

Supplementary Table 1. Principal component (PC) 1 loadings of significant metabolites from urine (*General Metabolism*) following FS-CR. Positive loadings (shaded) are correlated with **BAS1** and negative are correlated with **BAS2**. Numeric metabolites had a spectral match factor < 800.

Metabolite	PC1 (29.35%)
406846	-2.10E-01
401047	-2.05E-01
222303	-1.79E-01
34083	-1.75E-01
389988	-1.65E-01
18305	-1.64E-01
127665	-1.63E-01
520639	-1.56E-01
6376	-1.53E-01
33401	-1.52E-01
112261	-1.36E-01
356986	-1.27E-01
2,3-dihydroxybutanoic acid (tartaric acid)	-1.16E-01
arabitol	-1.16E-01
cellobiose	-1.08E-01
alanine-alanine	-9.84E-02
1981	-9.62E-02
34015	-9.22E-02
glycerol	-6.88E-02
pipecolic acid	8.18E-02
4929	8.28E-02
167348	8.28E-02
395930	9.19E-02
2'-deoxyguanosine	9.29E-02
piperidone	9.47E-02
122843	1.01E-01
cytosine	1.04E-01
118995	1.04E-01
glycylglycine	1.10E-01
glucose-6-phosphate	1.18E-01
209677	1.20E-01
189936	1.23E-01
117201	1.37E-01
131989	1.40E-01
20903	1.42E-01
7543	1.43E-01
N-acetylmethionine	1.46E-01
17143	1.58E-01
4983	1.62E-01
pentadecanoic acid	1.64E-01
118989	1.65E-01
209172	1.70E-01
105214	1.74E-01
404049	1.80E-01
uric acid	1.88E-01
nicotinamide	1.97E-01
379063	2.06E-01
210798	2.16E-01

Supplementary Table 2. Principal component (PC) 1 loadings of significant metabolites from stool (*General Metabolism*) following FS-CR. Negative loadings (shaded) are correlated with **BAS1** and positive are correlated with **BAS2**. Numeric metabolites had a spectral match factor < 800.

Variable	PC 1 (48.59%)
cadaverine	-1.58E-01
12444	-1.55E-01
87712	-1.53E-01
trans-4-hydroxyproline	-1.44E-01
tryptamine	-1.43E-01
isopalmitic acid	-1.22E-01
4550	-7.86E-02
480022	1.05E-01
fructose	1.07E-01
117201	1.09E-01
199109	1.23E-01
sinigrin	1.27E-01
sophorose	1.39E-01
371546	1.47E-01
416595	1.56E-01
pipecolinic acid	1.57E-01
209172	1.57E-01
110429	1.63E-01
87282	1.65E-01
20282	1.67E-01
220224	1.68E-01
3,6-anhydro-D-galactose	1.68E-01
phenylacetic acid	1.76E-01
114501	1.78E-01
127847	1.82E-01
372458	1.83E-01
erythrose	1.84E-01
palmitoleic acid	1.85E-01
N-acetyl-D-tryptophan	1.86E-01
528624	1.87E-01
146226	1.89E-01
389988	1.96E-01
2-deoxyerythritol	1.97E-01
UDP-glucuronic acid	2.03E-01
18157	2.03E-01
384914	2.04E-01
64891	2.05E-01

Supplementary Table 3. Principal component (PC) 1 loadings of significant metabolites from serum (*General Metabolism*) following FS-CR. Positive loadings (shaded) are correlated with **BAS1** and negative are correlated with **BAS2**. Numeric metabolites had a spectral match factor < 800.

Variable	PC1 (82.30%)
34089	-2.97E-01
346241	2.99E-01
31764	3.06E-01
1380	3.09E-01
354256	3.13E-01
124484	3.23E-01
3-Amino-2-piperidone	3.23E-01
345436	3.25E-01
372458	3.30E-01
2-picolinic acid	3.34E-01

Supplementary Table 4. Principal component (PC) 1 loadings of significant metabolites from urine (*Complex Lipids*) following FS-CR. Positive loadings (shaded) are correlated with **BAS1** and negative are correlated with **BAS2**.

Variable	PC 1 (41.83%)
0.18_172.99	-1.89E-01
0.19_148.10	-1.88E-01
0.19_245.15	-1.79E-01
0.24_312.22	-1.74E-01
0.21_305.16	-1.72E-01
0.23_260.22	-1.71E-01
0.21_569.31	-1.68E-01
0.24_215.03	-1.51E-01
0.19_212.00	-1.46E-01
0.20_192.07	-1.37E-01
0.20_238.02	-1.23E-01
3.84_934.79	9.61E-02
0.26_152.07	1.18E-01
0.25_382.26	1.21E-01
0.23_297.00	1.26E-01
0.18_135.03	1.44E-01
1.59_568.43	1.46E-01
1.43_584.42	1.59E-01
0.20_124.01	1.61E-01
TG 62:14 TG 20:4_20:4_22:6	1.62E-01
0.20_265.15	1.62E-01
TG 60:13 TG 20:4_20:4_20:5	1.67E-01
0.20_145.13	1.68E-01
2.48_123.06	1.72E-01
0.19_218.10	1.72E-01
0.20_230.12	1.73E-01
3.54_968.77	1.78E-01
1.52_123.06	1.81E-01
0.26_141.07	1.81E-01
0.60_123.06	1.82E-01
0.24_166.09	1.87E-01
0.21_123.06	1.87E-01
3.21_538.45	1.90E-01
0.21_138.09	1.95E-01
0.21_137.07	2.02E-01
0.30_297.15	2.03E-01

Supplementary Table 5. Principal component (PC) 1 loadings of significant metabolites from stool (*Complex Lipids*) following FS-CR. Positive loadings (shaded) are correlated with **BAS1** and negative are correlated with **BAS2**.

Variable	PC 1 (76.69%)
1.34_445.37	-1.72E-01
1.33_479.32	-1.66E-01
FA 17:0	-1.65E-01
0.94_355.29	-1.44E-01
0.23_324.23	1.30E-01
2.30_207.10	1.32E-01
2.30_490.43	1.33E-01
0.22_453.20	1.39E-01
FA 20:5 (eicosapentaenoic acid)	1.40E-01
0.47_380.31	1.40E-01
4.13_858.79	1.45E-01
3.78_896.83	1.52E-01
TG 48:4 Isomer A	1.55E-01
4.16_954.83	1.58E-01
0.22_168.07	1.60E-01
0.21_495.30	1.60E-01
0.23_496.31	1.63E-01
0.23_387.20	1.64E-01
3.87_974.82	1.64E-01
0.34_329.18	1.68E-01
4.07_822.81	1.74E-01
TG 46:3 Isomer A	1.75E-01
4.06_549.49	1.76E-01
TG 55:6 TG 17:1_18:1_20:4	1.78E-01
4.07_976.83	1.80E-01
0.23_309.16	1.80E-01
TG 62:12 TG 20:3_20:4_22:5	1.81E-01
0.75_304.30	1.82E-01
TG 46:5	1.82E-01
0.19_162.06	1.83E-01
0.19_206.05	1.84E-01
1.55_569.43	1.87E-01
1.59_568.43	1.87E-01
2.24_552.43	1.87E-01
1.36_568.43	1.89E-01
1.39_568.48	1.89E-01

Supplementary Table 6. Principal component (PC) 1 loadings of significant metabolites from serum (*Complex Lipids*) following FS-CR. Negative loadings (shaded) are correlated with **BAS1** and positive are correlated with **BAS2**.

Variable	PC 1 (82.63%)
PC 38:5 Isomer B	-1.92E-01
2.31_858.59	-1.89E-01
3.21_538.45	-1.88E-01
3.31_542.48	-1.86E-01
2.32_860.62	-1.85E-01
3.18_540.47	-1.84E-01
2.23_819.61	-1.84E-01
3.69_971.79	-1.82E-01
2.10_766.58	-1.82E-01
PC 40:7 Isomer B	-1.80E-01
2.39_836.67	-1.76E-01
2.08_832.65	-1.75E-01
1.47_569.43	-1.71E-01
2.31_837.61	-1.68E-01
2.50_814.68	1.74E-01
PC 37:4	1.75E-01
2.26_798.59	1.77E-01
PC 37:3	1.79E-01
2.49_813.57	1.80E-01
2.12_729.65	1.82E-01
2.33_780.59	1.83E-01
2.15_754.57	1.84E-01
2.13_1586.11	1.85E-01
2.47_749.59	1.85E-01
SM d36:2	1.86E-01
2.13_782.78	1.86E-01
PC 33:0	1.87E-01
2.56_774.61	1.87E-01
2.21_770.57	1.89E-01
1.98_727.58	1.94E-01

Supplementary Table 7. Principal component (PC) 1 loadings of significant metabolites from urine (*Biogenic Amines*) following FS-CR. Negative loadings (shaded) are correlated with **BAS1** and positive are correlated with **BAS2**.

Variable	PC 1 (46.35%)
1.43_137.07	-1.36E-01
1.43_136.65	-1.35E-01
1.43_139.08	-1.33E-01
1.43_94.06	-1.32E-01
(2-oxo-2,3-dihydro-1H-indol-3-yl)acetic acid	-1.24E-01
0.41_146.06	-1.23E-01
0.45_375.17	-1.22E-01
0.41_174.05	-1.21E-01
0.29_385.13	-1.18E-01
2.23_195.05	-1.14E-01
N-Acetylmannosamine	-1.14E-01
1.87_349.12	-1.13E-01
1.93_278.06	-1.08E-01
0.29_399.14	-1.07E-01
0.30_415.13	-1.06E-01
CMPF	-1.06E-01
His-Tyr	-1.06E-01
1.76_176.01	-1.05E-01
0.35_106.03	-1.05E-01
2.01_321.08	-1.05E-01
0.74_258.07	-1.04E-01
Ser-Arg	-1.04E-01
0.53_74.02	-1.03E-01
0.30_431.13	-1.02E-01
Ala-Pro	-1.01E-01
0.37_260.11	-1.00E-01
2.39_187.94	-9.90E-02
Threonic acid	-9.87E-02
1.03_135.03	-9.78E-02
Nicotinamide	-9.75E-02
1.23_264.04	-9.69E-02
0.31_415.22	-9.64E-02
2.20_710.24	-9.52E-02
2.18_458.05	-9.34E-02
1.03_175.00	-9.20E-02
N-Methylhistidine	-9.16E-02
1.91_242.09	-8.62E-02
Dopamine	-8.30E-02
0.36_431.22	-8.26E-02
0.47_312.97	-8.12E-02
1.29_495.32	-8.12E-02
Pyrrole-2-carboxylic acid	-8.07E-02
1.88_238.08	-8.05E-02
0.31_503.28	-7.84E-02
1.35_649.32	-7.79E-02
1.42_438.23	-7.77E-02
Asp-Asp	-7.60E-02
Phe-Val	7.91E-02
0.26_241.97	8.56E-02

1.86_245.15	8.57E-02
0.29_184.07	8.67E-02
0.30_572.41	8.78E-02
1.32_243.97	8.81E-02
1.62_143.05	9.02E-02
1.50_189.16	9.04E-02
2.32_149.01	9.17E-02
1.46_60.05	9.20E-02
1.90_315.27	9.22E-02
N-Methylphenylalanine	9.30E-02
0.62_407.11	9.39E-02
0.29_202.08	9.65E-02
1.21_306.90	9.84E-02
1.86_277.08	9.85E-02
1.48_314.18	9.88E-02
Phenyl glucuronide	1.02E-01
0.54_916.55	1.03E-01
1.79_245.15	1.04E-01
0.62_291.99	1.05E-01
Tartaric acid	1.05E-01
Mirtazapine	1.06E-01
0.43_206.08	1.10E-01
4-Aminomethylcyclohexanecarboxylic acid	1.11E-01
0.23_254.01	1.13E-01
0.29_514.36	1.14E-01
0.77_135.09	1.14E-01
1.86_184.09	1.17E-01
Propoxyphene	1.17E-01
0.32_460.04	1.17E-01
Methacholine cation	1.18E-01
1.87_185.10	1.18E-01
0.29_456.31	1.19E-01
1.86_125.02	1.20E-01
1.38_160.13	1.20E-01
Tyr-Phe	1.26E-01
1.39_279.08	1.28E-01
1.86_200.06	1.28E-01
1.86_369.10	1.28E-01
1.60_196.03	1.29E-01
1.30_258.17	1.33E-01
1.80_205.10	1.34E-01

Supplementary Table 8. Principal component (PC) 1 loadings of significant metabolites from stool (*Biogenic Amines*) following FS-CR. Positive loadings (shaded) are correlated with **BAS1** and negative are correlated with **BAS2**.

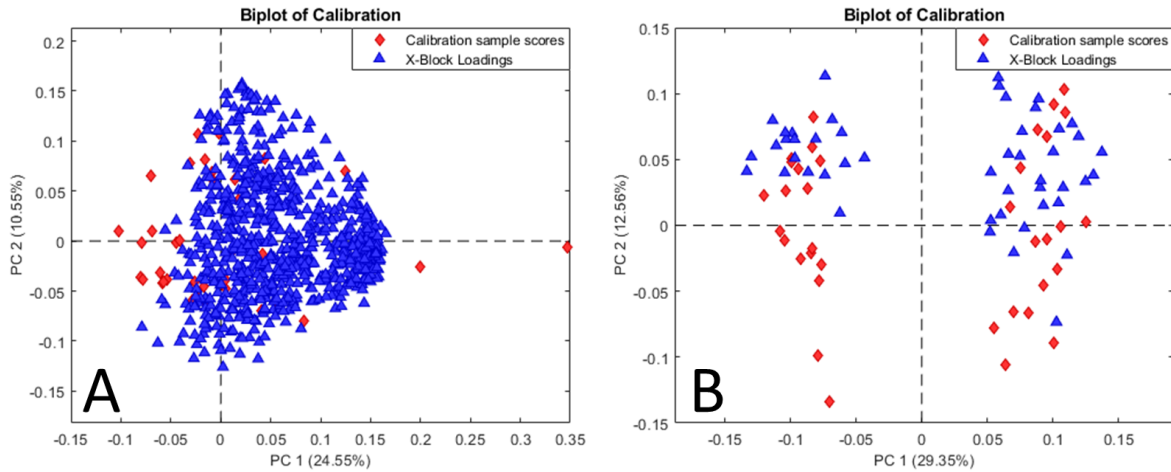
Variable	PC 1 (54.20%)
0.31_373.15	-1.33E-01
Prochlorperazine	-1.28E-01
1.79_186.05	-1.22E-01
2.09_449.17	-1.17E-01
2.50_403.92	-1.13E-01
0.41_164.03	-1.10E-01
1.59_359.07	-1.10E-01
2.12_491.17	-1.09E-01
0.31_631.26	-1.01E-01
0.30_572.41	-9.95E-02
2.24_373.24	-9.74E-02
Stachydrine	-9.60E-02
0.30_629.26	-9.30E-02
0.26_536.38	-8.51E-02
1.47_358.22	-8.37E-02
1.88_278.06	-7.82E-02
1.57_189.05	-7.31E-02
1.39_336.23	6.52E-02
Temozolomide	7.17E-02
CHEMBL1616521	7.88E-02
Glycerophosphocholine	8.13E-02
2-dGMP	8.38E-02
0.24_126.90	8.44E-02
0.33_73.00	8.66E-02
0.21_490.42	9.08E-02
alpha-Tocopheryl acetate	9.10E-02
3-Pyridinemethanol	9.73E-02
1.59_222.04	9.92E-02
0.90_219.01	1.00E-01
O-Acetylsalicylic acid	1.02E-01
1.25_703.57	1.02E-01
1.00_189.98	1.06E-01
1.47_184.10	1.07E-01
0.91_142.99	1.07E-01
0.40_213.12	1.08E-01
Benzene-1,2,4-triol	1.10E-01
0.36_509.16	1.15E-01
1.39_184.10	1.16E-01
1.43_317.13	1.21E-01
Caffeic acid	1.22E-01
3,4-Dihydroxybenzoic acid	1.24E-01
0.56_151.12	1.29E-01
Formononetine	1.30E-01
Tyr-His	1.30E-01
3-Hydroxyanthranilic acid	1.33E-01
Cytosine	1.37E-01
Kaempferol	1.37E-01
2,3-Dihydroxybenzoic acid B	1.40E-01
0.52_151.12	1.41E-01

1.16_577.36	1.42E-01
0.46_185.09	1.43E-01
0.54_244.08	1.44E-01
0.85_305.96	1.45E-01
1.26_539.27	1.45E-01
Cytarabine	1.46E-01
0.46_165.14	1.47E-01
Clonidine	1.47E-01
1.38_631.37	1.50E-01
1.26_533.24	1.50E-01
Glu-Ala	1.51E-01
3-(1-Pyrazolyl)-alanine	1.54E-01
1.28_110.06	1.55E-01
0.85_451.04	1.55E-01
0.85_696.05	1.55E-01
N-Ethyl-4-(dimethylamino)benzylamine	1.56E-01
Acetaminophen glucuronide	1.57E-01
3-Amino-3-(4-hydroxyphenyl)propionic acid	1.57E-01
1.87_349.12	1.57E-01

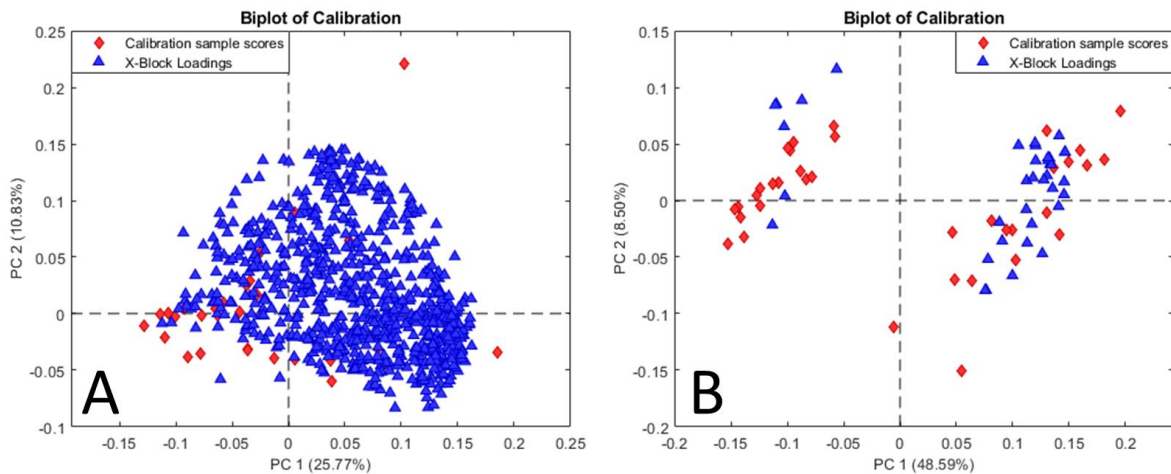
Supplementary Table 9. Principal component (PC) 1 loadings of significant metabolites from serum (*Biogenic Amines*) following FS-CR. Negative loadings (shaded) are correlated with **BAS1** and positive are correlated with **BAS2**.

Variable	PC 1 (69.17%)
4-Aminobenzoic acid	-2.29E-01
1.16_577.36	-2.01E-01
1.66_160.11	-1.98E-01
1.30_568.33	-1.97E-01
1.26_568.34	-1.97E-01
0.40_153.06	-1.95E-01
0.52_151.12	-1.94E-01
L-Histidinol	-1.93E-01
0.62_150.05	-1.92E-01
1.68_192.04	-1.81E-01
1.68_86.10	-1.81E-01
0.31_234.97	1.80E-01
Secnidazole	1.82E-01
1.32_510.35	1.82E-01
Ezetimibe	1.84E-01
4-Hydroxybenzylcyanide	1.85E-01
Vanillin	1.85E-01
0.23_231.00	1.86E-01
0.26_230.99	1.89E-01
1.41_179.05	1.96E-01
1.32_482.32	1.99E-01
2.38_149.01	2.05E-01
Tartaric acid	2.07E-01
0.58_207.05	2.08E-01
0.23_559.47	2.20E-01
0.23_557.45	2.21E-01

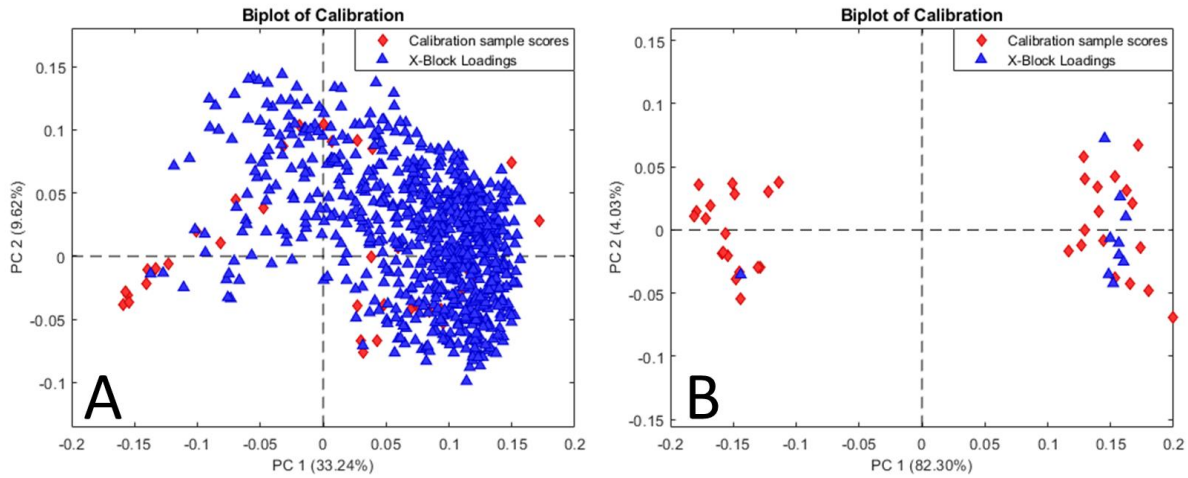
Supplementary Figure 1. Biplot of urine (*General Metabolism*) (A) before feature selection and (B) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).



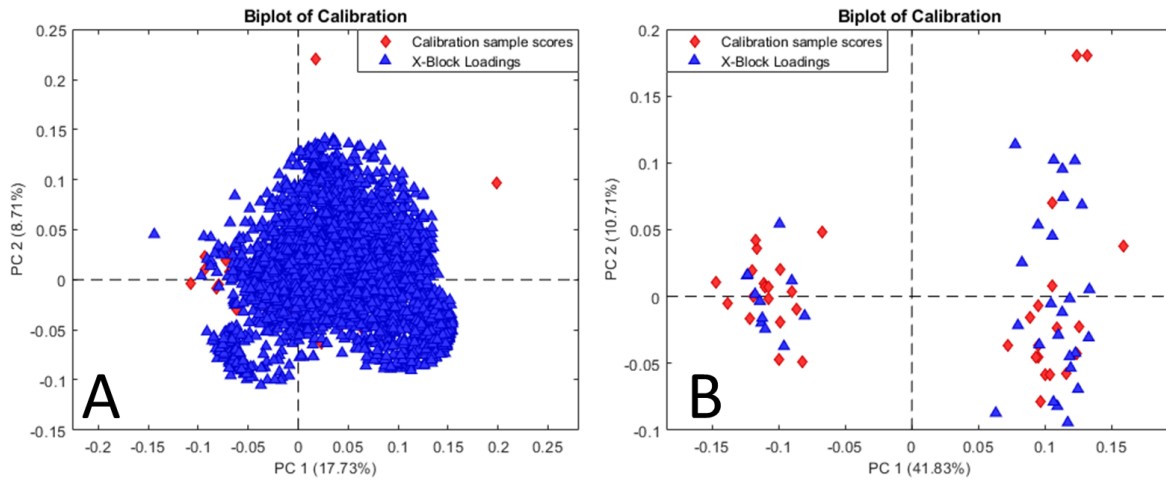
Supplementary Figure 2. Biplot of stool (*General Metabolism*) (A) before feature selection and (B) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).



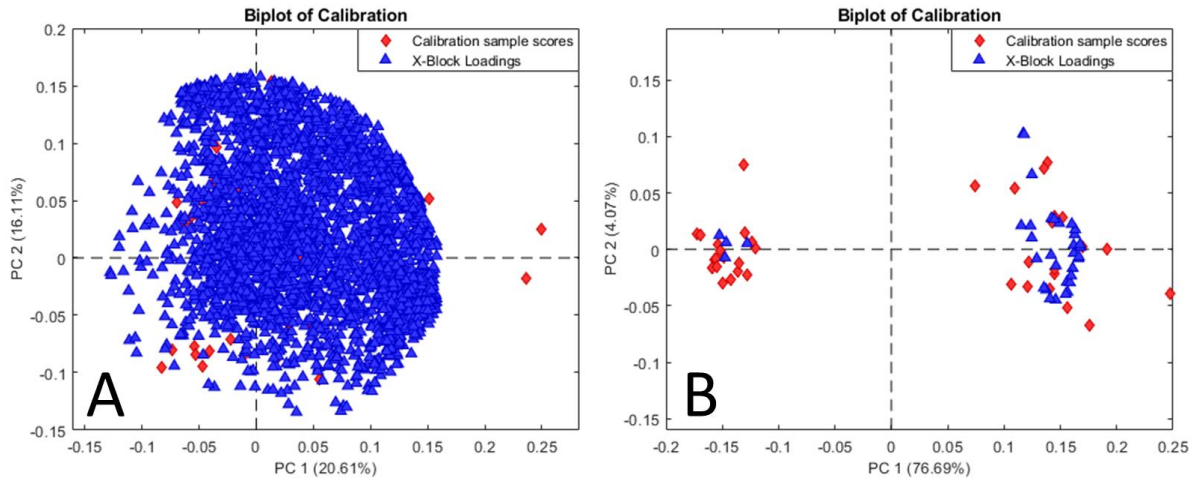
Supplementary Figure 3. Biplot of serum (*General Metabolism*) (A) before feature selection and (B) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).



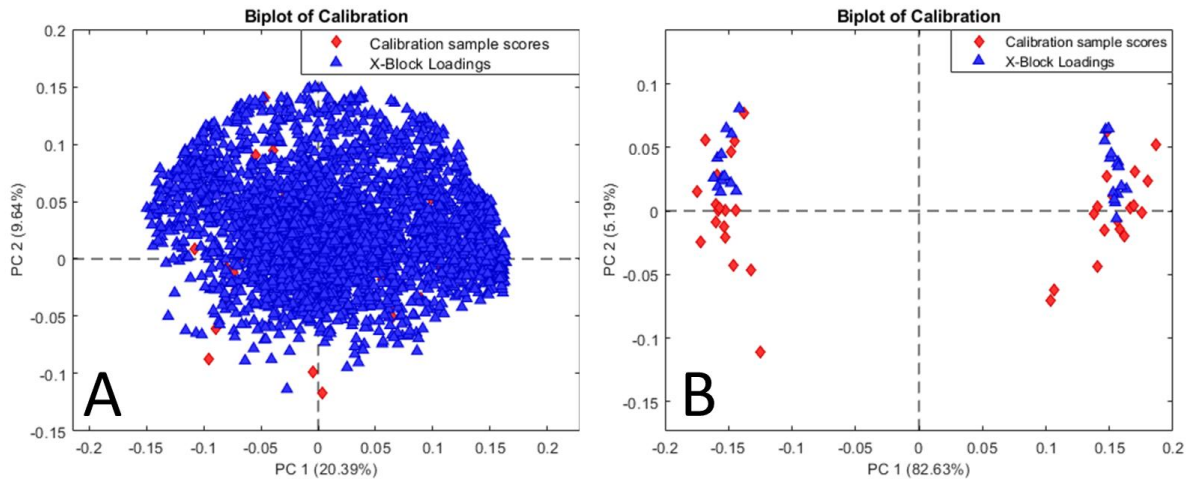
Supplementary Figure 4. Biplot of urine (*Complex Lipids*) (A) before feature selection and (B) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).



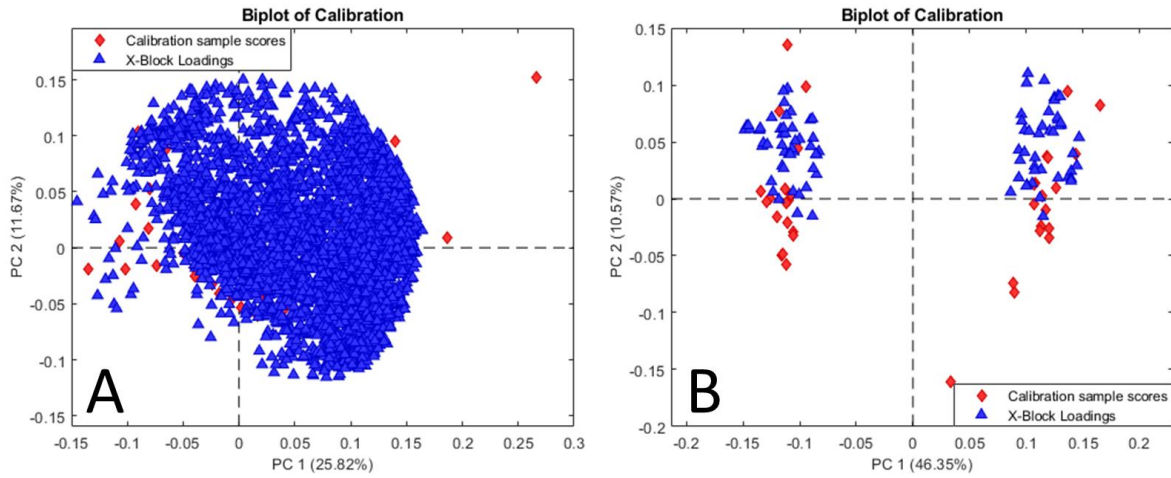
Supplementary Figure 5. Biplot of stool (*Complex Lipids*) (A) before feature selection and (B) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).



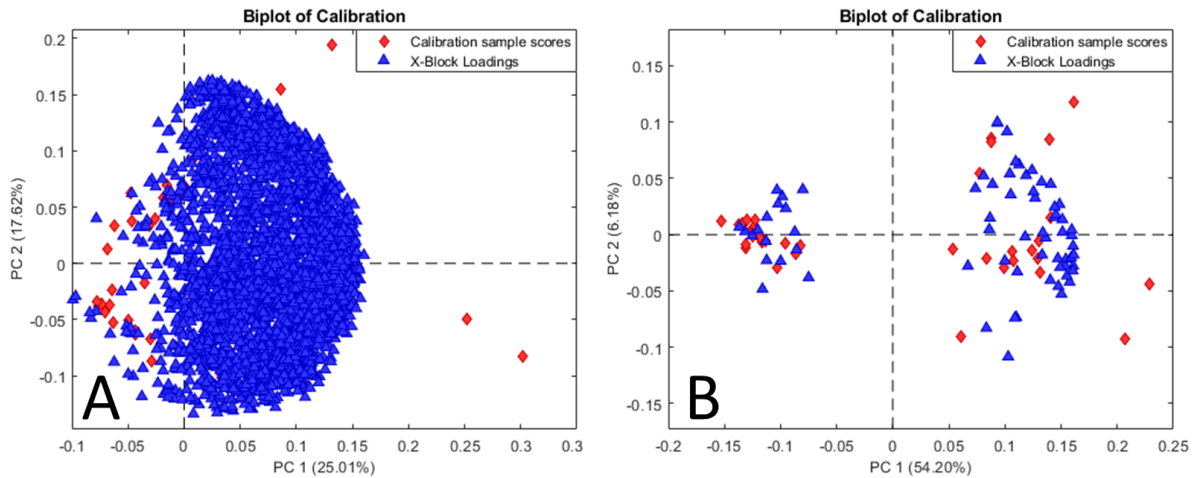
Supplementary Figure 6. Biplot of serum (*Complex Lipids*) (A) before feature selection and (B) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).



Supplementary Figure 7. Biplot of urine (*Biogenic Amines*) (A) before feature selection and (B) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).



Supplementary Figure 8. Biplot of stool (*Biogenic Amines*) (A) before feature selection and (B) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).



Supplementary Figure 9. Biplot of serum (*Biogenic Amines*) (**A**) before feature selection and (**B**) after feature selection. Red diamonds represent samples (scores), and blue triangles represent variables (loadings).

