0.66575497	4 Acetone
2.37500024" "	0.653419971	
4.12500048" "	0.641063988	
1.87500024" "	0.638963997	
8.47500038" "	0.622466981	
2.62500024" "	0.61709702	
1.82500029" "	0.612757027	
7.67500019" "	0.610632002	
3.47500038" "	0.605764985	
2.97500038" "	0.602792025	
2.02500033" "	0.602522016	
1.62500024" "	0.592383027	
7.72500038" "	0.58287698	
1.52500021" "	0.577071011	
6.82500029" "	0.553602993	
4.37500048" "	0.549178004	
1.37500024" "	0.540980995	
2.92500019" "	0.532335997	
4.22500038" "	0.511853993	

1.67500031" "	0.486193001	
7.22500038" "	0.484183013	
1.57500029" "	0.483810991	
0.97500026" "	0.483559996	
1.77500021" "	0.475443989	
6.87500048" "	0.450325012	
8.62500000" "	0.433279008	
2.07500029" "	0.431243986	
7.27500057" "	0.427237988	
8.87500000" "	0.422962993	
7.77500057" "	0.416563988	
2.27500033" "	0.412259996	
6.62500048" "	0.399426997	
1.72500026" "	0.397323012	
6.77500057" "	0.39261201	
1.12500024" "	0.382423997	
8.17500019" "	0.37281099	
2.72500038" "	0.36721599	1 Dimethylamine
	1	
7.87500048" "	0.338402987	
0.82500023" "	0.333602995	
8.37500000" "	0.326135993	
0.62500024"	0.319480002	
6.57500029" "	0.308353007	
6.52500010" "	0.306014001	
0.67500025" "	0.304387987	
8.52500057" "	0.303461999	
8.22500038" "	0.300437003	
6.92500019" "	0.298218995	
7.92500019" "	0.288340986	
1.97500026" "	0.281796992	
6.67500019" "	0.279828995	
0.77500021" "	0.262273997	
6.72500038" "	0.257734001	
8.32500076" "	0.257587999	
8.27500057" "	0.218898997	
8.02500057" "	0.214447007	
8.12500000" "	0.206196994	
8.42500019" "	0.165461004	
8.67500019" "	0.132401004	
9.02500057" "	0.115324996	
8.77500057" "	0.109944999	
9.72500038" "	0.108014002	
8.97500038" "	0.100500003	
9.27500057" "	0.096881799	
8.92500019" "	0.093246996	
9.67500019" "	0.092921101	

9.97500038" "	0.0894325	
8.72500038" "	0.088609204	
9.22500038" "	0.087710597	
9.82500076" "	0.085960403	
9.17500019" "	0.085089602	
9.87500000" "	0.085039802	
9.07500076" "	0.084417097	
9.42500019" "	0.081428401	
9.62500000" "	0.076260403	
9.37500000" "	0.075103603	
9.92500019" "	0.0707964	
9.52500057" "	0.069924198	
9.77500057" "	0.068051398	
9.32500076" "	0.067642398	
9.57500076" "	0.067051597	
9.47500038" "	0.0628362	
4.52500010" "	0.050185699	

VIP for PLS-DA regarding cognitive component of FIM

Primary ID (chemical shift)	VIP	Targeted metabolites
2.17500019" "	3.580670118	Paracetamol (Acetaminophen) + Acetaminophen glucuronide
3.27500033" "	3.120130062	
3.62500024" "	2.989099979	
7.12500048" "	2.876940012	Acetaminophen derivatives
4.07500029" "	2.445760012	
7.32500029" "	2.128540039	
7.17500019" "	2.019740105	Acetaminophen derivatives
3.02500033" "	2.00109005	
4.02500010" "	1.971529961	
3.87500024" "	1.906350017	
1.92500031" "	1.833989978	
2.12500024" "	1.819540024	
7.82500029" "	1.796790004	
3.97500038" "	1.785560012	
7.22500038" "	1.718140006	
3.77500033" "	1.674640059	
7.37500048" "	1.636000037	
4.42500019" "	1.60066998	
7.57500029" "	1.496700048	
3.92500019" "	1.38609004	

7.92500019" "	1.316509962	
3.17500019" "	1.300420046	
2.22500038" "	1.22109997 3	Acetone
3.72500038" "	1.21239996	
7.47500038" "	1.189399958	
2.72500038" "	1.12205004 7	Dimethylamine
7.27500057" "	1.077280045	
2.87500024" "	1.062770009	
7.62500048" "	1.054219961	
3.42500019" "	1.052209973	
3.47500038" "	1.045979977	
1.17500019" "	1.036749959	
1.42500031" "	1.016250014	
3.52500033" "	1.015699983	
3.37500024" "	0.979201019	
3.07500029" "	0.972541988	
3.82500029" "	0.956556976	
0.87500024" "	0.953836024	
1.87500024" "	0.94491601	
6.62500048" "	0.942669988	
8.82500076" "	0.917770982	
4.17500019" "	0.914976001	
7.42500019" "	0.910874009	
3.57500029" "	0.882044971	
2.57500029" "	0.869125009	
1.32500029" "	0.850059986	
2.27500033" "	0.849956989	
0.97500026" "	0.833805978	
2.67500019" "	0.829720974	
1.22500026" "	0.818176985	
9.12500000" "	0.804977	
3.67500019" "	0.803331017	
4.12500048" "	0.798340976	
2.62500024" "	0.798174977	
1.72500026" "	0.790269017	
1.67500031" "	0.776252985	
7.52500057" "	0.769765973	
2.52500033" "	0.756511986	
4.37500048" "	0.752882004	
3.12500024" "	0.742497027	
3.22500038" "	0.739880979	
6.67500019" "	0.734220982	
2.07500029" "	0.728034973	
1.77500021" "	0.721665025	
8.87500000" "	0.697538972	

1.62500024" "	0.694299996	
1.47500026" "	0.685970008	
2.32500029" "	0.676155984	
8.02500057" "	0.675288975	
1.02500021" "	0.674024999	
4.22500038" "	0.666764975	
1.57500029" "	0.663012981	
6.92500019" "	0.659008026	
1.12500024" "	0.658065021	
2.37500024" "	0.649703026	
4.47500038" "	0.646278977	
1.27500021" "	0.639084995	
2.92500019" "	0.639055014	
4.32500029" "	0.634131014	
2.47500038" "	0.632076979	
1.82500029" "	0.62866497	
2.97500038" "	0.619919002	
1.97500026" "	0.616255999	
2.82500029" "	0.599489987	
7.02500057" "	0.598078012	
2.77500033" "	0.574346006	
7.07500029" "	0.566619992	
0.92500025" "	0.564047992	
3.32500029" "	0.560163975	
1.07500029" "	0.559525013	
1.37500024" "	0.539552987	
7.67500019" "	0.536579013	
6.82500029" "	0.529246986	
4.27500010" "	0.516021013	
7.97500038" "	0.507849991	
1.52500021" "	0.501192987	
6.57500029" "	0.485552996	
2.42500019" "	0.482279003	
8.07500076" "	0.473531991	
2.02500033" "	0.468286991	
6.52500010" "	0.450183988	
0.77500021" "	0.448561013	
6.72500038" "	0.4444444001	
0.72500026" "	0.439058006	
0.82500023" "	0.388603002	
7.77500057" "	0.385067999	
8.47500038" "	0.382245988	
8.57500076" "	0.380443007	
8.17500019" "	0.379078001	
7.72500038" "	0.372675002	
8.62500000" "	0.365193993	

0.67500025" "	0.363397002	
6.87500048" "	0.361054987	
6.77500057" "	0.343887001	
0.62500024"	0.322932988	
8.12500000" "	0.279980004	
8.52500057" "	0.246543005	
8.37500000" "	0.234124005	
6.97500038" "	0.198933005	
8.22500038" "	0.191062003	
7.87500048" "	0.179527	
8.32500076" "	0.168852001	
8.27500057" "	0.166382998	
8.67500019" "	0.118749	
9.17500019" "	0.101682	
9.97500038" "	0.084938802	
8.92500019" "	0.079984598	
9.37500000" "	0.075677097	
9.47500038" "	0.071273603	
9.62500000" "	0.070294097	
9.42500019" "	0.070078	
8.77500057" "	0.068929501	
9.87500000" "	0.068564601	
8.72500038" "	0.0683439	
9.57500076" "	0.068337001	
9.07500076" "	0.0666508	
9.77500057" "	0.064819098	
9.67500019" "	0.061509501	
9.92500019" "	0.0606381	
9.32500076" "	0.060236402	
9.02500057" "	0.056683999	
8.97500038" "	0.0558246	
9.82500076" "	0.055767801	
9.52500057" "	0.055245999	
9.27500057" "	0.0551618	
9.72500038" "	0.048636999	
9.22500038" "	0.0460383	
4.52500010" "	0.044241302	
8.42500019" "	0.042750999	

VIP for PLS-DA regarding SPPB at baseline
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Primary ID (chemical shift)	VIP	Targeted metabolites
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2.17500019 " "	3.51290988 9	Paracetamol (Acetaminophen) + Acetaminophen glucuronide
3.62500024" "	2.815459967	
3.27500033" "	2.596070051	
4.07500029" "	2.400540113	
3.77500033" "	2.246860027	
7.12500048" "	2.225270033	
7.82500029" "	2.221560001	
7.32500029" "	2.199219942	
3.87500024" "	2.149600029	
3.97500038" "	2.070549965	
2.67500019" "	2.01748991	
4.02500010" "	2.000869989	
3.82500029" "	1.882419944	
7.37500048" "	1.854269981	
3.72500038" "	1.827110052	
7.57500029" "	1.667490005	
3.92500019" "	1.649359941	
3.52500033" "	1.584100008	
3.57500029" "	1.533220053	
3.22500038" "	1.506680012	
7.17500019" "	1.505849957	
7.62500048" "	1.421370029	
7.52500057" "	1.420379996	
3.02500033" "	1.413159966	
3.67500019" "	1.398100019	
1.92500031 " "	1.37223005 3	Acetate
0.87500024" "	1.334879994	
8.82500076" "	1.33265996	
4.42500019" "	1.307279944	
7.02500057" "	1.277809978	
1.42500031" "	1.210500002	
1.17500019" "	1.181879997	
1.37500024 " "	1.16726005 1	Lactate
1.22500026" "	1.148399949	
1.27500021" "	1.101240039	
7.27500057" "	1.069120049	
6.97500038" "	1.057010055	
1.07500029" "	1.017740011	
2.57500029" "	0.996105015	
1.52500021" "	0.989895999	
2.52500033" "	0.974425972	
9.12500000" "	0.892669022	
3.42500019" "	0.891768992	
2.87500024" "	0.871680021	

7.77500057" "	0.865637004	
3.07500029" "	0.858089983	
1.32500029" "	0.831487	
2.22500038" "	0.815463006	Acetone
2.47500038" "	0.764791012	
3.32500029" "	0.763934016	
4.32500029" "	0.755107999	
2.32500029" "	0.741243005	
2.92500019" "	0.739591002	
7.07500029" "	0.738407016	
3.37500024" "	0.738063991	
7.42500019" "	0.720871985	
3.17500019" "	0.712769985	
8.07500076" "	0.700515985	
4.47500038" "	0.690396011	
3.47500038" "	0.68800801	
7.47500038" "	0.682518005	
8.57500076" "	0.666337013	
4.27500010" "	0.657073021	
2.62500024" "	0.650548995	
6.87500048" "	0.64408499	
2.72500038" "	0.641593993	
0.72500026" "	0.631887019	
3.12500024" "	0.627487004	
4.17500019" "	0.626119971	
4.12500048" "	0.623179972	
1.47500026" "	0.609432995	Alanine
7.22500038" "	0.606330991	
2.02500033" "	0.601077974	
2.12500024" "	0.592585027	
2.42500019" "	0.581004977	
4.22500038" "	0.574449003	
4.37500048" "	0.562601984	
1.02500021" "	0.560297012	
2.82500029" "	0.559713006	
7.97500038" "	0.544098973	
8.22500038" "	0.542212009	
1.97500026" "	0.542168975	
8.02500057" "	0.533838987	
1.67500031" "	0.516384006	
1.82500029" "	0.499345988	
2.07500029" "	0.492547989	
7.67500019" "	0.479490995	
2.37500024" "	0.470099002	
0.97500026" "	0.468342006	

1.72500026" "	0.454252005	
1.87500024" "	0.429001004	
1.62500024" "	0.422419995	
2.77500033" "	0.410780996	
0.92500025" "	0.404621005	
1.57500029" "	0.403654993	
7.72500038" "	0.399958014	
8.62500000" "	0.391770989	
2.97500038" "	0.388238013	
1.12500024" "	0.362291008	
1.77500021" "	0.361378014	
7.92500019" "	0.342976004	
6.82500029" "	0.33495301	
8.87500000" "	0.306769013	
0.82500023" "	0.301243991	
6.92500019" "	0.288818002	
8.27500057" "	0.255508006	
0.77500021" "	0.242476001	
8.32500076" "	0.239109993	
0.67500025" "	0.232228994	
0.62500024"	0.229100004	
2.27500033" "	0.222666994	
6.62500048" "	0.215443999	
8.52500057" "	0.205983996	
6.77500057" "	0.181765005	
8.12500000" "	0.177134007	
8.47500038" "	0.173688993	
8.37500000" "	0.168236002	
7.87500048" "	0.166931003	
6.67500019" "	0.166602999	
9.72500038" "	0.139479995	
8.77500057" "	0.138460994	
6.72500038" "	0.136855006	
6.57500029" "	0.107058004	
9.82500076" "	0.101692997	
9.07500076" "	0.098023199	
8.17500019" "	0.0966281	
6.52500010" "	0.095339902	
9.77500057" "	0.091663398	
9.92500019" "	0.087485597	
9.22500038" "	0.0857803	
9.52500057" "	0.080743998	
9.87500000" "	0.076461099	
9.62500000" "	0.076252401	
8.72500038" "	0.074013397	
9.67500019" "	0.072376303	

9.32500076" "	0.072365902	
9.27500057" "	0.0679399	
9.57500076" "	0.065350302	
4.52500010" "	0.063555896	
8.67500019" "	0.0601914	
9.97500038" "	0.059533998	
9.37500000" "	0.059182301	
8.97500038" "	0.055453699	
8.92500019" "	0.055011801	
9.02500057" "	0.054043699	
9.42500019" "	0.052002799	
8.42500019" "	0.0471517	
9.47500038" "	0.046968799	
9.17500019" "	0.0388784	

VIP for PLS-DA regarding SPPB after 12 months

Primary ID (chemical shift)	VIP	Targeted metabolites
4.07500029" "	3.433180094	
3.27500033" "	3.269949913	TMAO
2.17500019" "	2.837589979	
7.82500029" "	2.326329947	
7.52500057" "	2.282910109	
7.17500019" "	2.20314002	
7.12500048" "	2.202950001	
2.67500019" "	2.023780107	
3.22500038" "	1.941140056	
8.82500076" "	1.932309985	
3.97500038" "	1.86135006	
4.42500019" "	1.837069988	
3.57500029" "	1.817579985	
4.02500010" "	1.726169944	
2.87500024" "	1.627320051	
3.12500024" "	1.618720055	
1.87500024" "	1.594799995	
7.62500048" "	1.590489984	Hippuric acid
3.72500038" "	1.562039971	
3.62500024" "	1.526039958	
2.52500033" "	1.450109959	
7.37500048" "	1.435490012	
7.32500029" "	1.426010013	
0.87500024" "	1.396839976	
9.12500000" "	1.360780001	

4.27500010" "	1.336619973	
2.57500029" "	1.331959963	
1.27500021" "	1.304810047	
1.42500031" "	1.197999954	
7.57500029" "	1.13301003	
2.32500029" "	1.125509977	
2.47500038" "	1.118489981	
3.07500029" "	1.111829996	
3.52500033" "	1.107740045	
3.67500019" "	1.063949943	
2.42500019" "	1.056030035	
4.47500038" "	1.047000051	
2.12500024" "	1.034809947	
2.02500033" "	1.019330025	
3.02500033" "	0.98951	
7.92500019" "	0.988188028	
3.17500019" "	0.972037971	
1.92500031" "	0.952609003	Acetate
8.57500076" "	0.928424001	
7.02500057" "	0.922134995	
3.37500024" "	0.917999029	
4.32500029" "	0.859907985	
2.22500038" "	0.855675995	Acetone
3.87500024" "	0.84246701	
3.42500019" "	0.837758005	
8.07500076" "	0.826223016	
7.07500029" "	0.808574975	
4.22500038" "	0.801088989	
4.17500019" "	0.793448985	
4.12500048" "	0.790503979	
3.77500033" "	0.757955015	
7.27500057" "	0.756859004	
4.37500048" "	0.742093027	
1.07500029" "	0.730614007	
1.37500024" "	0.722832024	
3.32500029" "	0.691488981	
6.97500038" "	0.690173984	
1.17500019" "	0.675261974	
1.52500021" "	0.674032986	
1.47500026" "	0.658580005	
2.97500038" "	0.651938975	
2.92500019" "	0.625930011	
2.27500033" "	0.623319983	
2.77500033" "	0.619596004	
1.22500026" "	0.616451025	
7.47500038" "	0.615541995	

3.82500029" "	0.613763988	
1.02500021" "	0.604955971	
1.32500029" "	0.593318999	Lactate
2.37500024" "	0.586853981	
8.17500019" "	0.586709976	
6.82500029" "	0.584164023	
7.67500019" "	0.579671979	
1.72500026" "	0.566438973	
1.62500024" "	0.554705977	
2.72500038" "	0.550706983	
3.92500019" "	0.536671996	
2.07500029" "	0.529794991	
1.82500029" "	0.528501987	
6.62500048" "	0.523881972	
7.42500019" "	0.515685976	
6.87500048" "	0.5111116028	
0.92500025" "	0.504585981	
1.67500031" "	0.488467008	
7.77500057" "	0.482813001	
8.22500038" "	0.480168015	
7.87500048" "	0.473710001	
6.92500019" "	0.461053014	
1.77500021" "	0.457747012	
8.87500000" "	0.457242012	
8.47500038" "	0.451622993	
8.37500000" "	0.440632999	
1.57500029" "	0.417923987	
1.97500026" "	0.408549011	
2.82500029" "	0.408241004	
6.77500057" "	0.390648007	
3.47500038" "	0.383183002	
0.97500026" "	0.382909	Valine
8.62500000" "	0.373353004	
6.72500038" "	0.365529001	
7.22500038" "	0.364944994	
0.72500026" "	0.360915989	
8.27500057" "	0.356056988	
7.72500038" "	0.315138996	
6.67500019" "	0.313432008	
8.52500057" "	0.304044008	
6.57500029" "	0.295473993	
0.82500023" "	0.292849988	
7.97500038" "	0.291307002	
0.67500025" "	0.267298013	
0.62500024"	0.26086399	
2.62500024" "	0.254456013	

0.77500021" "	0.237210006	
6.52500010" "	0.231463999	
8.32500076" "	0.205871001	
8.12500000" "	0.205523998	
1.12500024" "	0.199608997	
8.42500019" "	0.175608993	
8.02500057" "	0.144948006	
8.67500019" "	0.111160003	
8.77500057" "	0.107490003	
9.72500038" "	0.102008	
9.02500057" "	0.090320602	
9.07500076" "	0.077213898	
9.82500076" "	0.076349102	
4.52500010" "	0.075899497	
9.77500057" "	0.070663698	
9.92500019" "	0.061778601	
9.27500057" "	0.061314501	
8.97500038" "	0.058582202	
8.72500038" "	0.0576168	
8.92500019" "	0.054319501	
9.52500057" "	0.050620198	
9.17500019" "	0.047325801	
9.97500038" "	0.046857402	
9.87500000" "	0.046033502	
9.22500038" "	0.045117699	
9.32500076" "	0.043583799	
9.67500019" "	0.043511599	
9.42500019" "	0.036835201	
9.47500038" "	0.036793798	
9.37500000" "	0.0359479	
9.57500076" "	0.033355899	
9.62500000" "	0.033151899	