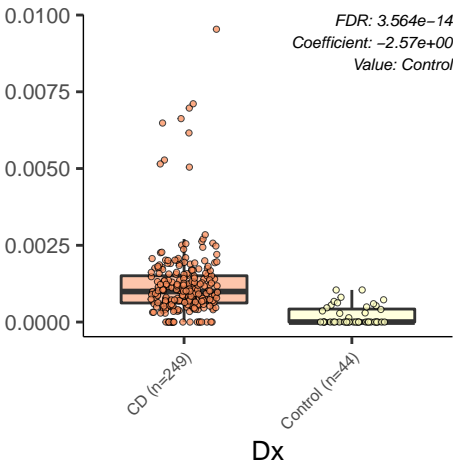
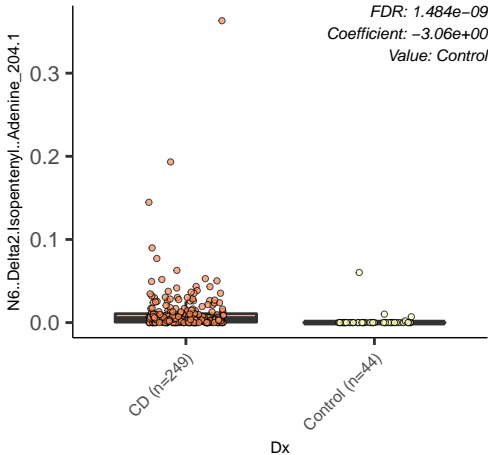


Threitol_121.1





N-Formyl-L-Methionine_176

FDR: $1.561e-07$
Coefficient: $2.78e+00$
Value: Control

0.10

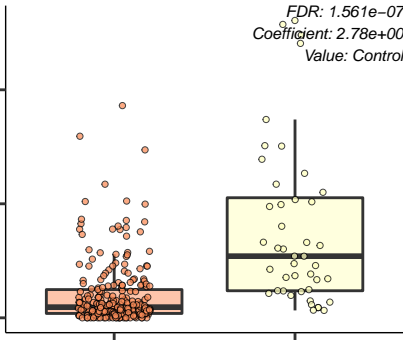
0.05

0.00

CD (n=249)

Control (n=44)

Dx



Homoserine_120.1

FDR: 3.386e-07

Coefficient: -1.03e+00

Value: Control

0.10

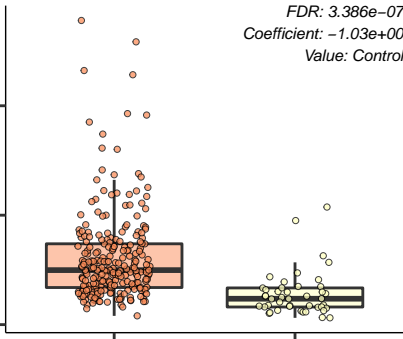
0.05

0.00

CD (n=249)

Control (n=44)

Dx



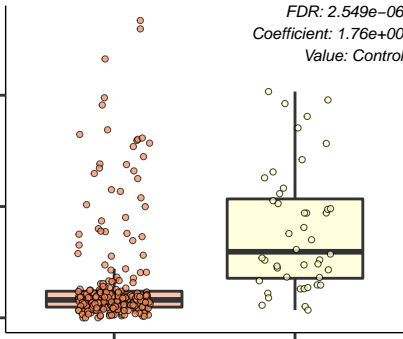
N.Formylglycine_102

FDR: 2.549e-06
Coefficient: 1.76e+00
Value: Control

CD (n=249)

Control (n=44)

Dx



Pyridoxine_170.1

FDR: 2.549e-06

Coefficient: -1.50e+00

Value: Control

1.5

1.0

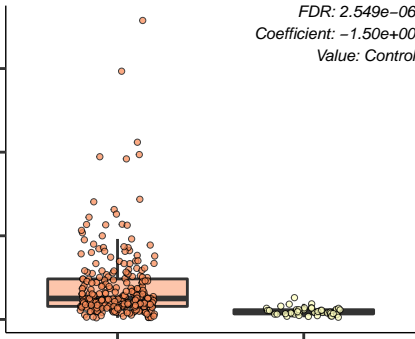
0.5

0.0

CD (n=249)

Control (n=44)

Dx



Methionine.Sulfoximine_181.1

FDR: 5.745e-05
Coefficient: -1.25e+00
Value: Control

0.02

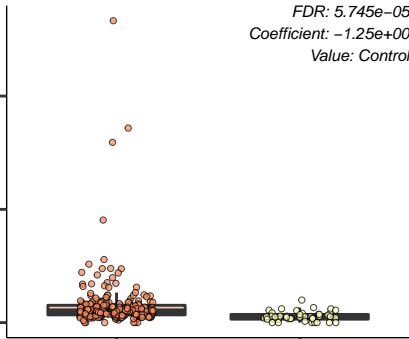
0.01

0.00

CD (n=249)

Control (n=44)

Dx



cis.5.Dodecenoic.acid_197.2

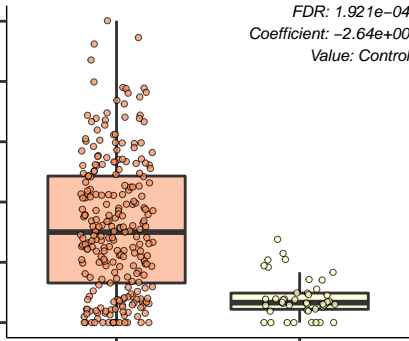
0.25
0.20
0.15
0.10
0.05
0.00

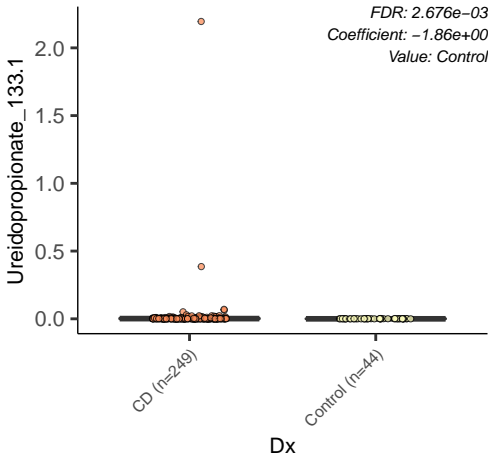
CD (n=249)

Control (n=44)

Dx

FDR: $1.921e-04$
Coefficient: $-2.64e+00$
Value: Control





X2.Aminophenol_108

0.020

0.015

0.010

0.005

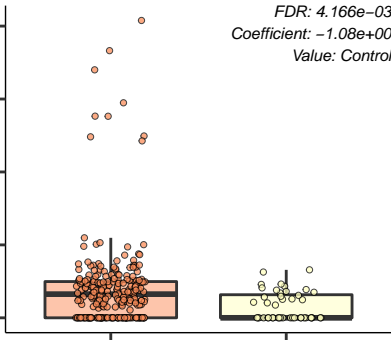
0.000

CD (n=249)

Control (n=44)

Dx

FDR: 4.166e-03
Coefficient: -1.08e+00
Value: Control



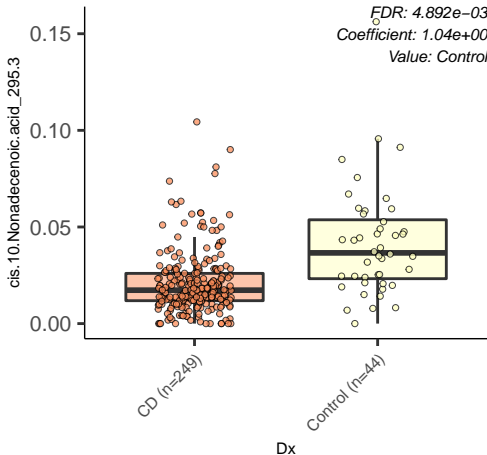
cis.10.Nonadecenoic.acid_295.3

FDR: 4.892e-03
Coefficient: 1.04e+00
Value: Control

CD (n=249)

Control (n=44)

Dx



Beta.hydroxyvaleric.Acid_117.1

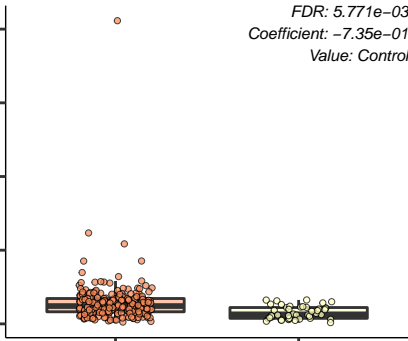
1.00
0.75
0.50
0.25
0.00

FDR: 5.771e-03
Coefficient: -7.35e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



Gulonolactone_177

FDR: 5.771e-03

Coefficient: -7.73e-01

Value: Control

0.15

0.10

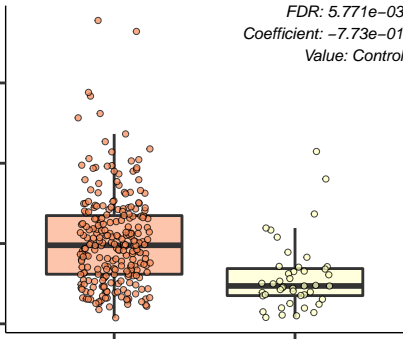
0.05

0.00

CD (n=249)

Control (n=44)

Dx



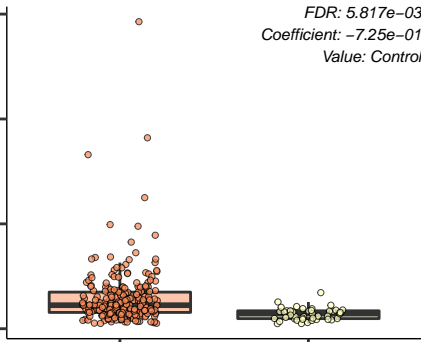
X3.hydroxybutyric.acid_103

FDR: 5.817e-03
Coefficient: -7.25e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



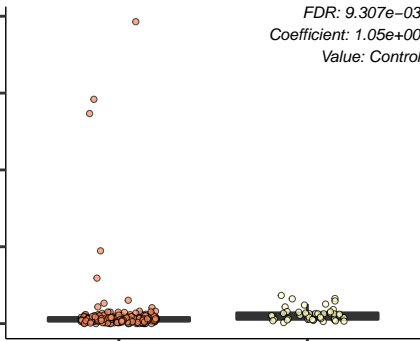
Eicosapentaenoic.acid_301.2

FDR: 9.307e-03
Coefficient: 1.05e+00
Value: Control

CD (n=249)

Control (n=44)

Dx



Deoxycarnitine_146.1

FDR: 1.043e-02

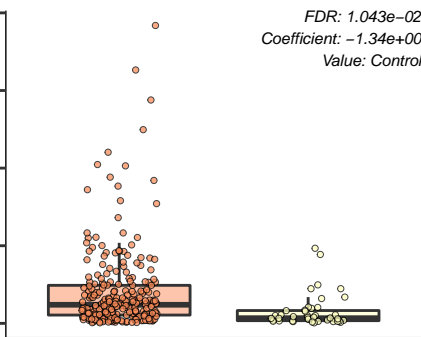
Coefficient: -1.34e+00

Value: Control

CD (n=249)

Control (n=44)

Dx



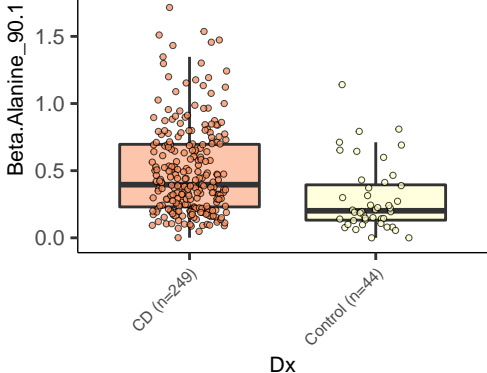
Beta.Alanine_90.1

FDR: 1.070e-02
Coefficient: -1.03e+00
Value: Control

CD (n=249)

Control (n=44)

Dx



N.AcetylIleucine_172.1

FDR: 1.070e-02
Coefficient: -8.86e-01
Value: Control

0.2

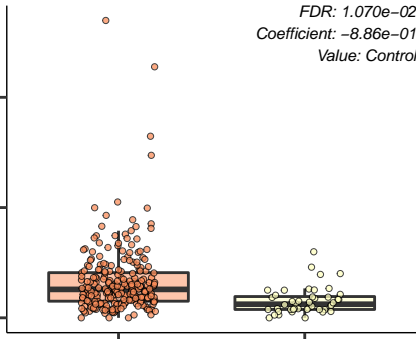
0.1

0.0

CD (n=249)

Control (n=44)

Dx



N.Acetylneuraminate_310.1

0.75

0.50

0.25

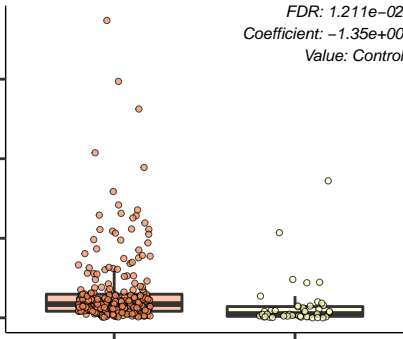
0.00

CD (n=249)

Control (n=44)

Dx

FDR: 1.211e-02
Coefficient: -1.35e+00
Value: Control



Isoleucine_132.1

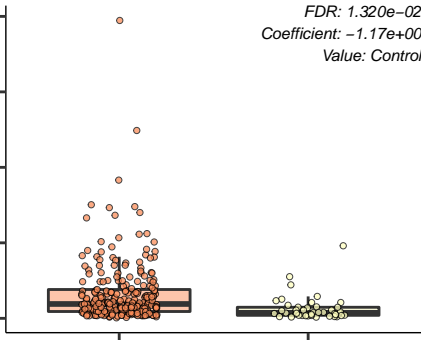
20
15
10
5
0

FDR: 1.320e-02
Coefficient: -1.17e+00
Value: Control

CD (n=249)

Control (n=44)

Dx



Mannitol_181.1

FDR: 1.320e-02

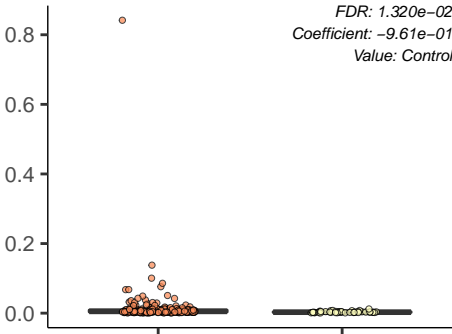
Coefficient: -9.61e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



Octanoic.acid_143.1

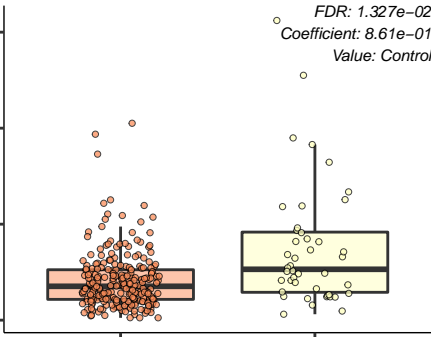
6
4
2
0

CD (n=249)

Control (n=44)

Dx

FDR: 1.327e-02
Coefficient: 8.61e-01
Value: Control



Indole.3.Pyruvate_204.1

0.100

0.075

0.050

0.025

0.000

FDR: $1.474e-02$

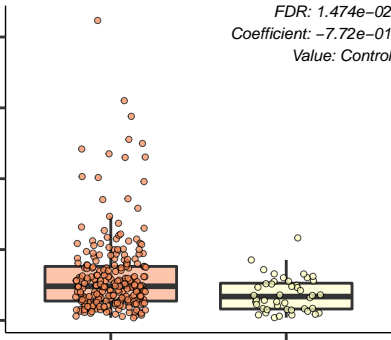
Coefficient: $-7.72e-01$

Value: Control

CD (n=249)

Control (n=44)

Dx



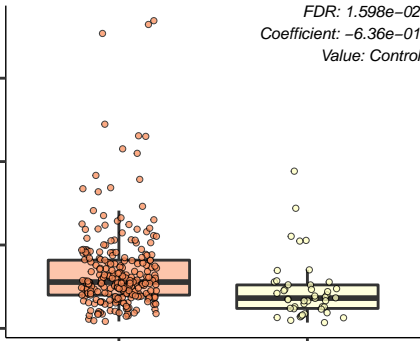
X3..2.Hydroxyphenyl.I.Propanoate_165.1

FDR: 1.598e-02
Coefficient: -6.36e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



Thiopurine.S.Methylether_167

0.15

0.10

0.05

0.00

CD (n=249)

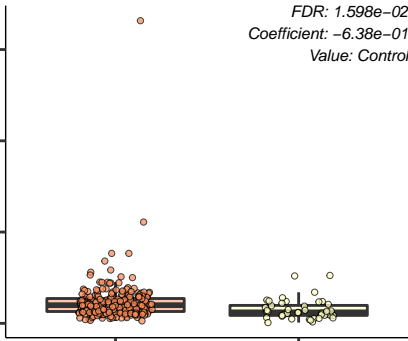
Control (n=44)

Dx

FDR: 1.598e-02

Coefficient: -6.38e-01

Value: Control



Threonine_120.1

FDR: 1.598e-02

Coefficient: -7.96e-01

Value: Control

1.0

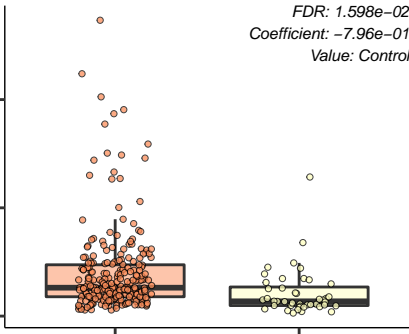
0.5

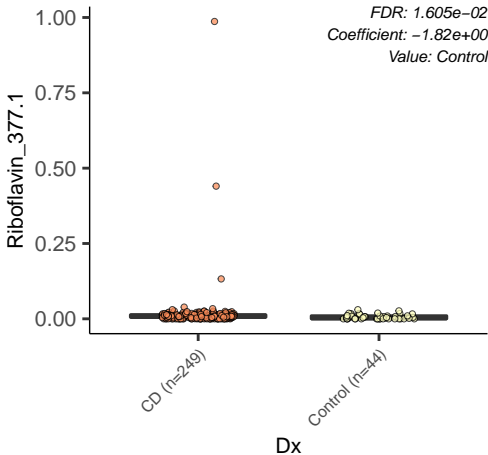
0.0

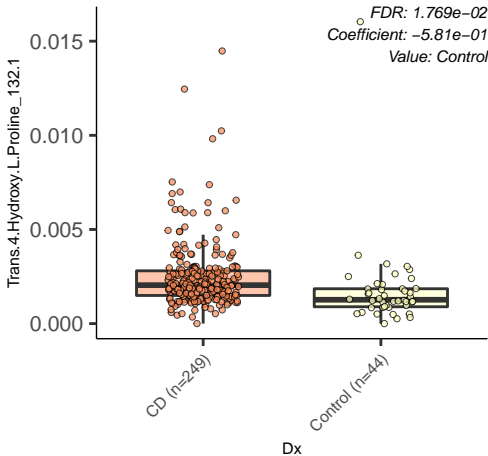
CD (n=249)

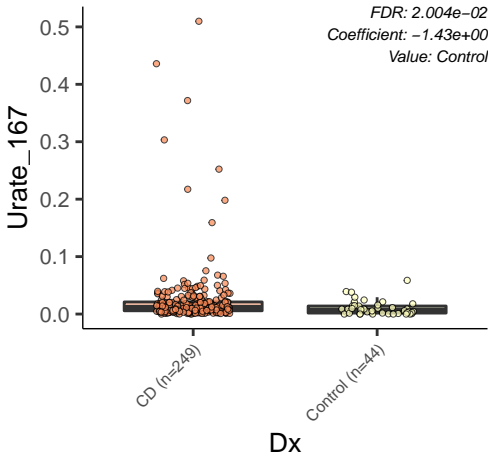
Control (n=44)

Dx









Phenylalanine_166.1

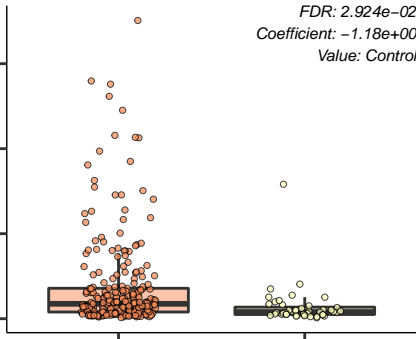
FDR: 2.924e-02
Coefficient: -1.18e+00
Value: Control

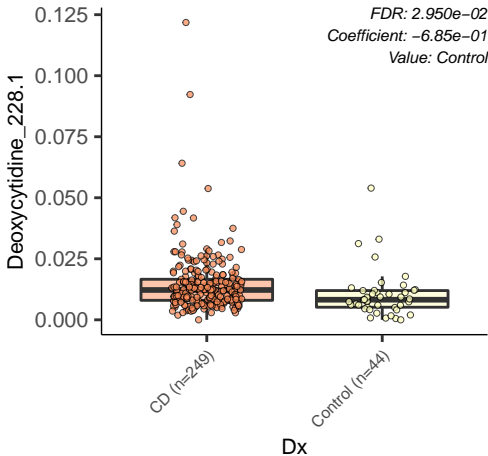
7.5
5.0
2.5
0.0

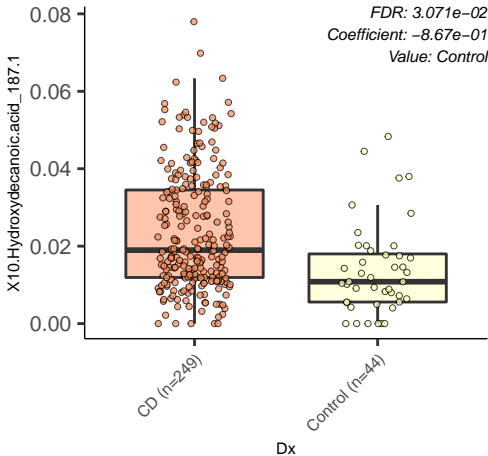
CD (n=249)

Control (n=44)

Dx







X6.Carboxyhexanoate_159.1

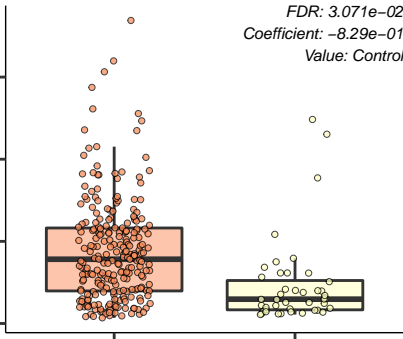
FDR: $3.071\text{e-}02$
Coefficient: $-8.29\text{e-}01$
Value: Control

0.09
0.06
0.03
0.00

CD (n=249)

Control (n=44)

Dx



Rhamnose_163.1

FDR: 3.071e-02
Coefficient: -5.54e-01
Value: Control

0.10

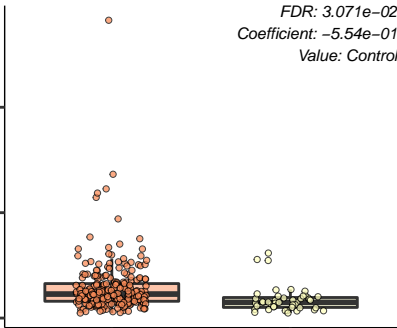
0.05

0.00

CD (n=249)

Control (n=44)

Dx



X5.Aminopentanoate_118.1

FDR: $3.296e-02$

Coefficient: $-9.25e-01$

Value: Control

10

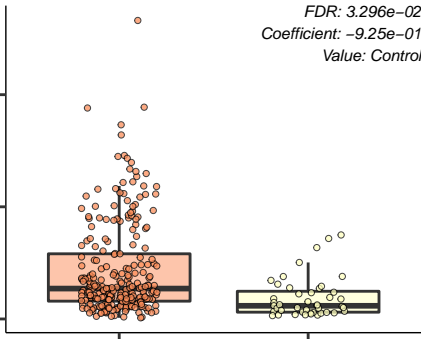
5

0

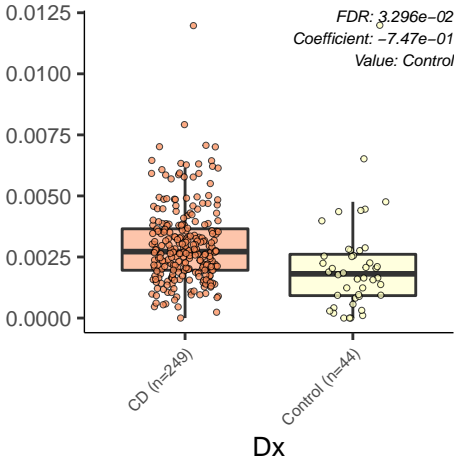
CD (n=249)

Control (n=44)

Dx



Cys.Gly_177



Methionine_150.1

3

2

1

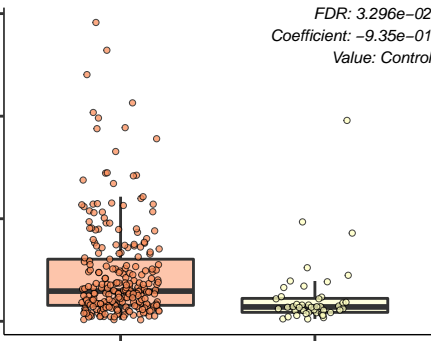
0

CD (n=249)

Control (n=44)

Dx

FDR: $3.296e-02$
Coefficient: $-9.35e-01$
Value: Control



Linoleic.acid_279.2

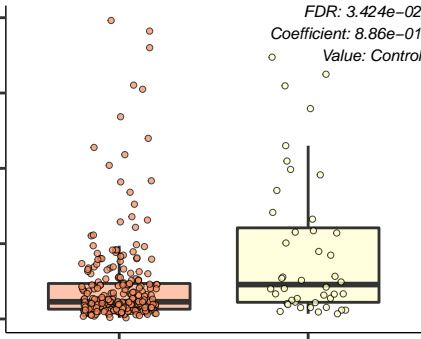
20
15
10
5
0

CD (n=249)

Control (n=44)

Dx

FDR: $3.424e-02$
Coefficient: $8.86e-01$
Value: Control



Nicotinamide_123.1

FDR: 3.778e-02

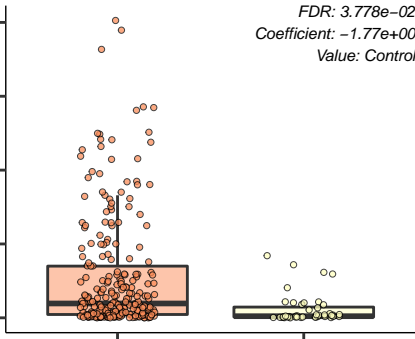
Coefficient: -1.77e+00

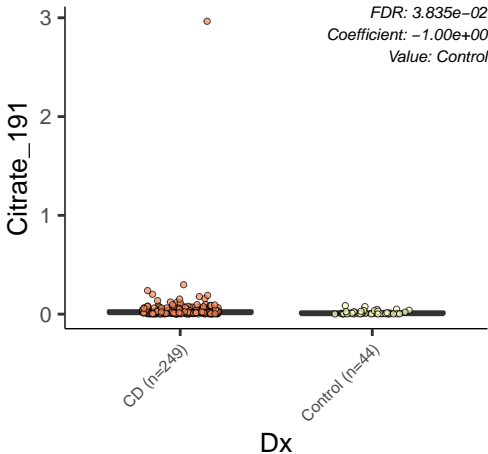
Value: Control

CD (n=249)

Control (n=44)

Dx





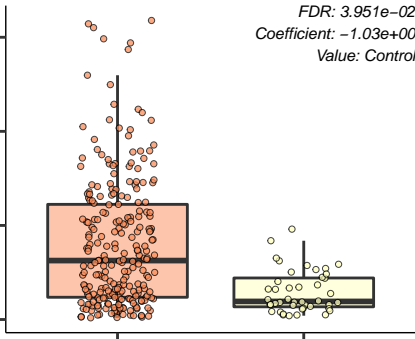
Glucuronolactone_175

FDR: 3.951e-02
Coefficient: -1.03e+00
Value: Control

CD (n=249)

Control (n=44)

Dx



Indoxyl.Glucoside_294.1

FDR: 3.951e-02
Coefficient: -1.04e+00
Value: Control

CD (n=249)

Control (n=44)

Dx

0.020

0.015

0.010

0.005

0.000

X14.Methylhexadecanoic.acid_269.2

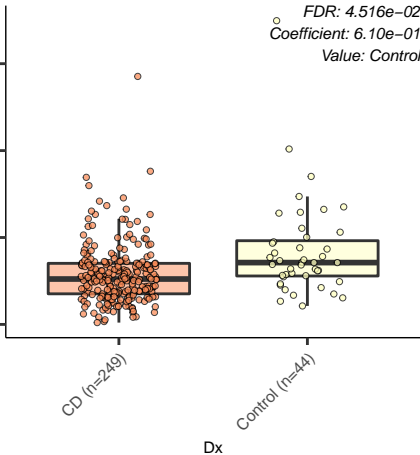
FDR: 4.516e-02
Coefficient: 6.10e-01
Value: Control

CD (n=249)

Control (n=44)

Dx

1.5
1.0
0.5
0.0



Raffinose_503.2

FDR: 4.516e-02

Coefficient: -1.07e+00

Value: Control

0.3

0.2

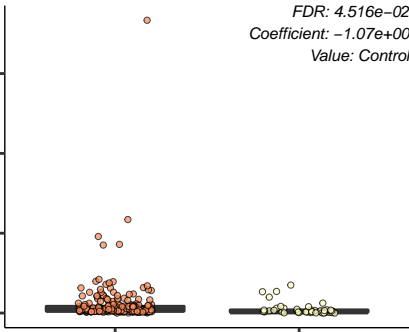
0.1

0.0

CD (n=249)

Control (n=44)

Dx



Citramalate_147

FDR: 4.943e-02

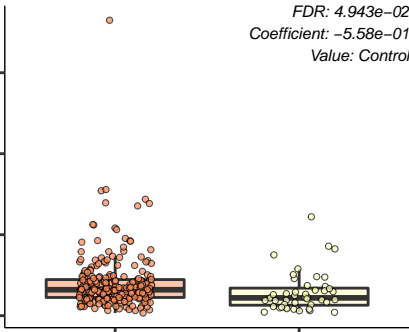
Coefficient: -5.58e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



Mesaconic.acid_129

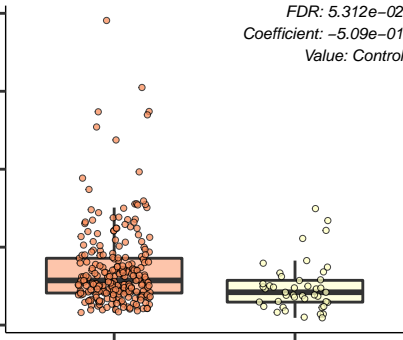
0.04
0.03
0.02
0.01
0.00

FDR: 5.312e-02
Coefficient: -5.09e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



X2.hydroxyglutarate_147

FDR: 5.613e-02

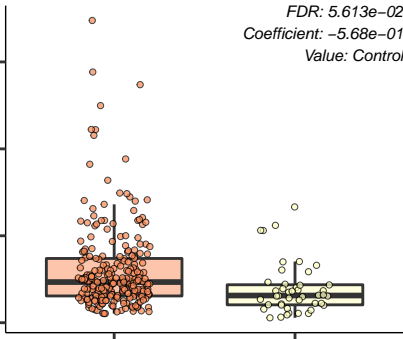
Coefficient: -5.68e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



Fructose_179.1

FDR: 5.613e-02

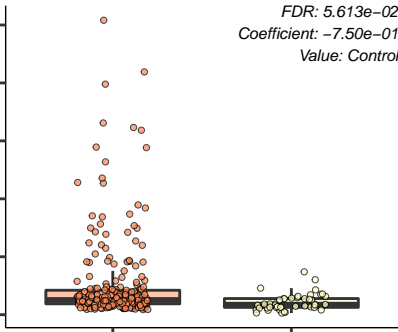
Coefficient: -7.50e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



Tyrosine_182.1

FDR: 5.613e-02

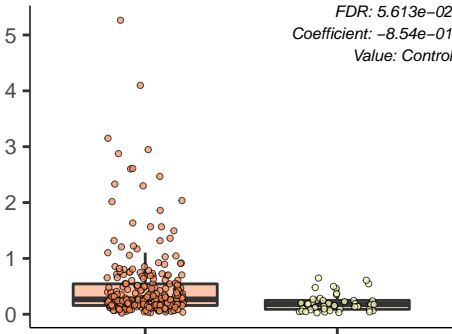
Coefficient: -8.54e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



N.Acetylputrescine_131.1

FDR: $6.002e-02$

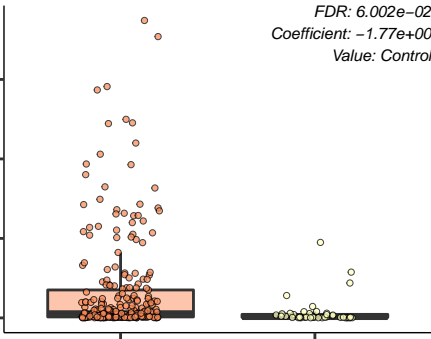
Coefficient: $-1.77e+00$

Value: Control

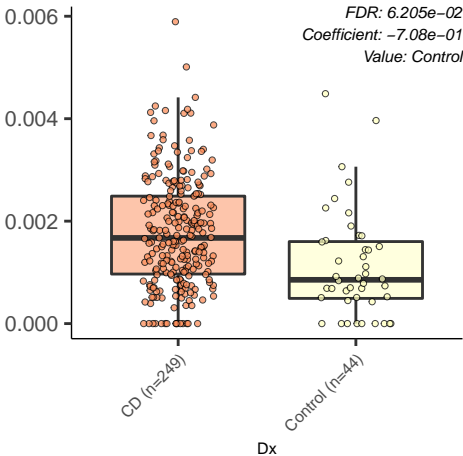
CD (n=249)

Control (n=44)

Dx



X2.4.Dihydroxypteridine_163



Oxalate_89

FDR: 6.214e-02

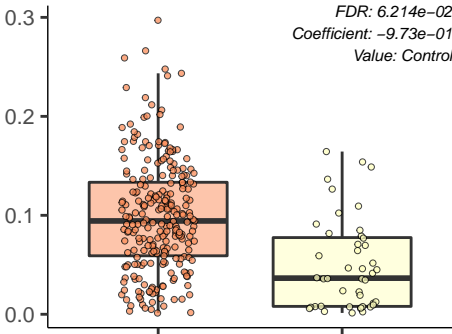
Coefficient: -9.73e-01

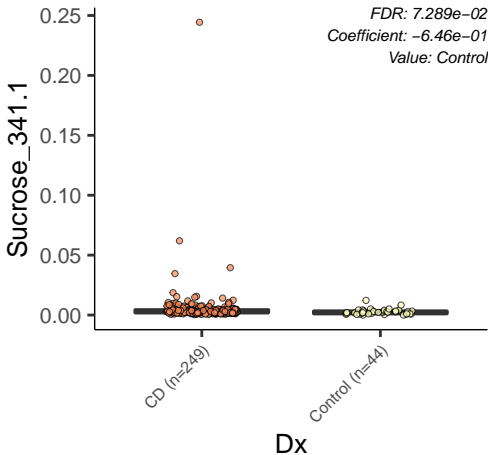
Value: Control

CD (n=249)

Control (n=44)

Dx





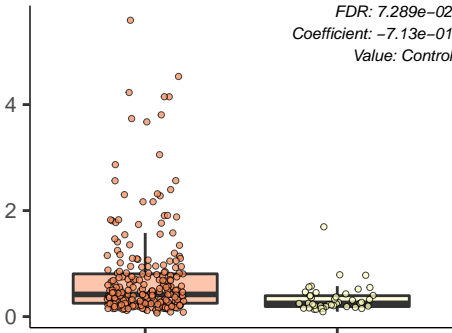
Valine_118.1

FDR: $7.289\text{e-}02$
Coefficient: $-7.13\text{e-}01$
Value: Control

CD (n=249)

Control (n=44)

Dx



Indole.3.Acetamide_175.1

FDR: $7.317e-02$
Coefficient: $-8.11e-01$
Value: Control

0.0100

0.0075

0.0050

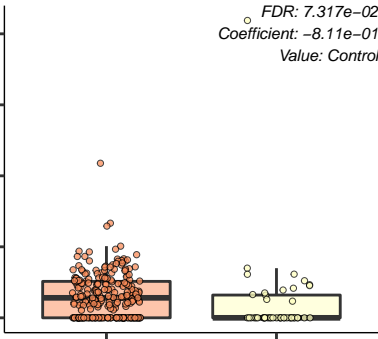
0.0025

0.0000

CD (n=249)

Control (n=44)

Dx



Methyl.Galactoside_193.1

FDR: 7.319e-02

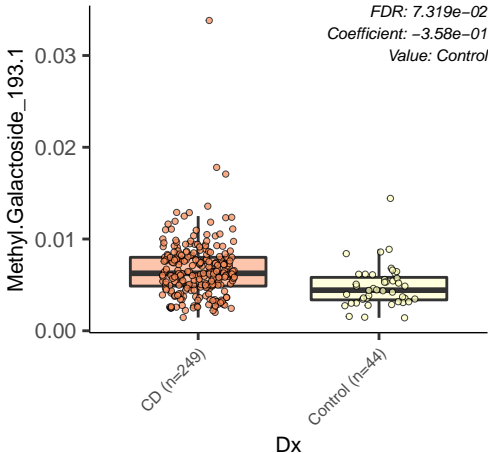
Coefficient: -3.58e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



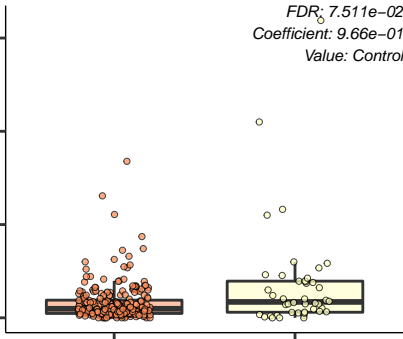
Asparagine_133.1

FDR: 7.511e-02
Coefficient: 9.66e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



Tyramine_138.1

FDR: 7.543e-02

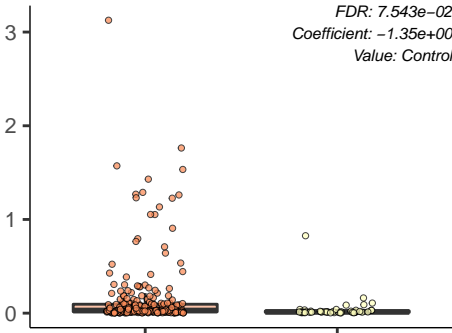
Coefficient: -1.35e+00

Value: Control

CD (n=249)

Control (n=44)

Dx



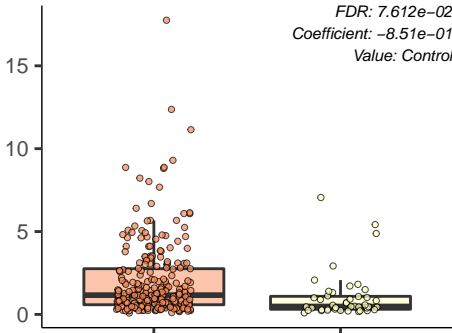
Leucine_132.1

FDR: 7.612e-02
Coefficient: -8.51e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



Galactarate_209

FDR: 7.755e-02

Coefficient: -8.58e-01

Value: Control

0.020

0.015

0.010

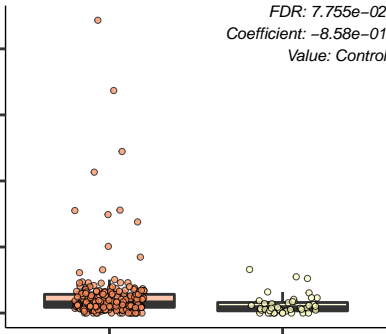
0.005

0.000

CD (n=249)

Control (n=44)

Dx



D.Pinitol_193.1

FDR: 7.951e-02

Coefficient: -8.21e-01

Value: Control

0.20

0.15

0.10

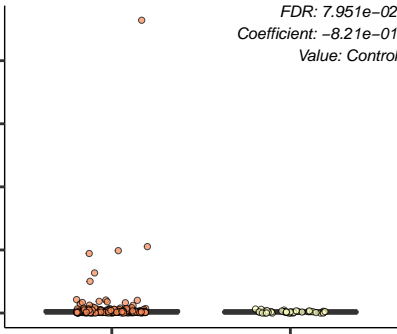
0.05

0.00

CD (n=249)

Control (n=44)

Dx



Oleic.acid_281.2

30

20

10

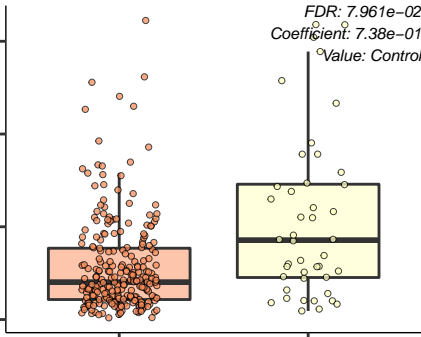
0

CD (n=249)

Control (n=44)

Dx

FDR: $7.961e-02$
Coefficient: $7.38e-01$
Value: Control



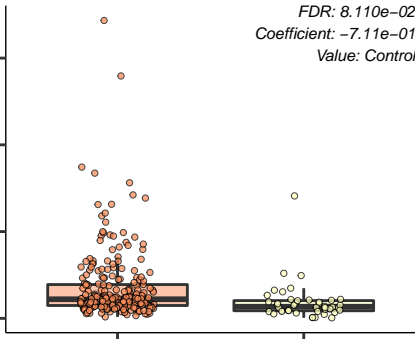
Galacturonate_193

FDR: 8.110e-02
Coefficient: -7.11e-01
Value: Control

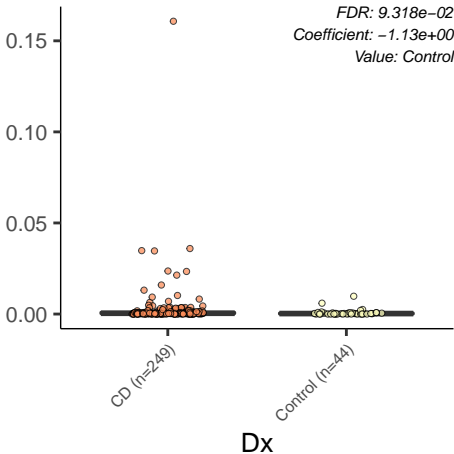
CD (n=249)

Control (n=44)

Dx



Lactose_343.1



X2.Deoxy.D.Glucose_163.1

FDR: $9.613e-02$

Coefficient: $-7.54e-01$

○ Value: Control

0.09

0.06

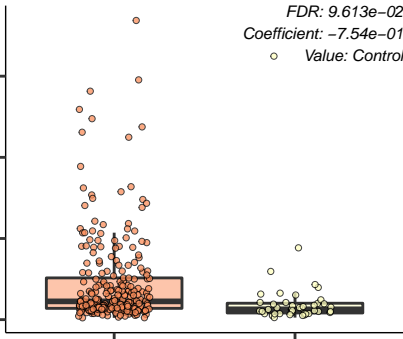
0.03

0.00

CD (n=249)

Control (n=44)

Dx



Carnitine_162.1

FDR: 9.613e-02

Coefficient: -7.00e-01

Value: Control

4

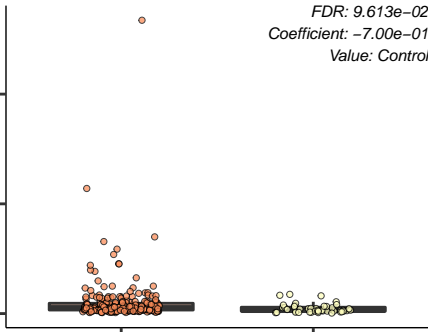
2

0

CD (n=249)

Control (n=44)

Dx



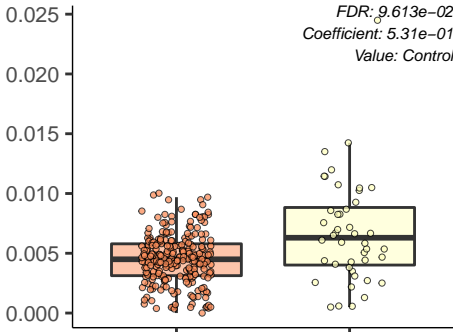
Glycerate_105

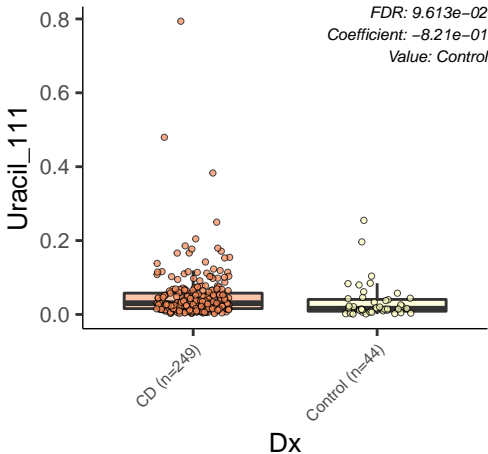
FDR: 9.613e-02
Coefficient: 5.31e-01
Value: Control

CD (n=249)

Control (n=44)

Dx





Saccharate_209

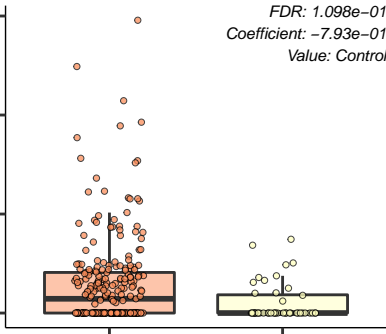
0.003
0.002
0.001
0.000

FDR: 1.098e-01
Coefficient: -7.93e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



N.Acetylserine_146

0.2

0.1

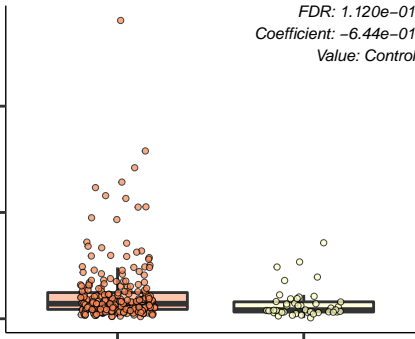
0.0

CD (n=249)

Control (n=44)

Dx

FDR: 1.120e-01
Coefficient: -6.44e-01
Value: Control



Sedoheptulose.7.phosphate_289

FDR: 1.205e-01
Coefficient: -1.30e+00
Value: Control

0.02

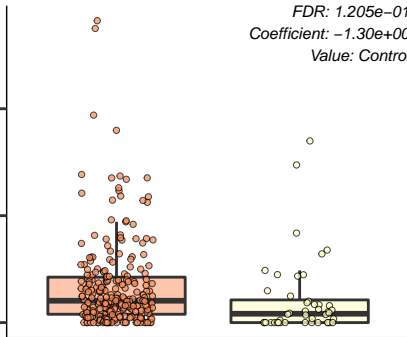
0.01

0.00

CD (n=249)

Control (n=44)

Dx



X2.Aminoisobutyrate_104.1

FDR: 1.321e-01

Coefficient: -3.78e-01

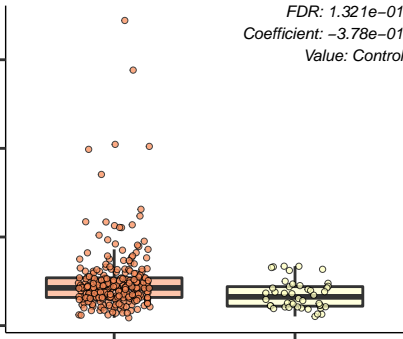
Value: Control

0.75
0.50
0.25
0.00

CD (n=249)

Control (n=44)

Dx



Deoxyguanosine_268.1

0.15

0.10

0.05

0.00

CD (n=249)

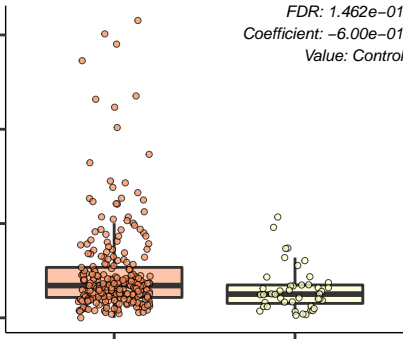
Control (n=44)

Dx

FDR: 1.462e-01

Coefficient: -6.00e-01

Value: Control



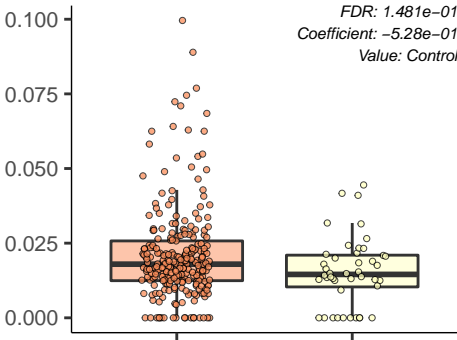
Myristoleic.acid_225.2

FDR: 1.481e-01
Coefficient: -5.28e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



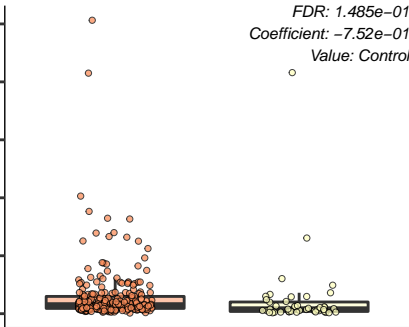
Trehalose_341.1

FDR: 1.485e-01
Coefficient: -7.52e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



N.Acetylglucine_116

0.02

0.01

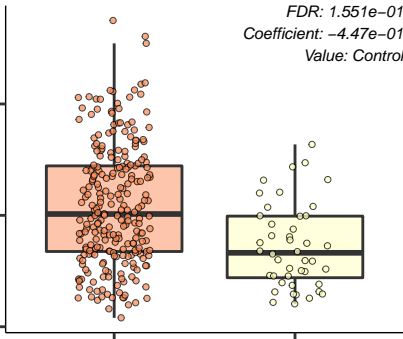
0.00

CD (n=249)

Control (n=44)

Dx

FDR: 1.551e-01
Coefficient: -4.47e-01
Value: Control



Thymine_125

FDR: 1.594e-01

Coefficient: -6.89e-01

Value: Control

0.6

0.4

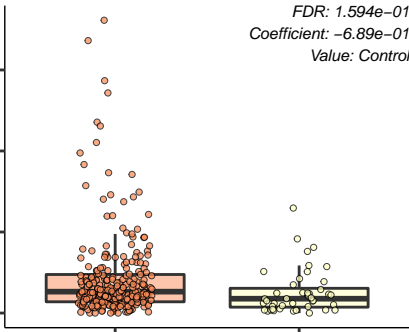
0.2

0.0

CD (n=249)

Control (n=44)

Dx



Caffeate_179

FDR: 1.726e-01

Coefficient: -3.55e-01

Value: Control

0.010

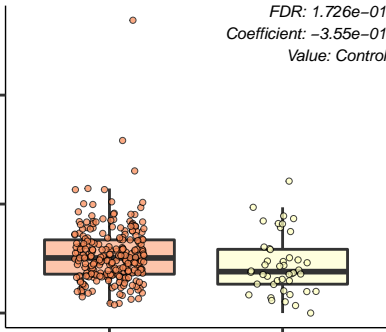
0.005

0.000

CD (n=249)

Control (n=44)

Dx



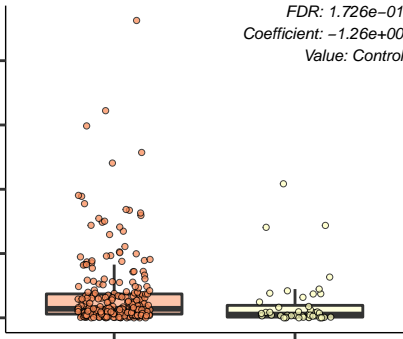
Glucose.6.Phosphate_259

FDR: 1.726e-01
Coefficient: -1.26e+00
Value: Control

CD (n=249)

Control (n=44)

Dx



methyI.lysine_161.1

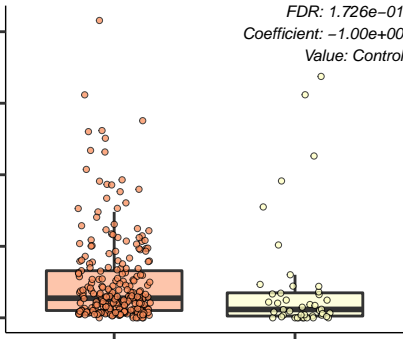
0.08
0.06
0.04
0.02
0.00

CD (n=249)

Control (n=44)

Dx

FDR: 1.726e-01
Coefficient: -1.00e+00
Value: Control



Lysine_147.1

FDR: 1.785e-01

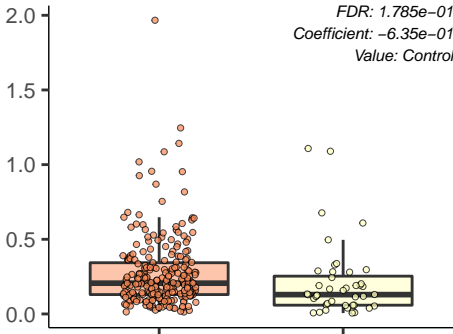
Coefficient: -6.35e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



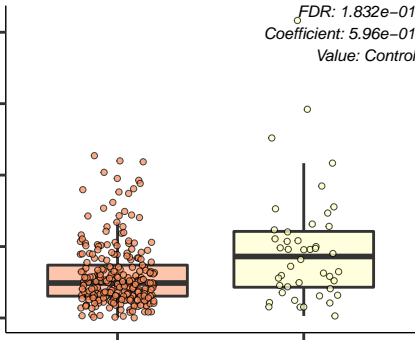
Arachidic.acid_311.3

FDR: 1.832e-01
Coefficient: 5.96e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



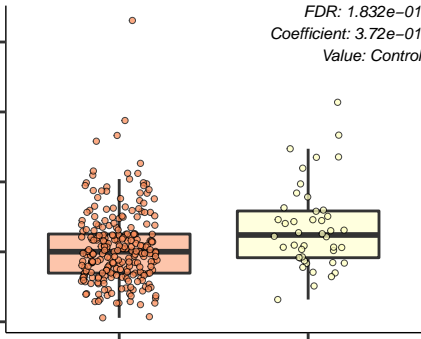
Palmitic.acid_255.2

FDR: 1.832e-01
Coefficient: 3.72e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



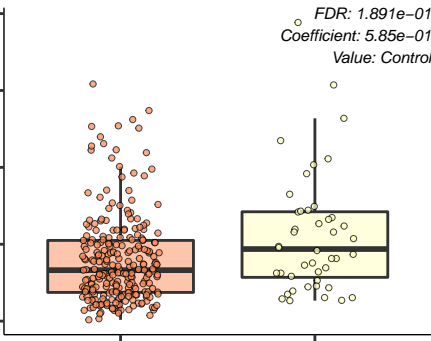
Pentadecanoic.acid_241.2

FDR: 1.891e-01
Coefficient: 5.85e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



Oleoyl.Glycerol_355.3

FDR: 1.897e-01

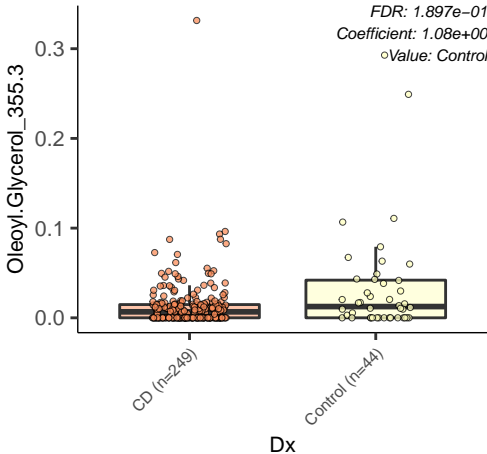
Coefficient: 1.08e+00

○ Value: Control

CD (n=249)

Control (n=44)

Dx



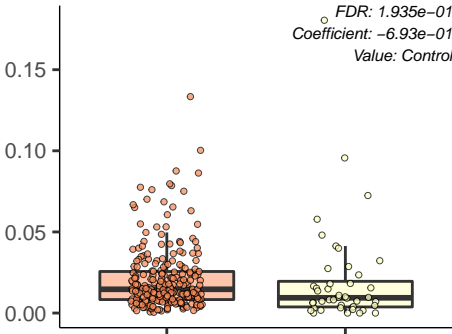
Guanosine_284.1

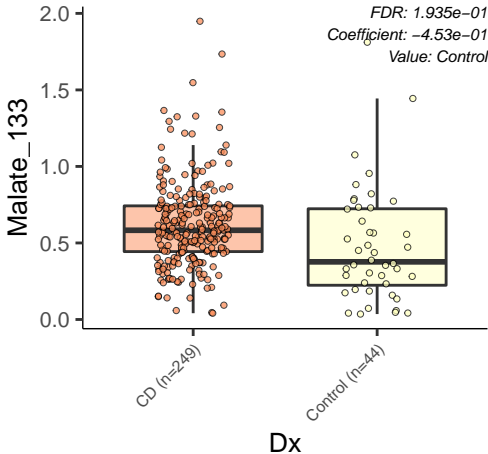
FDR: 1.935e-01
Coefficient: -6.93e-01
Value: Control

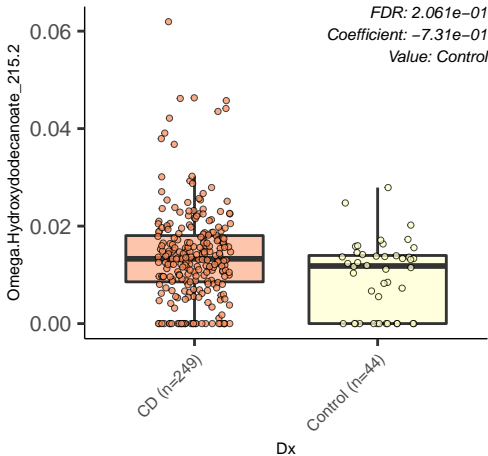
CD (n=249)

Control (n=44)

Dx







Stachyose_665.2

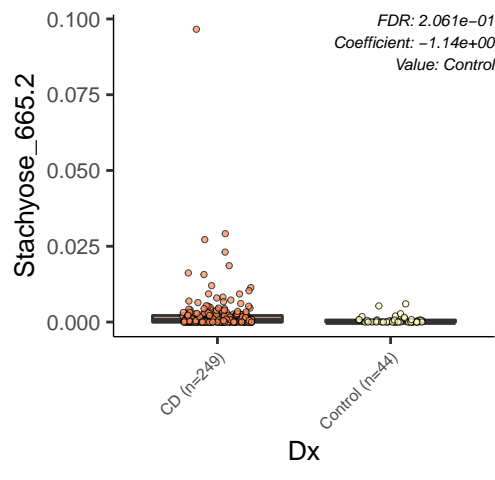
0.100
0.075
0.050
0.025
0.000

FDR: 2.061e-01
Coefficient: -1.14e+00
Value: Control

CD (n=249)

Control (n=44)

Dx



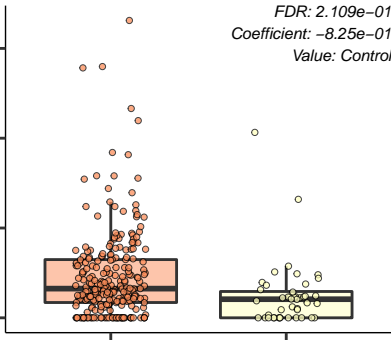
Methylarginine_189.1

FDR: 2.109e-01
Coefficient: -8.25e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



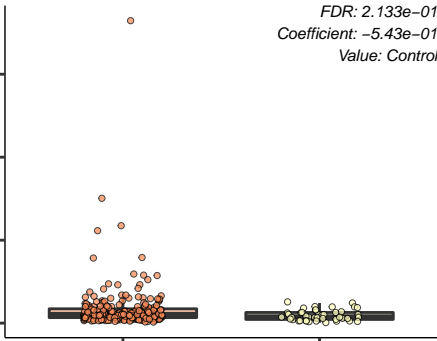
X2.Hydroxyisocaproic.acid_131.1

FDR: 2.133e-01
Coefficient: -5.43e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



Homocysteine_136

FDR: 2.133e-01

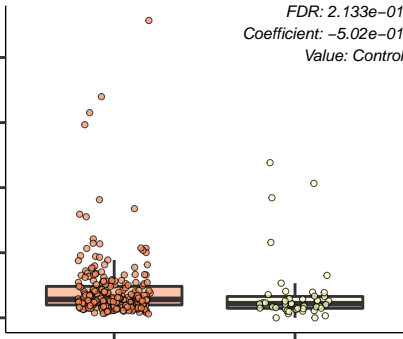
Coefficient: -5.02e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



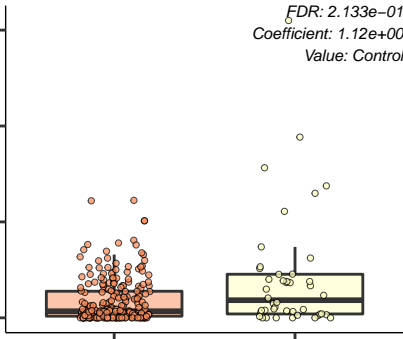
Tricosanoic.acid_353.3

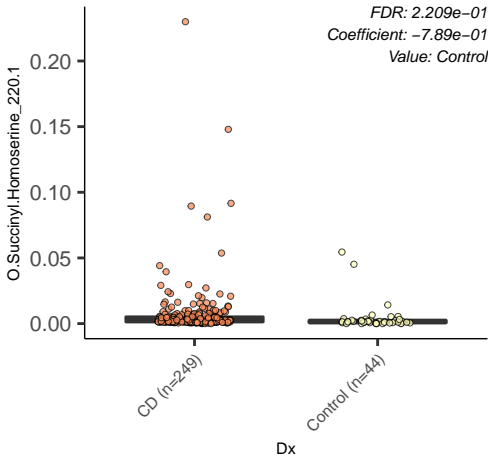
FDR: 2.133e-01
Coefficient: 1.12e+00
Value: Control

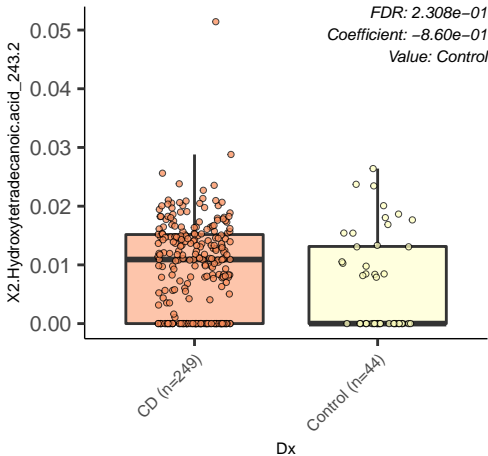
CD (n=249)

Control (n=44)

Dx







X2.Methylmaleate_129

FDR: 2.308e-01

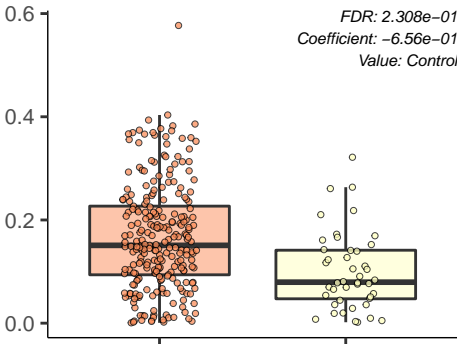
Coefficient: -6.56e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



Dodecanoic.acid_199.2

FDR: 2.308e-01

Coefficient: -4.75e-01

Value: Control

10

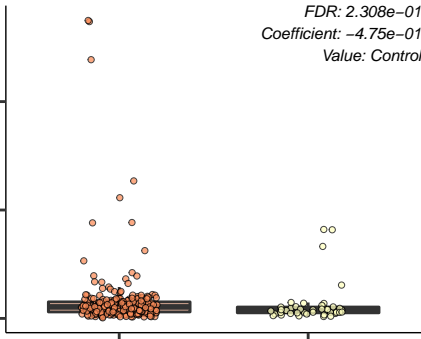
5

0

CD (n=249)

Control (n=44)

Dx



Guanine_152.1

FDR: 2.308e-01

Coefficient: -5.00e-01

Value: Control

0.3

0.2

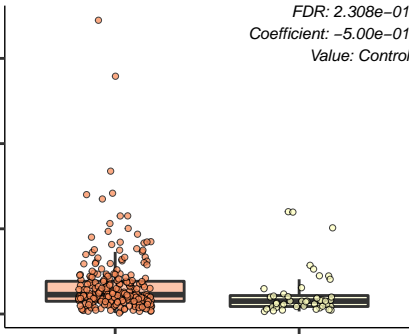
0.1

0.0

CD (n=249)

Control (n=44)

Dx



Histamine_112.1

FDR: 2.308e-01

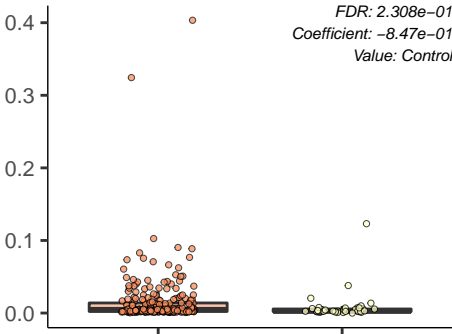
Coefficient: -8.47e-01

Value: Control

CD (n=249)

Control (n=44)

Dx



Hypoxanthine_137

3

2

1

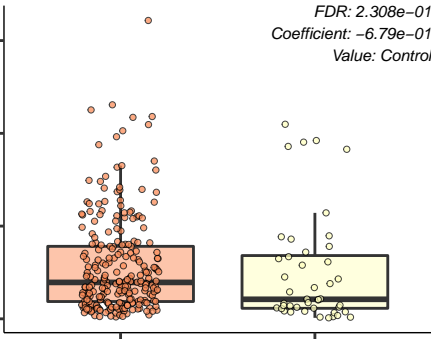
0

CD (n=249)

Control (n=44)

Dx

FDR: 2.308e-01
Coefficient: -6.79e-01
Value: Control



Maleamate_114

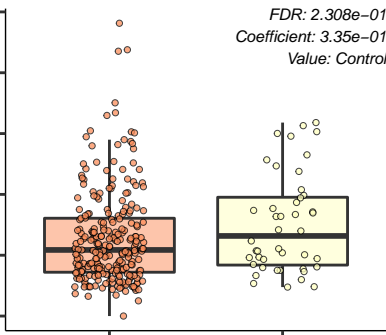
0.005
0.004
0.003
0.002
0.001
0.000

FDR: 2.308e-01
Coefficient: 3.35e-01
Value: Control

CD (n=249)

Control (n=44)

Dx



Adipate_145.1

FDR: 2.456e-01
Coefficient: 5.23e-01
Value: Control

1.0
0.5
0.0

CD (n=249)

Control (n=44)

Dx

