

Pyridoxine\_170.1

*FDR: 1.934e-05*

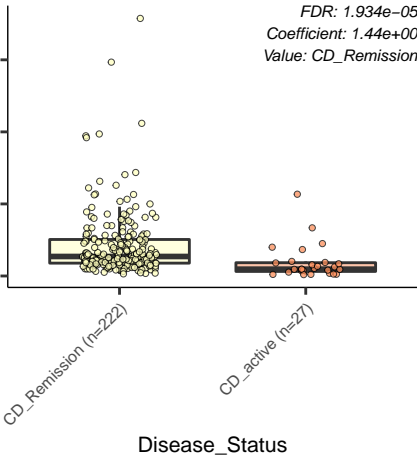
*Coefficient: 1.44e+00*

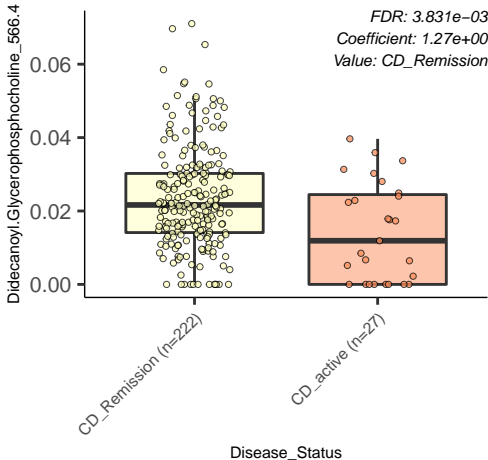
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





N.Acetylglycine\_116

0.02

0.01

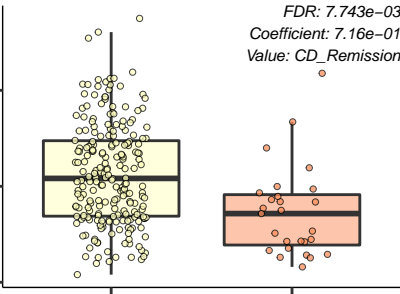
0.00

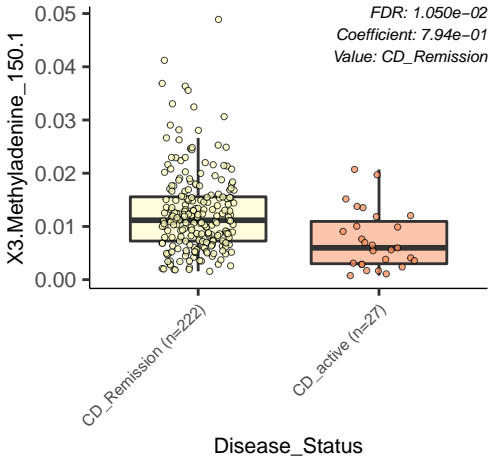
CD\_Remission (n=222)

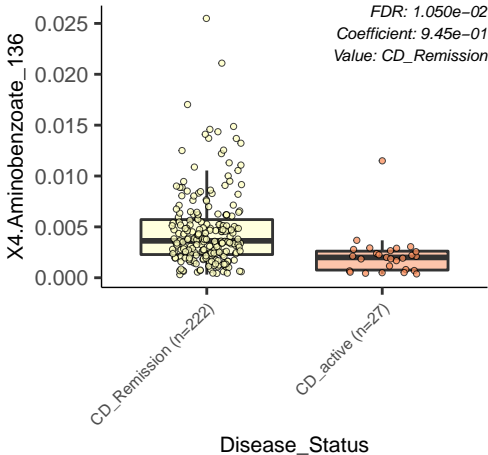
CD\_active (n=27)

Disease\_Status

FDR: 7.743e-03  
Coefficient: 7.16e-01  
Value: CD\_Remission







cis.5.Dodecenoic.acid\_197.2

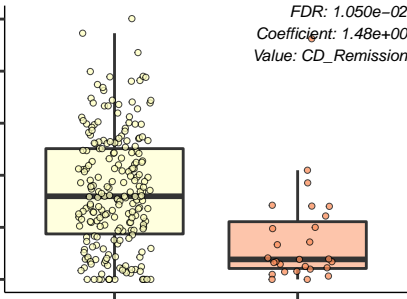
0.25  
0.20  
0.15  
0.10  
0.05  
0.00

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

FDR: 1.050e-02  
Coefficient: 1.48e+00  
Value: CD\_Remission



Heptanoic.acid\_129.1

FDR: 1.050e-02

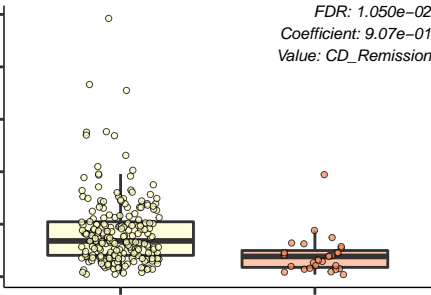
Coefficient: 9.07e-01

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





trans.3.Hexenoic.acid\_113.1

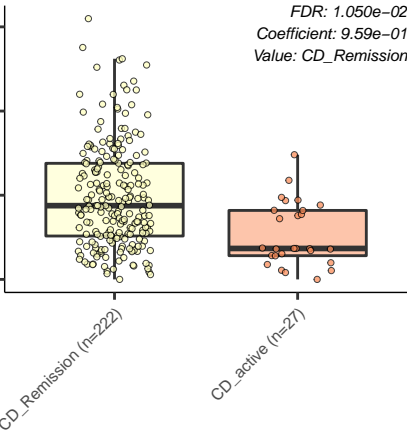
0.06  
0.04  
0.02  
0.00

*FDR: 1.050e-02*  
*Coefficient: 9.59e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Acetylcysteine\_164

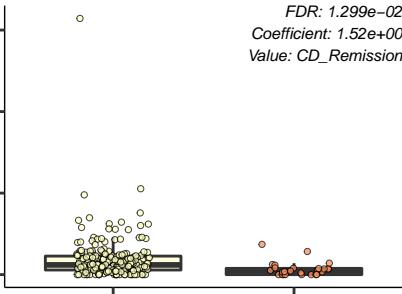
0.06  
0.04  
0.02  
0.00

*FDR: 1.299e-02*  
*Coefficient: 1.52e+00*  
*Value: CD\_Remission*

CD\_Remission (n=222)

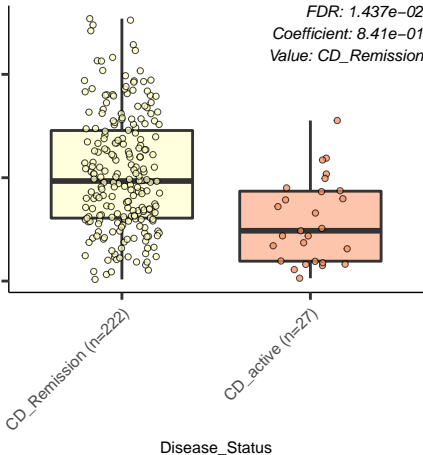
CD\_active (n=27)

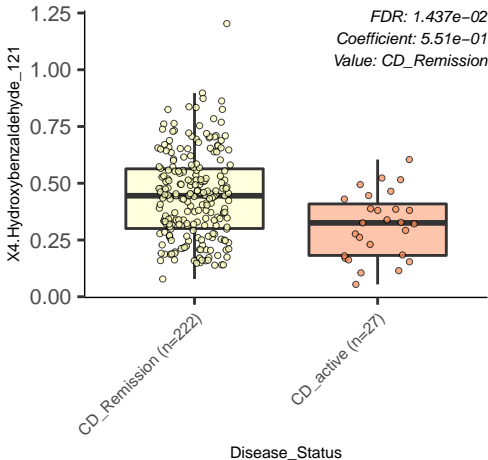
Disease\_Status



X3..4.Hydroxyphenyl.Pyruvate\_179

*FDR: 1.437e-02*  
*Coefficient: 8.41e-01*  
*Value: CD\_Remission*





Decanoic.acid\_171.1

*FDR: 1.437e-02*

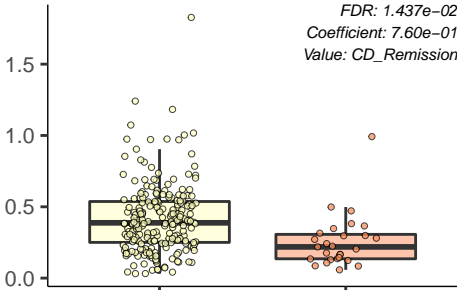
*Coefficient: 7.60e-01*

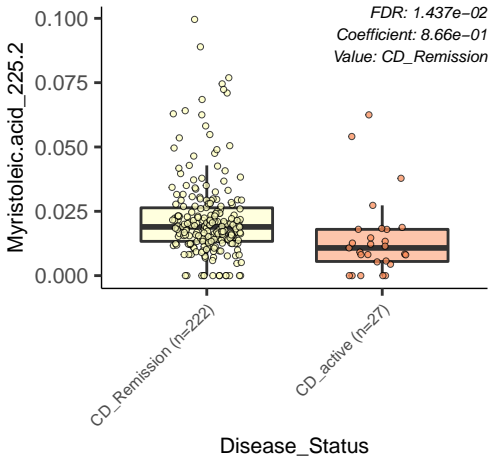
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





Sorbate\_111

FDR: 1.437e-02

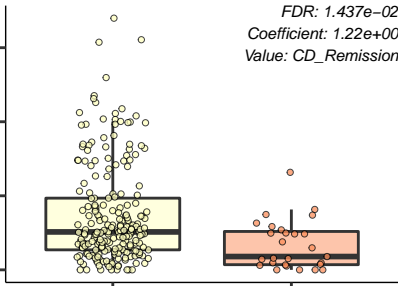
Coefficient: 1.22e+00

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



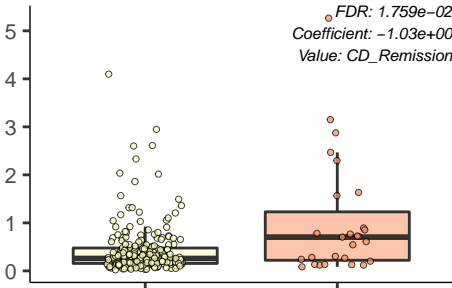
Tyrosine\_182.1

FDR:  $1.759\text{e-}02$   
Coefficient:  $-1.03\text{e}+00$   
Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





Cysteate\_170

FDR: 2.161e-02

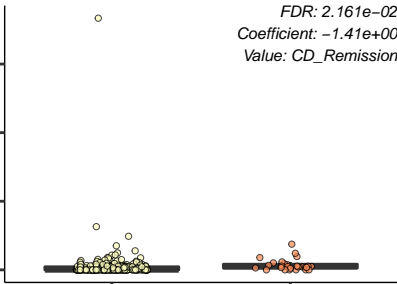
Coefficient: -1.41e+00

Value: CD\_Remission

CD\_Remission (n=222)

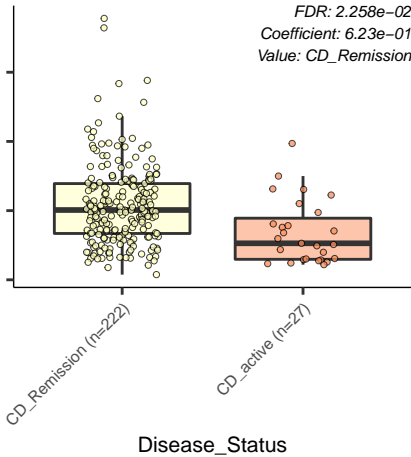
CD\_active (n=27)

Disease\_Status



Gulonolactone\_177

FDR: 2.258e-02  
Coefficient: 6.23e-01  
Value: CD\_Remission



Suberate\_173.1

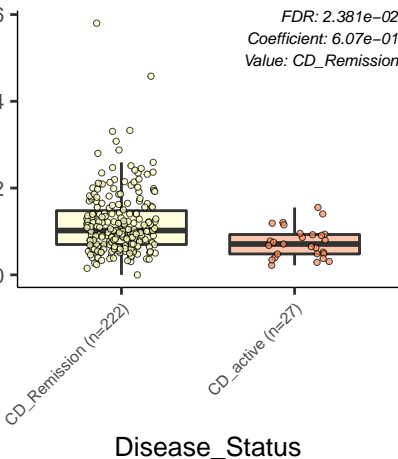
0.006  
0.004  
0.002  
0.000

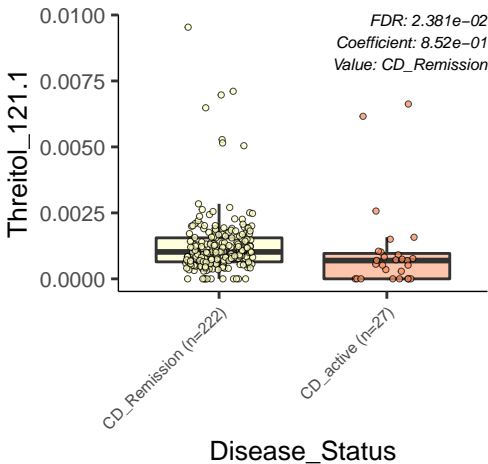
*FDR: 2.381e-02*  
*Coefficient: 6.07e-01*  
*Value: CD\_Remission*

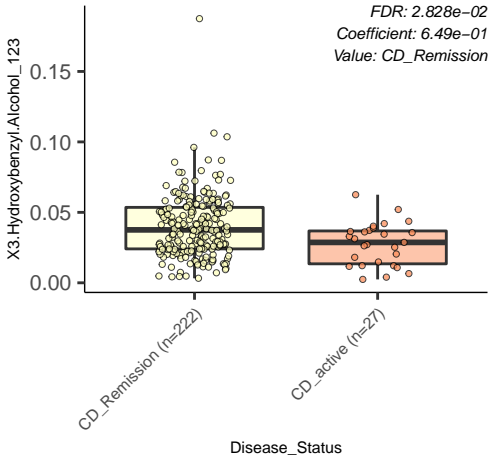
CD\_Remission (n=222)

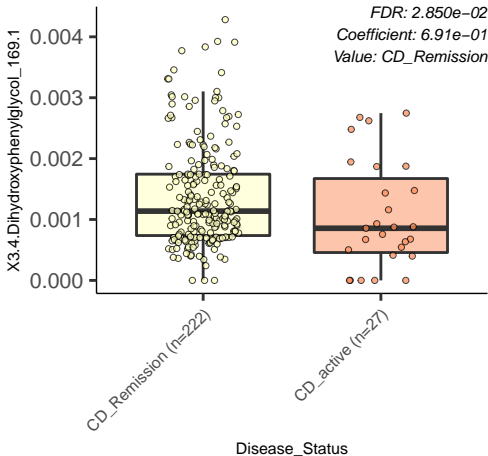
CD\_active (n=27)

Disease\_Status

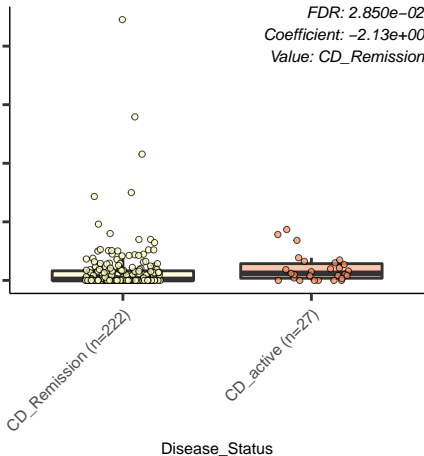


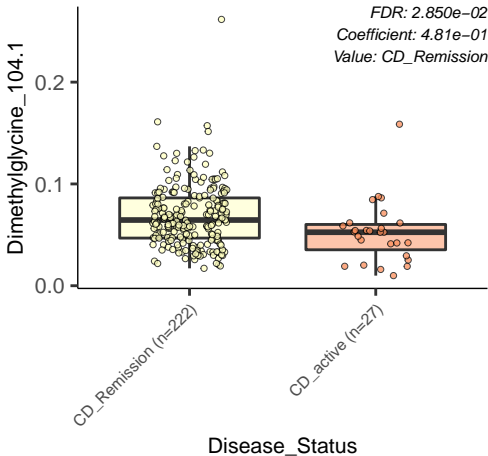




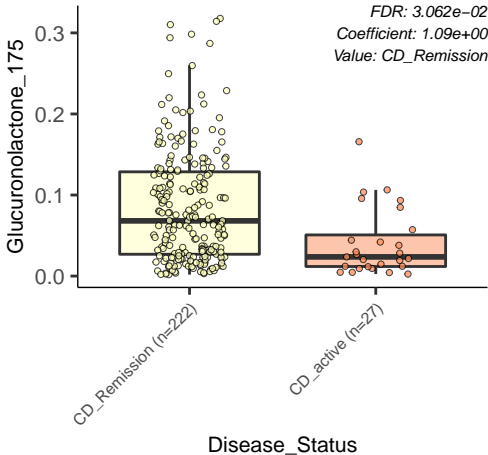


cis.7.10.13.16.Docosatetraenoic.acid\_331.3









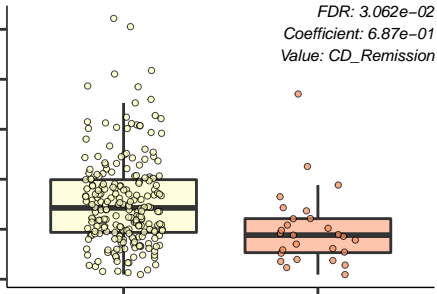
Nonanoic.acid\_157.1

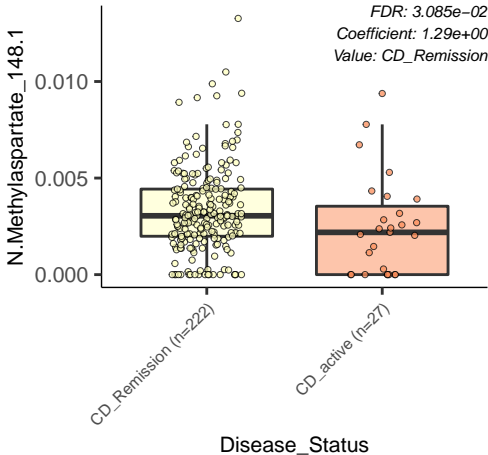
FDR: 3.062e-02  
Coefficient: 6.87e-01  
Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





Choline\_104.1

FDR: 3.235e-02

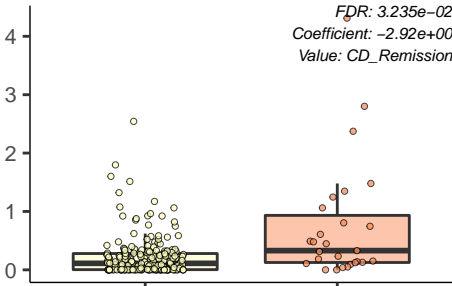
Coefficient: -2.92e+00

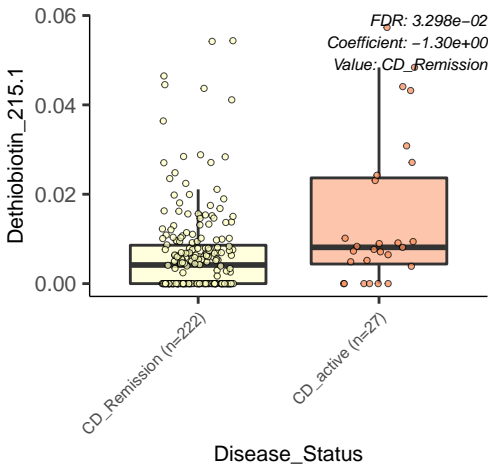
Value: CD\_Remission

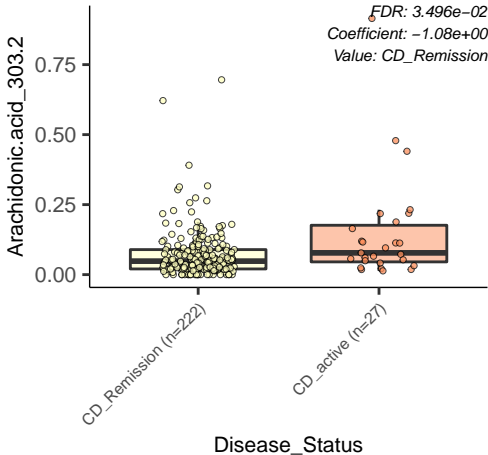
CD\_Remission (n=222)

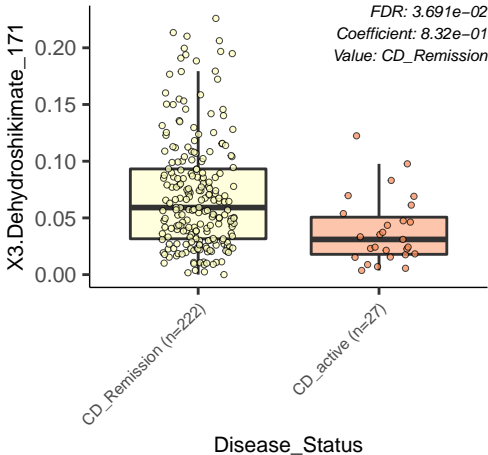
CD\_active (n=27)

Disease\_Status









Hexanoic.acid\_115.1

*FDR: 3.691e-02*

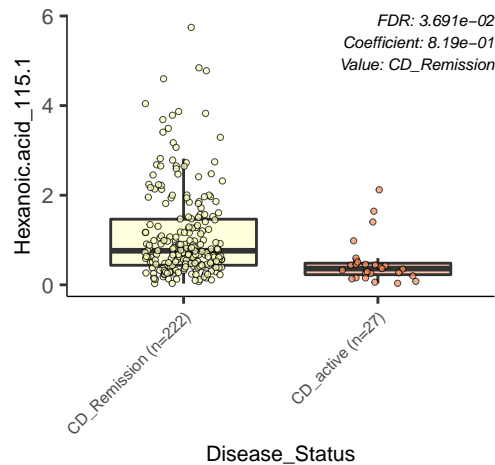
*Coefficient: 8.19e-01*

*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



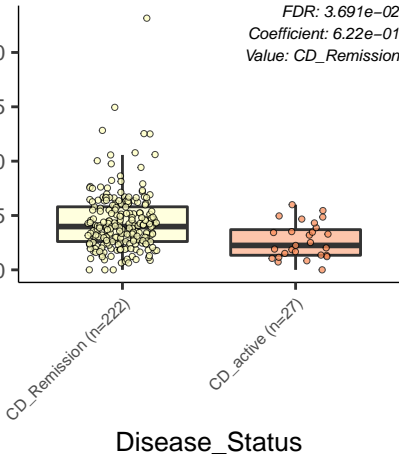


L.Dopa\_198.1

FDR: 3.691e-02

Coefficient: 6.22e-01

Value: CD\_Remission



Nervonic.acid\_365.3

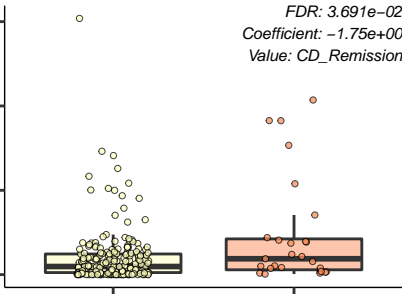
0.15  
0.10  
0.05  
0.00

*FDR: 3.691e-02*  
*Coefficient: -1.75e+00*  
*Value: CD\_Remission*

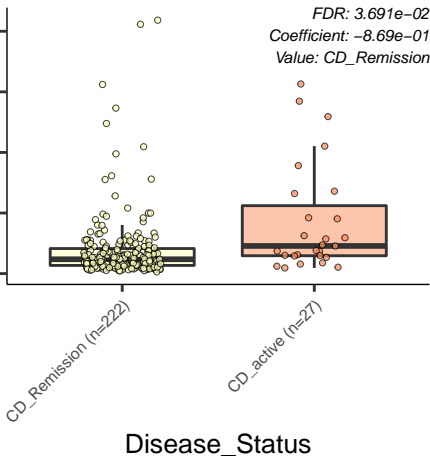
CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Proline\_116.1



Salsolinol\_180.1

*FDR: 3.691e-02*

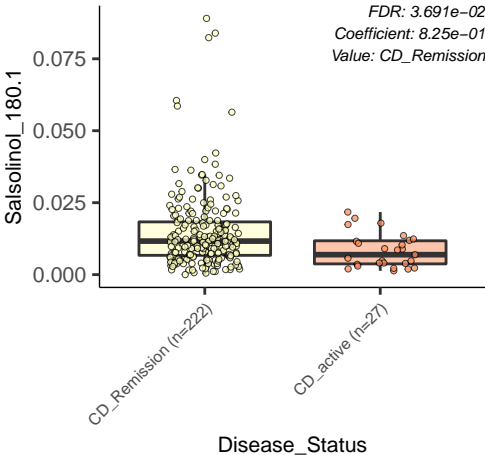
*Coefficient: 8.25e-01*

*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



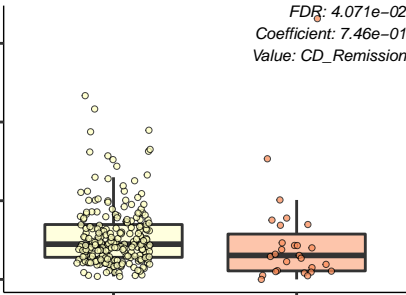
X2.3.Dihydroxybenzoate\_153

*FDR: 4.071e-02*  
*Coefficient: 7.46e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



X2.4.Dihydroxypteridine\_163

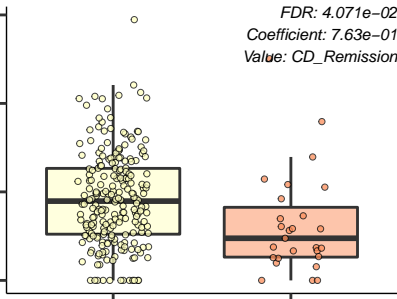
0.006  
0.004  
0.002  
0.000

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

FDR: 4.071e-02  
Coefficient: 7.63e-01  
Value: CD\_Remission



Lumichrome\_241.1

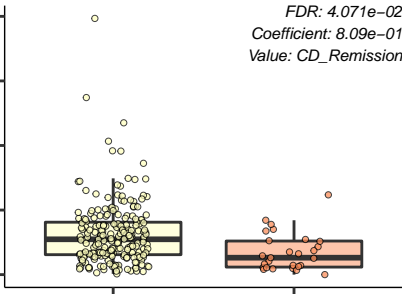
0.20  
0.15  
0.10  
0.05  
0.00

*FDR: 4.071e-02*  
*Coefficient: 8.09e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Glycerol\_91

FDR: 4.142e-02

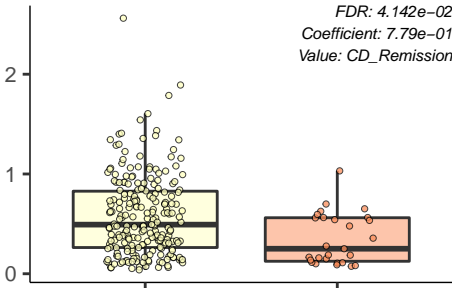
Coefficient: 7.79e-01

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





Maleimide\_98

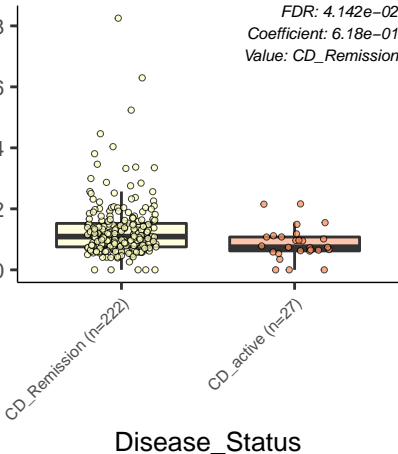
0.008  
0.006  
0.004  
0.002  
0.000

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

FDR:  $4.142 \times 10^{-2}$   
Coefficient:  $6.18 \times 10^{-1}$   
Value: CD\_Remission



methyI.lysine\_161.1

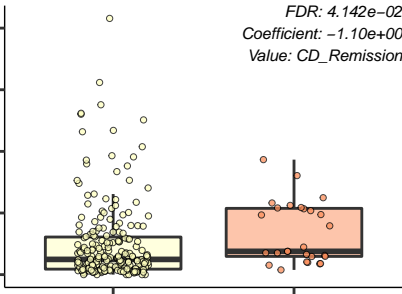
0.08  
0.06  
0.04  
0.02  
0.00

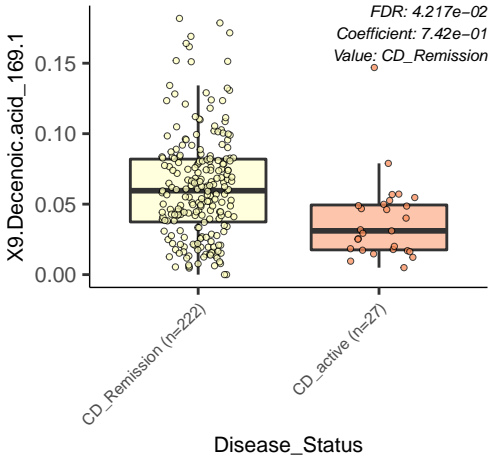
*FDR: 4.142e-02*  
*Coefficient: -1.10e+00*  
*Value: CD\_Remission*

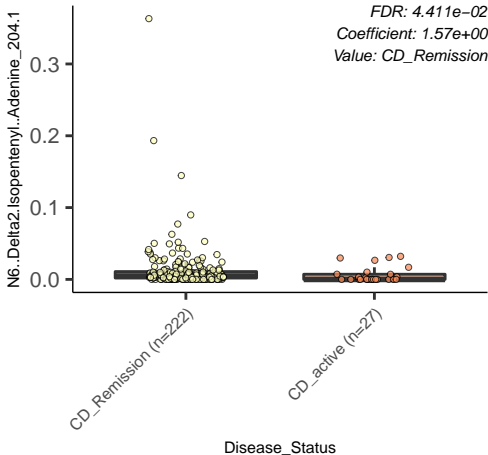
CD\_Remission (n=222)

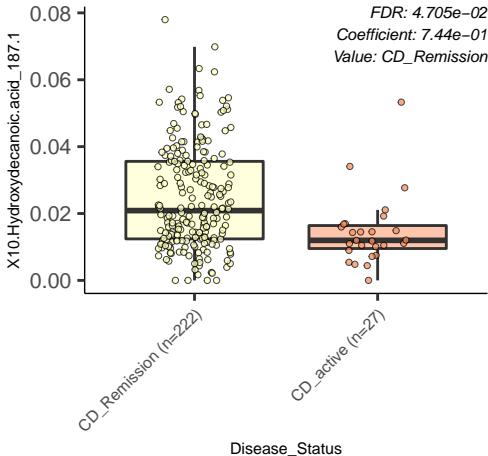
CD\_active (n=27)

Disease\_Status









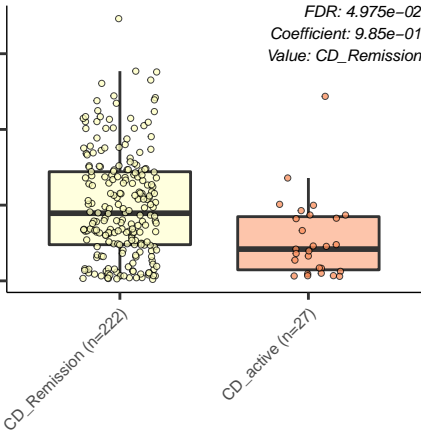
X2.6.Dihydropyridine\_112

*FDR: 4.975e-02*  
*Coefficient: 9.85e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Octanoic.acid\_143.1

FDR: 4.975e-02

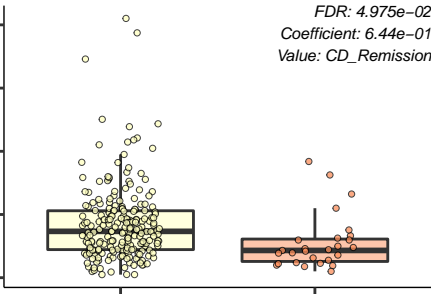
Coefficient: 6.44e-01

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Methyl.Vanillate\_181.1

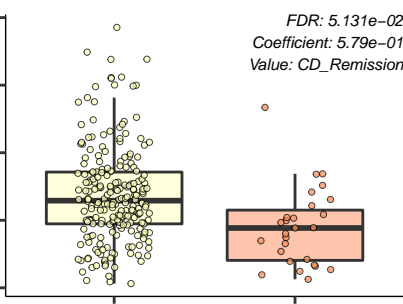
0.12  
0.09  
0.06  
0.03  
0.00

*FDR: 5.131e-02*  
*Coefficient: 5.79e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





Phenylalanine\_166.1

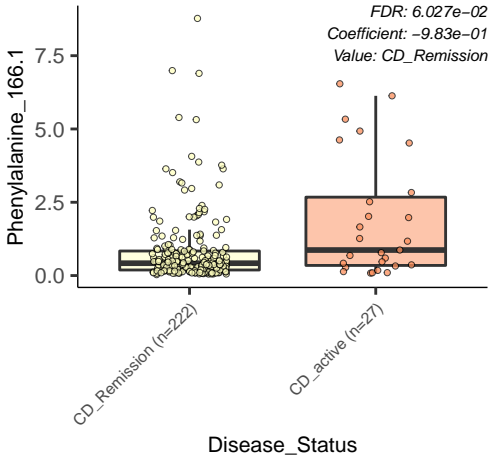
7.5  
5.0  
2.5  
0.0

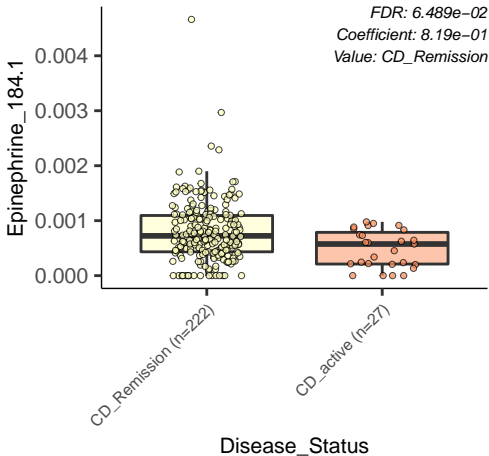
CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

*FDR: 6.027e-02*  
*Coefficient: -9.83e-01*  
*Value: CD\_Remission*





Dopamine\_154.1

FDR: 6.547e-02

Coefficient: 5.68e-01

Value: CD\_Remission

0.02

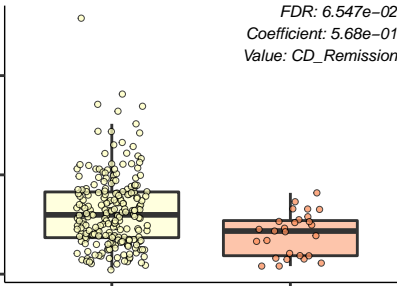
0.01

0.00

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Methylglutarate\_145.1

FDR: 6.547e-02

Coefficient: 4.85e-01

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

0.010

0.005

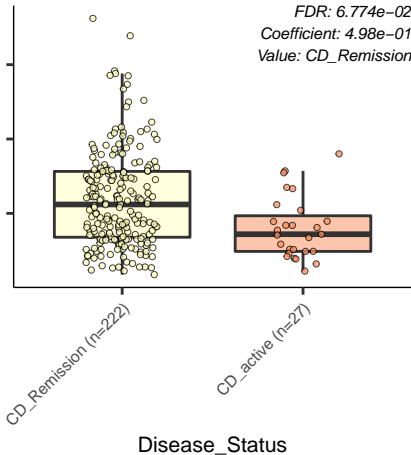
0.000

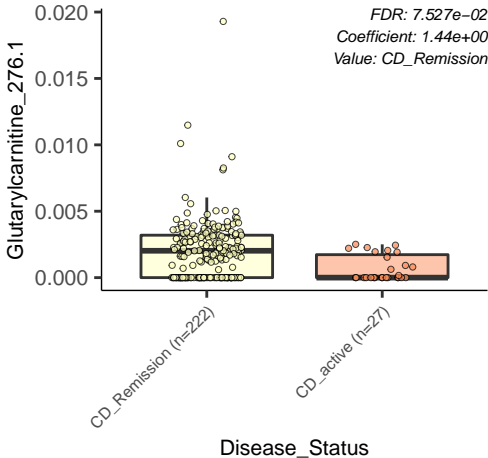
Acetoacetate\_101

*FDR: 6.774e-02*

*Coefficient: 4.98e-01*

*Value: CD\_Remission*





Glycolate\_75

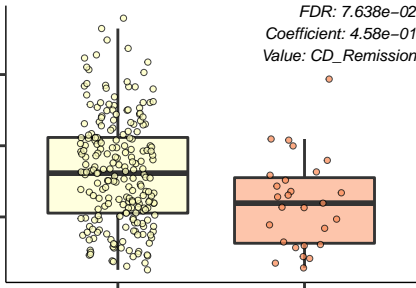
12  
8  
4

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

FDR: 7.638e-02  
Coefficient: 4.58e-01  
Value: CD\_Remission



Pyridoxal\_168.1

*FDR: 7.711e-02*

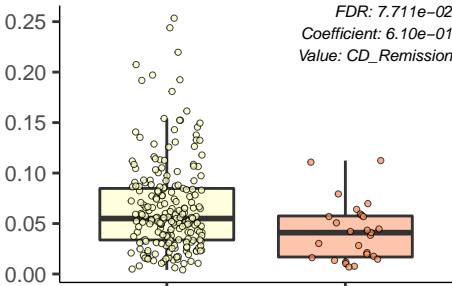
*Coefficient: 6.10e-01*

*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





Azela\_187.1

FDR:  $8.374e-02$

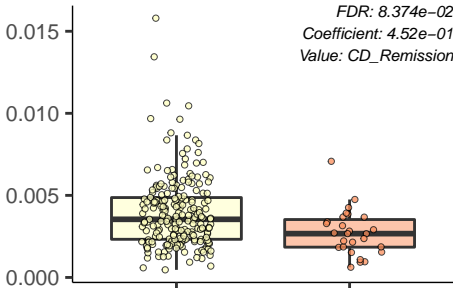
Coefficient:  $4.52e-01$

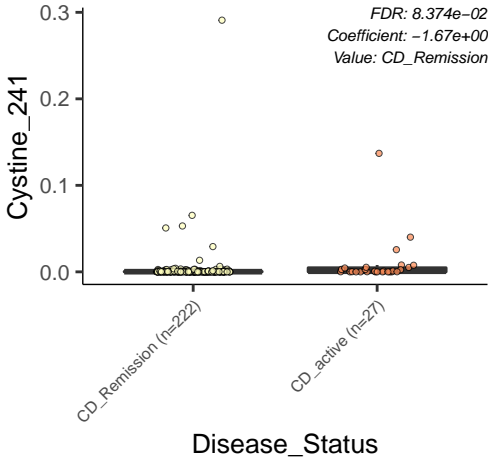
Value: CD\_Remission

CD\_Remission (n=222)

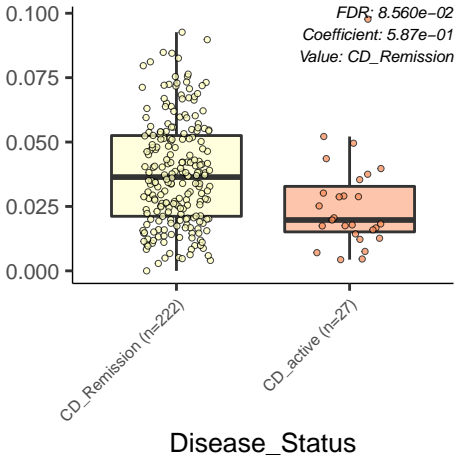
CD\_active (n=27)

Disease\_Status





X10.HAD\_185.1



Tryptophan\_205.1

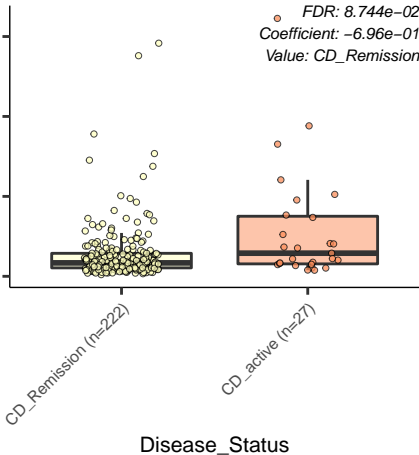
1.5  
1.0  
0.5  
0.0

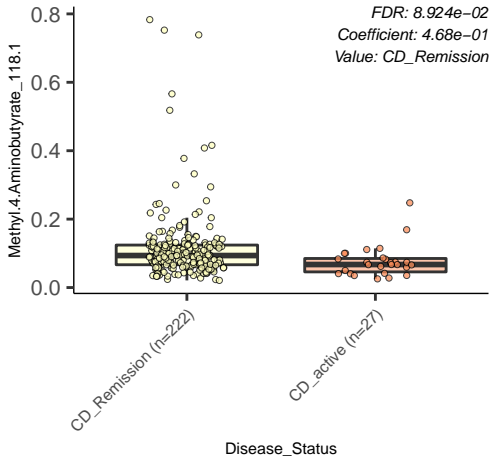
CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

FDR:  $8.744e-02$   
Coefficient:  $-6.96e-01$   
Value: CD\_Remission





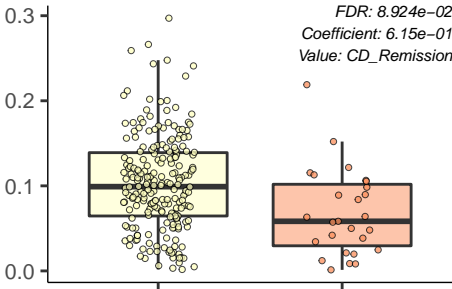
Oxalate\_89

FDR: 8.924e-02  
Coefficient: 6.15e-01  
Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



trans.trans.Muconic.acid\_141

0.008

0.006

0.004

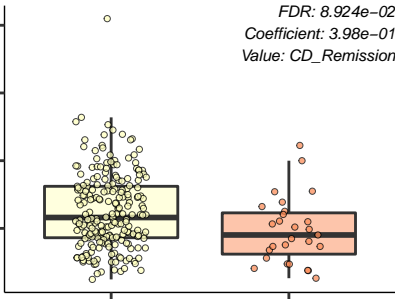
0.002

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

FDR:  $8.924e-02$   
Coefficient:  $3.98e-01$   
Value: CD\_Remission



Urocanate\_139.1

FDR:  $8.924e-02$

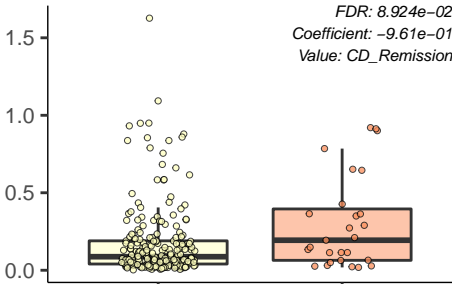
Coefficient:  $-9.61e-01$

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





X3.Methoxytyrosine\_210.1

FDR:  $9.338e-02$

Coefficient:  $4.61e-01$

Value: CD\_Remission

0.03

0.02

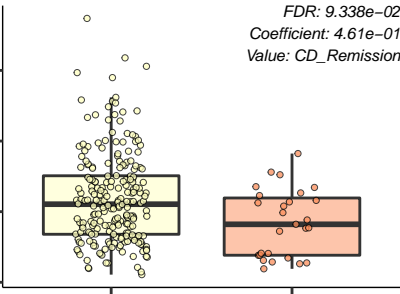
0.01

0.00

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



X6.Hydroxynicotinate\_138

*FDR: 9.338e-02*

*Coefficient: 4.22e-01*

*Value: CD\_Remission*

0.010

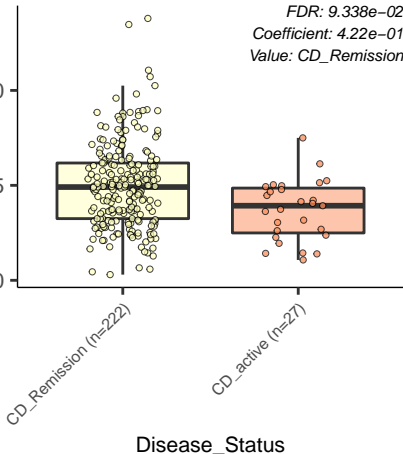
0.005

0.000

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

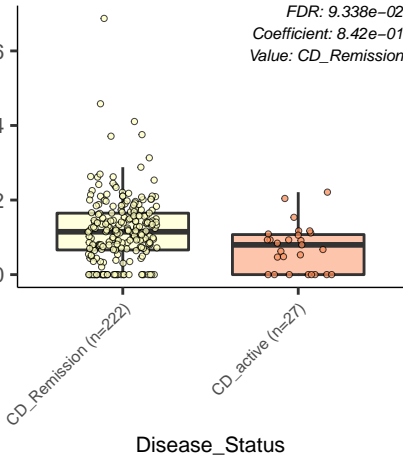


Glucosamine\_196.1

FDR: 9.338e-02

Coefficient: 8.42e-01

Value: CD\_Remission



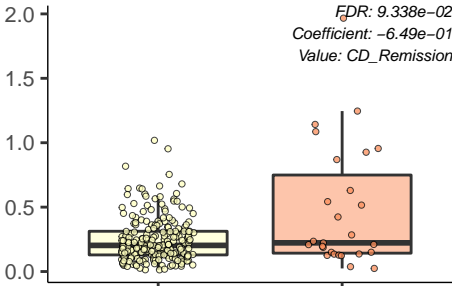
Lysine\_147.1

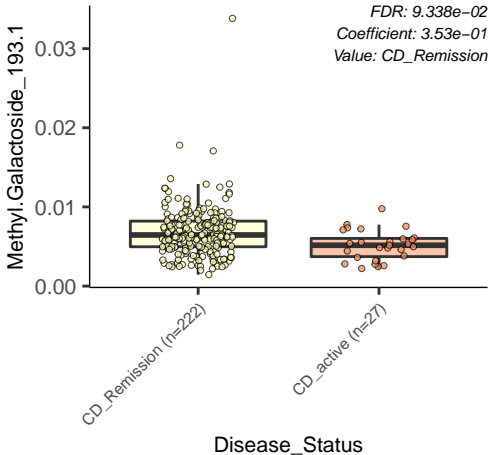
FDR:  $9.338e-02$   
Coefficient:  $-6.49e-01$   
Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





Tartrate\_149

FDR:  $9.338e-02$

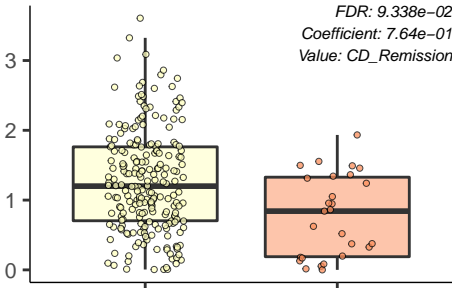
Coefficient:  $7.64e-01$

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



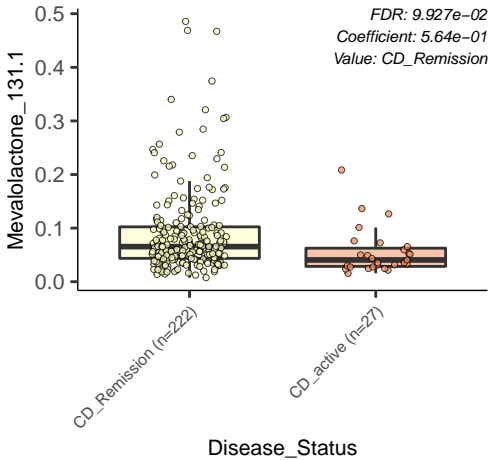
Mevalolactone\_131.1

FDR: 9.927e-02  
Coefficient: 5.64e-01  
Value: CD\_Remission

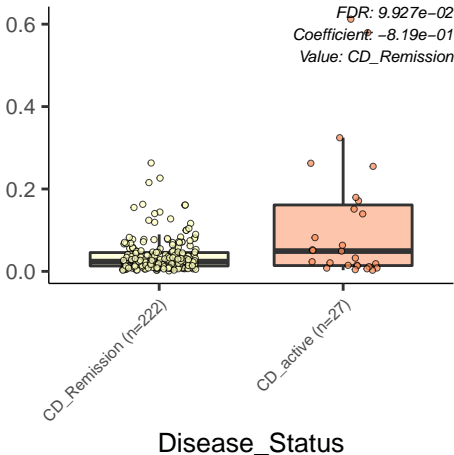
CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Ornithine\_133.1





X3.Methylglutaconate\_143

FDR: 1.004e-01

Coefficient: 4.82e-01

Value: CD\_Remission

0.10

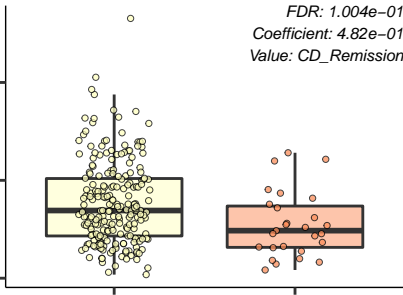
0.05

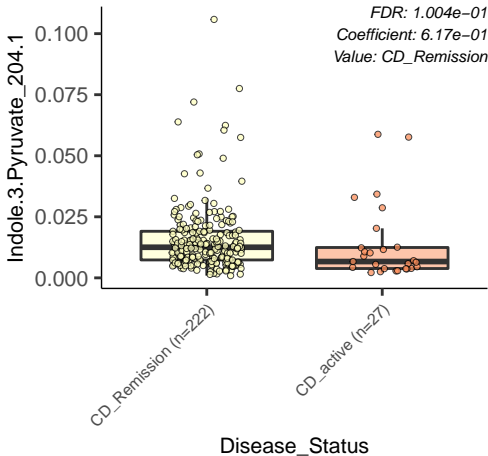
0.00

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





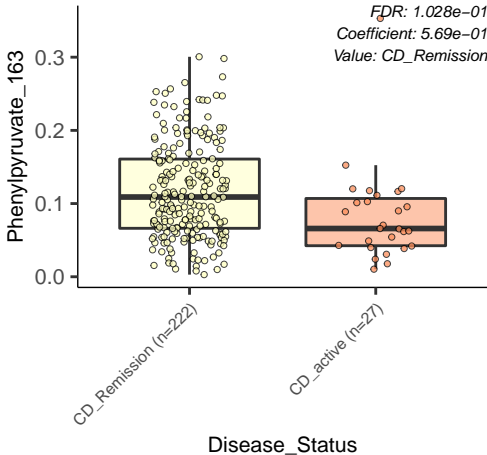
Phenylpyruvate\_163

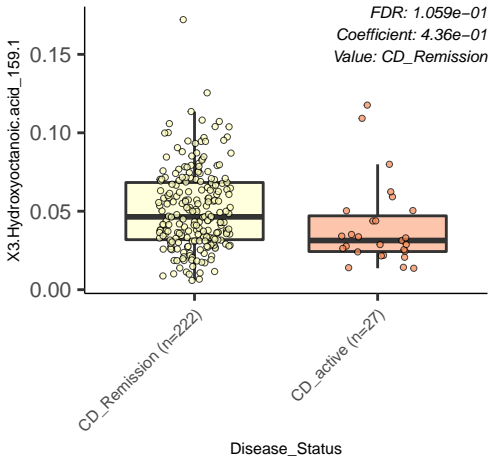
FDR: 1.028e-01  
Coefficient: 5.69e-01  
Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





X3.4.Dihydroxybenzoate\_153

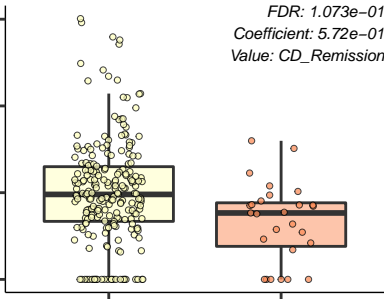
0.0015  
0.0010  
0.0005  
0.0000

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

FDR: 1.073e-01  
Coefficient: 5.72e-01  
Value: CD\_Remission



Caffeate\_179

*FDR: 1.073e-01*

*Coefficient: 3.80e-01*

*Value: CD\_Remission*

0.010

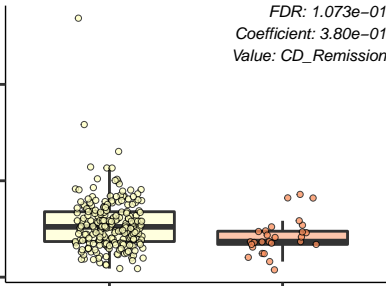
0.005

0.000

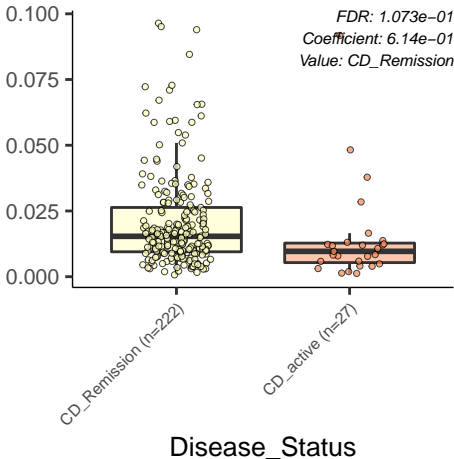
CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Cytidine\_244.1



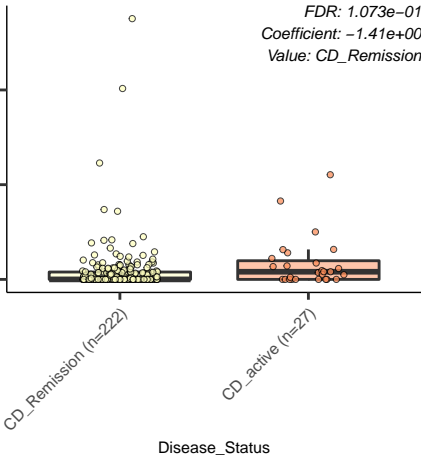
Docosahexaenoic.acid\_327.2

FDR: 1.073e-01  
Coefficient: -1.41e+00  
Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





Picolinate\_122

*FDR: 1.073e-01*

*Coefficient: 3.33e-01*

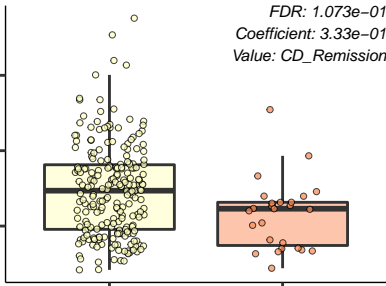
*Value: CD\_Remission*

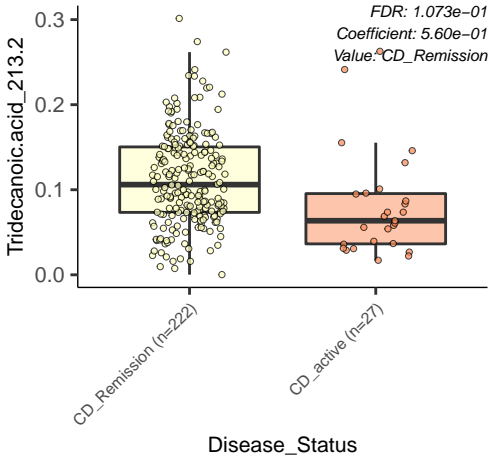
CD\_Remission (n=222)

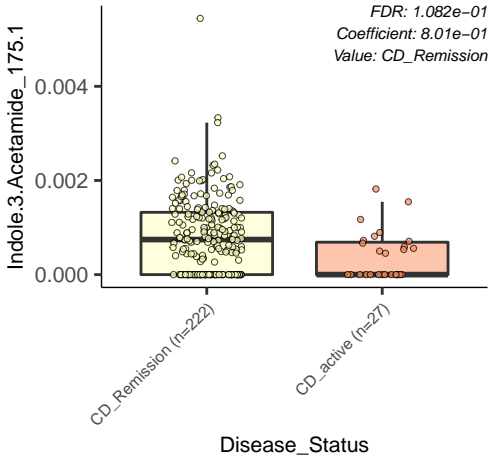
CD\_active (n=27)

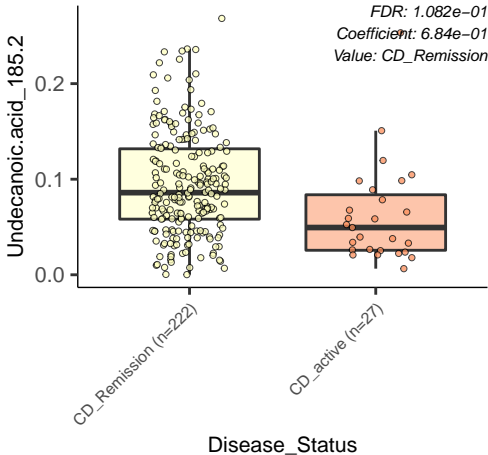
Disease\_Status

0.006  
0.004  
0.002









X2.Aminophenol\_108

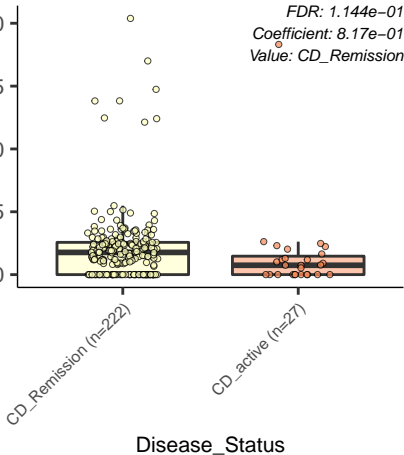
0.020  
0.015  
0.010  
0.005  
0.000

*FDR: 1.144e-01*  
*Coefficient: 8.17e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Cysteine\_122

*FDR: 1.144e-01*

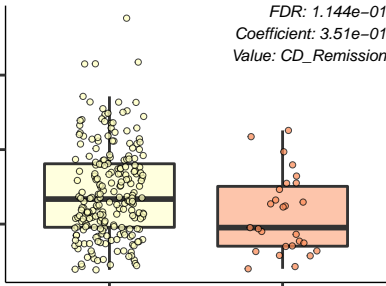
*Coefficient: 3.51e-01*

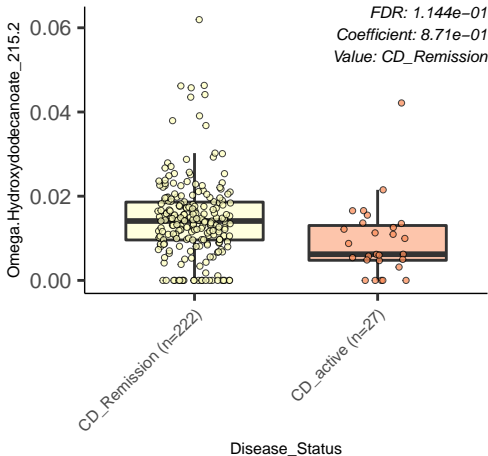
*Value: CD\_Remission*

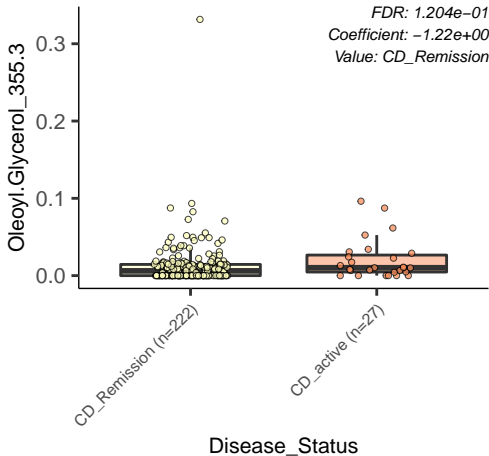
CD\_Remission (n=222)

CD\_active (n=27)

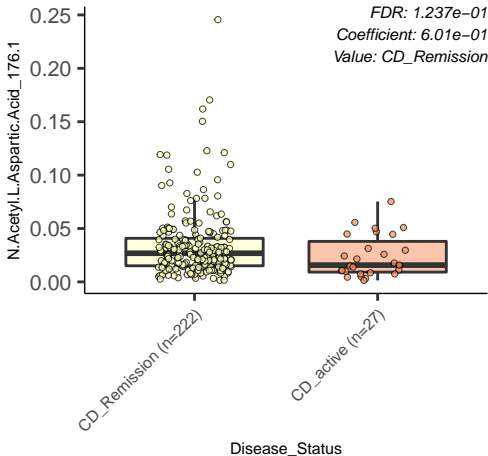
Disease\_Status

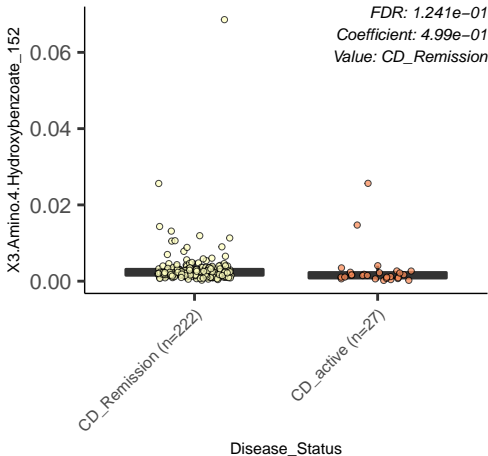


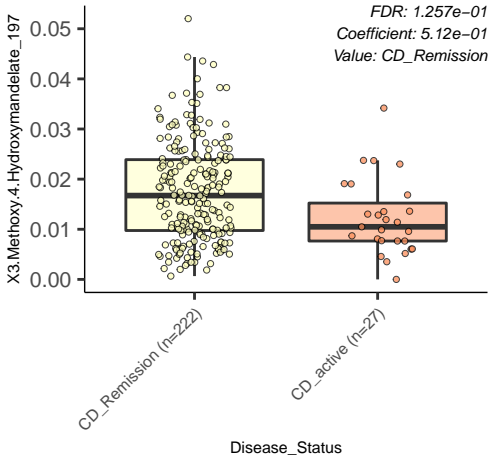












Mannitol\_181.1

FDR: 1.257e-01

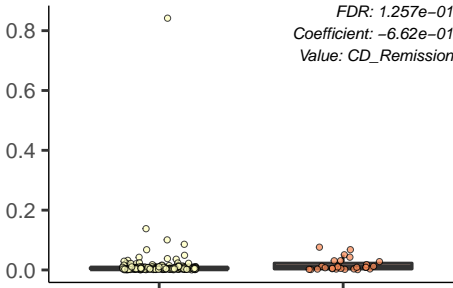
Coefficient: -6.62e-01

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Norepinephrine\_170.1

*FDR: 1.282e-01*

*Coefficient: 6.81e-01*

*Value: CD\_Remission*

0.015

0.010

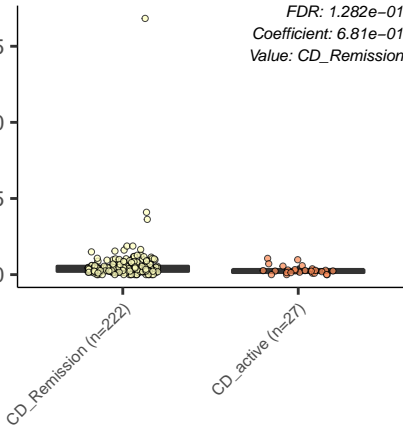
0.005

0.000

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



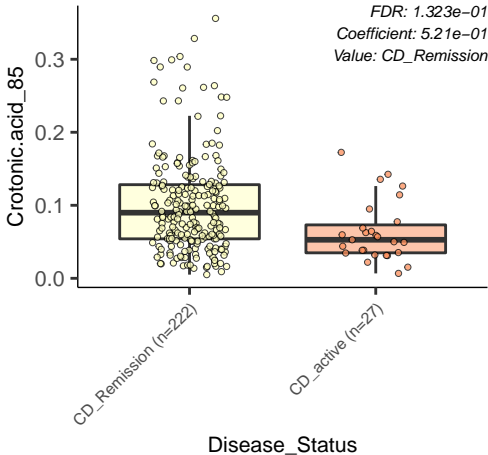
Crotonic.acid\_85

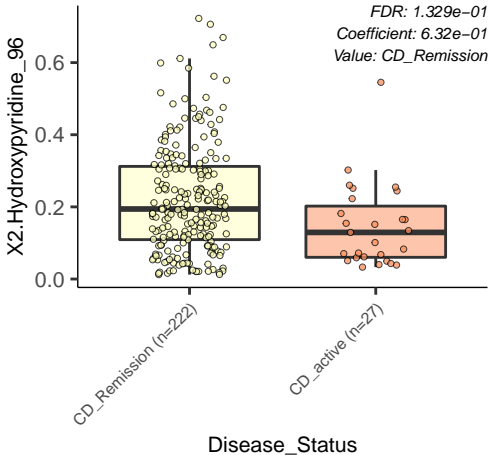
*FDR: 1.323e-01*  
*Coefficient: 5.21e-01*  
*Value: CD\_Remission*

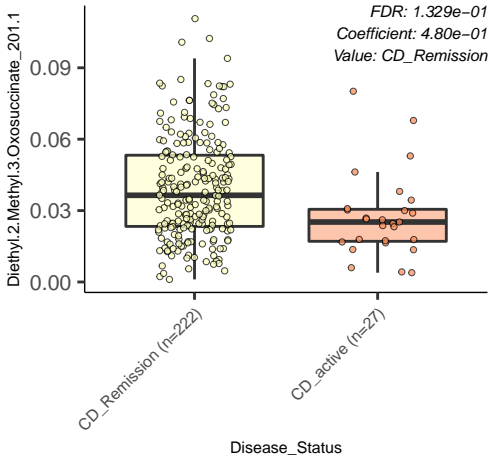
CD\_Remission (n=222)

CD\_active (n=27)

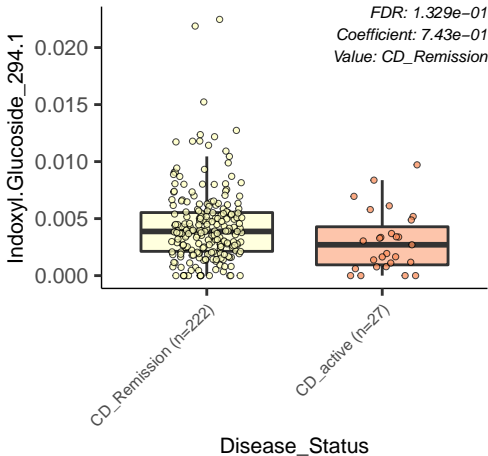
Disease\_Status











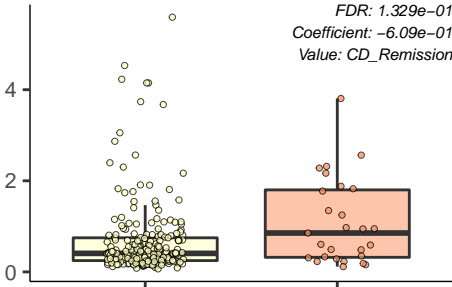
Valine\_118.1

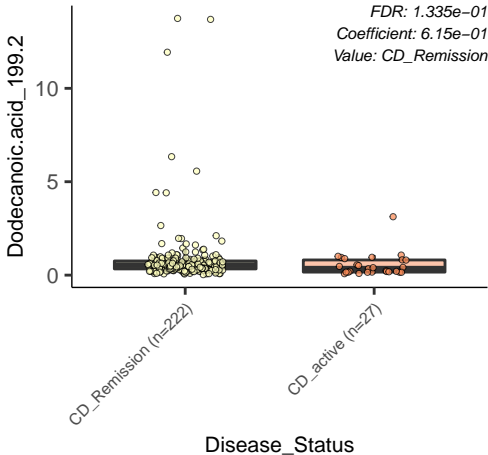
FDR: 1.329e-01  
Coefficient: -6.09e-01  
Value: CD\_Remission

CD\_Remission (n=222)

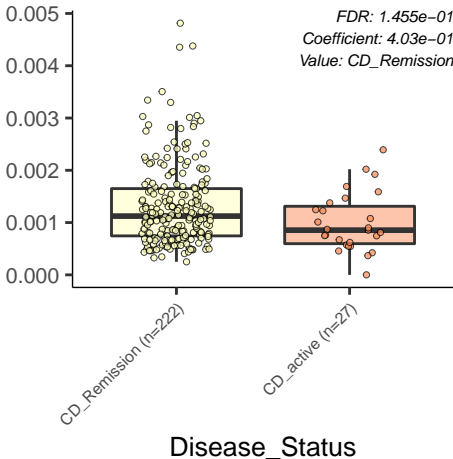
CD\_active (n=27)

Disease\_Status





Maleamate\_114



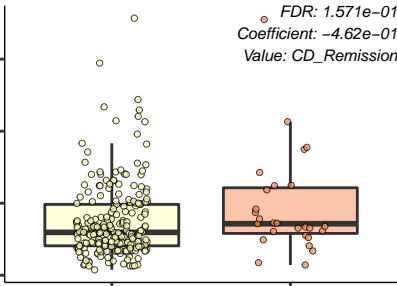
Serine\_106

FDR:  $1.571e-01$   
Coefficient:  $-4.62e-01$   
Value: CD\_Remission

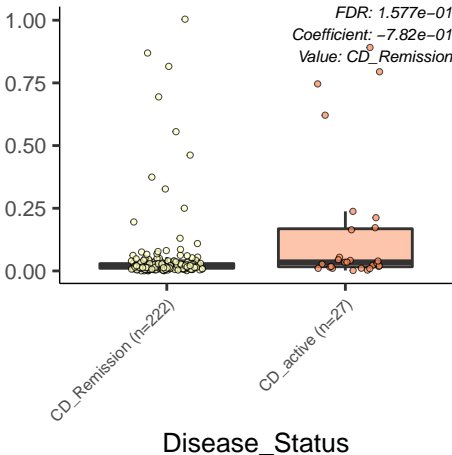
CD\_Remission (n=222)

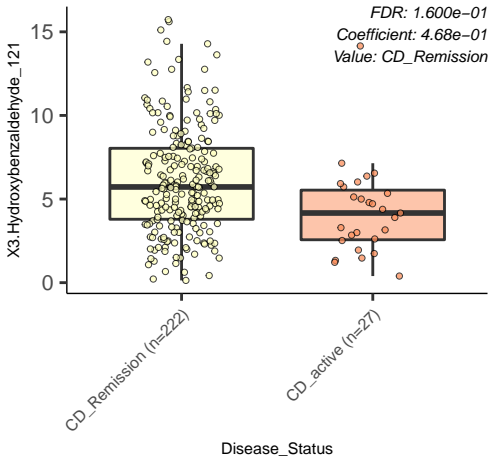
CD\_active (n=27)

Disease\_Status



Histidine\_156.1



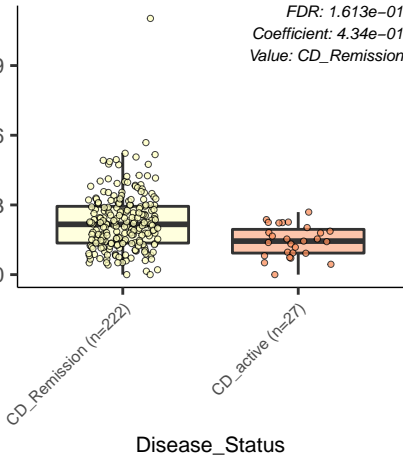


X2.Methylcitrate\_205

FDR: 1.613e-01

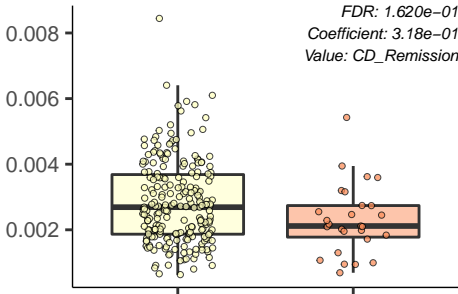
Coefficient: 4.34e-01

Value: CD\_Remission





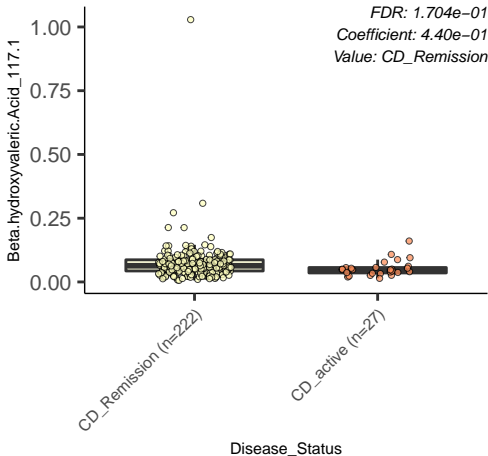
P.Octopamine\_154.1

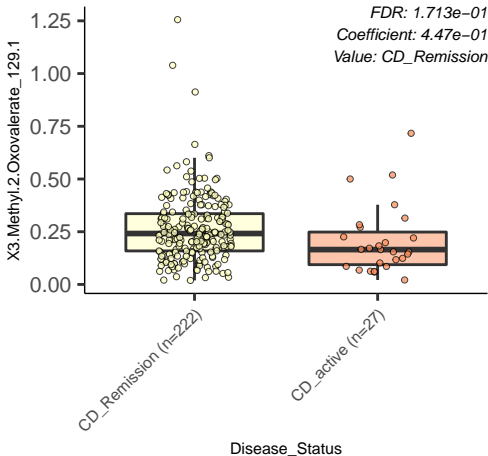


CD\_Remission (n=222)

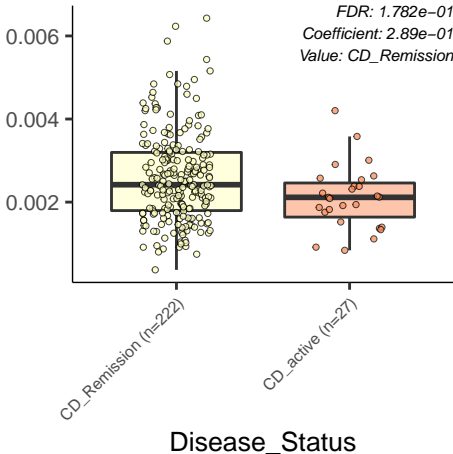
CD\_active (n=27)

Disease\_Status

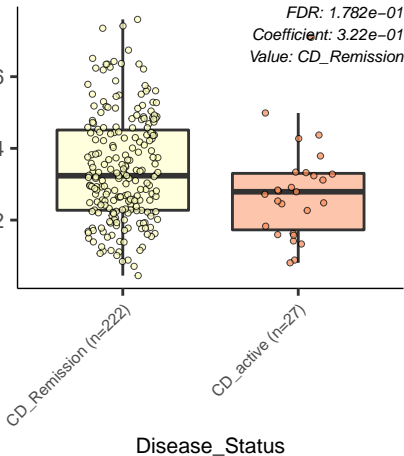




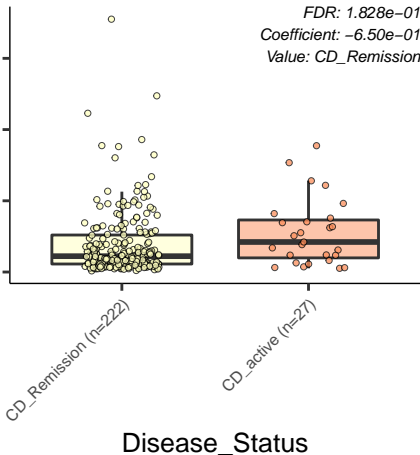
Itaconate\_129



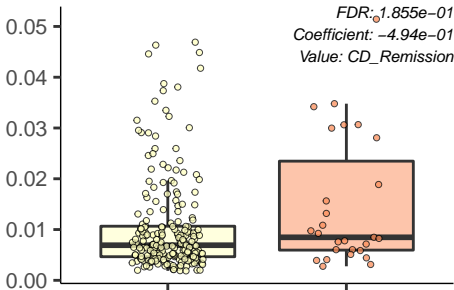
Methylmalonate\_117



Leucine\_132.1



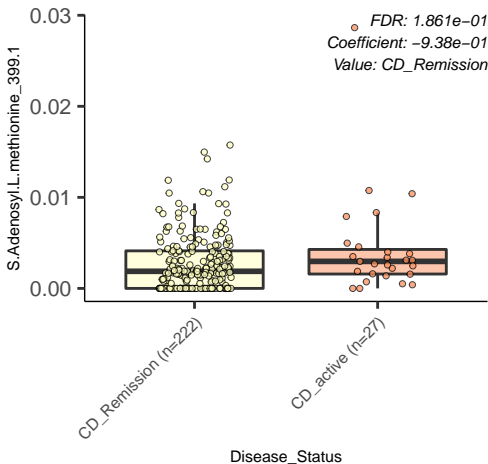
Ribose\_149



CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status





cis.11.Eicosenoic.acid\_309.3

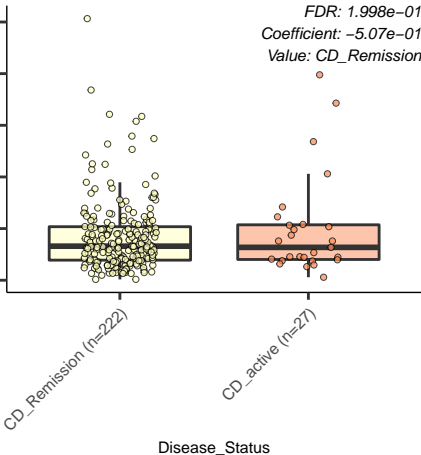
0.5  
0.4  
0.3  
0.2  
0.1  
0.0

*FDR: 1.998e-01*  
*Coefficient: -5.07e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Xanthine\_151

FDR: 2.029e-01

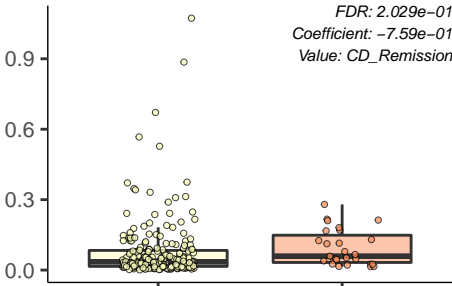
Coefficient: -7.59e-01

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Xanthurenate\_206

*FDR: 2.130e-01*

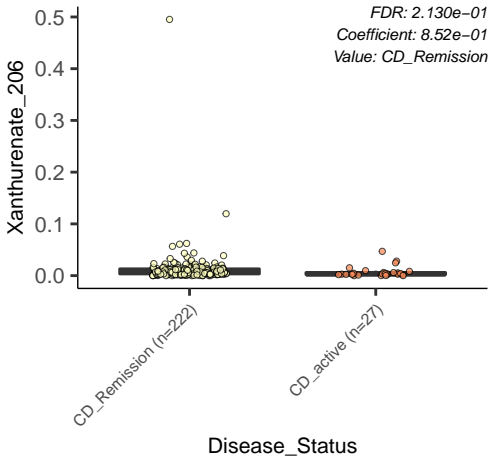
*Coefficient: 8.52e-01*

*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



X4.Pyridoxate\_184.1

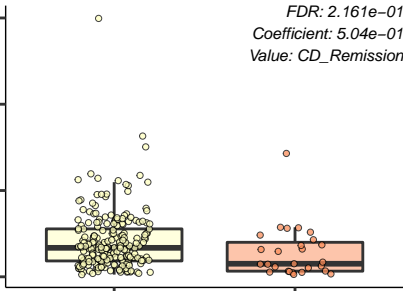
0.15  
0.10  
0.05  
0.00

*FDR: 2.161e-01*  
*Coefficient: 5.04e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



N.Acetyl.L.Aspartic.Acid\_174

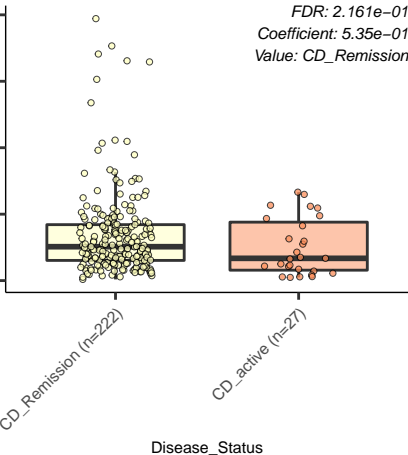
1.00  
0.75  
0.50  
0.25  
0.00

*FDR: 2.161e-01*  
*Coefficient: 5.35e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Biotin\_245.1

FDR: 2.174e-01

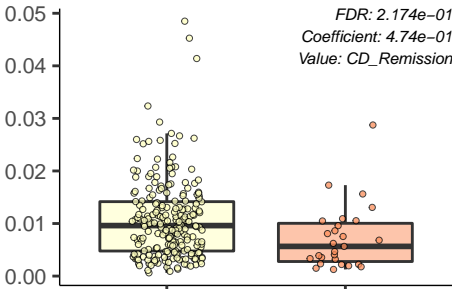
Coefficient: 4.74e-01

Value: CD\_Remission

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Galactosamine\_180.1

FDR: 2.230e-01

Coefficient: -4.92e-01

Value: CD\_Remission

0.10

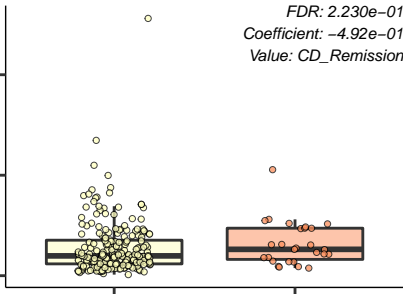
0.05

0.00

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



N.Acetylanaline\_130.1

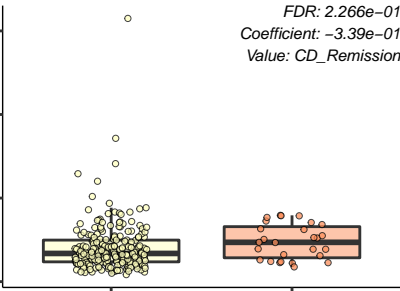
0.06  
0.04  
0.02  
0.00

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status

FDR: 2.266e-01  
Coefficient: -3.39e-01  
Value: CD\_Remission





Oxoadipate\_159

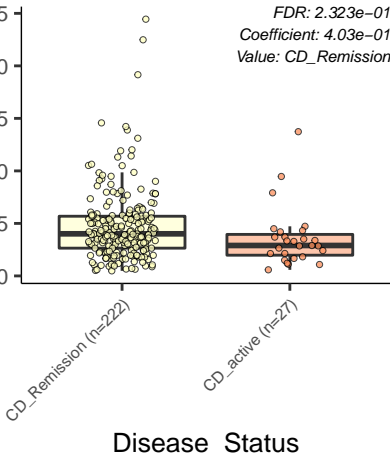
0.0125  
0.0100  
0.0075  
0.0050  
0.0025  
0.0000

*FDR: 2.323e-01*  
*Coefficient: 4.03e-01*  
*Value: CD\_Remission*

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Guaiacol\_123

*FDR: 2.336e-01*

*Coefficient: 3.91e-01*

*Value: CD\_Remission*

0.0100

0.0075

0.0050

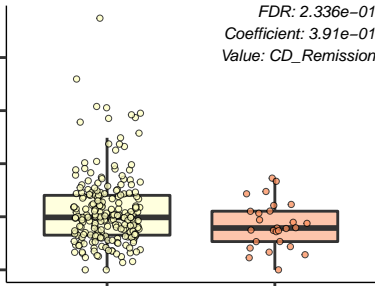
0.0025

0.0000

CD\_Remission (n=222)

CD\_active (n=27)

Disease\_Status



Hydroquinone\_109

