

C18.neg\_Cluster\_2021...urobilin

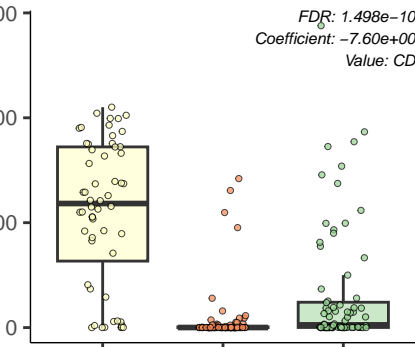
*FDR: 1.498e-10*  
*Coefficient: -7.60e+00*  
*Value: CD*

Control (n=56)

CD (n=88)

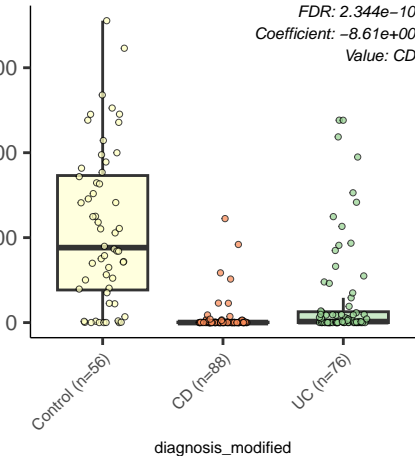
UC (n=76)

diagnosis\_modified



HILIC\_pos\_Cluster\_2093..urobilin.

FDR:  $2.344e-10$   
Coefficient:  $-8.61e+00$   
Value: CD



HILIC.pos\_Cluster\_1486..C16.carnitine

*FDR: 1.128e-07*  
*Coefficient: 4.37e+00*  
*Value: CD*

4000

2000

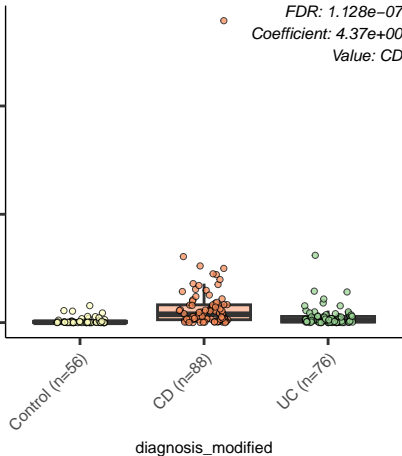
0

Control (n=56)

CD (n=88)

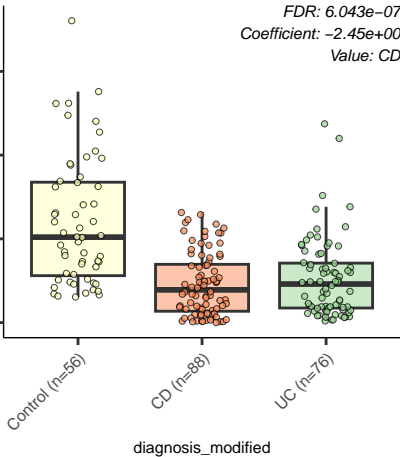
UC (n=76)

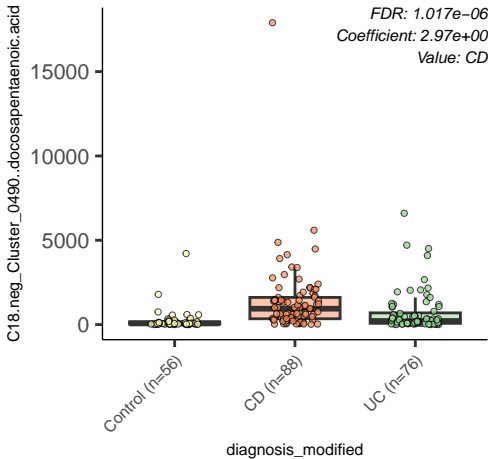
diagnosis\_modified

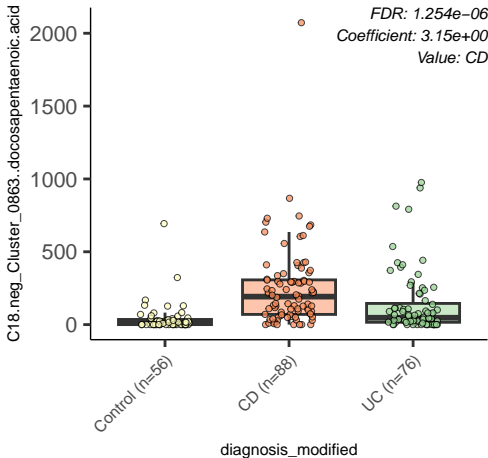


HILIC\_pos\_Cluster\_0268..pyridoxamine

FDR:  $6.043e-07$   
Coefficient:  $-2.45e+00$   
Value: CD







C8.pos\_Cluster\_0988...sphingosine

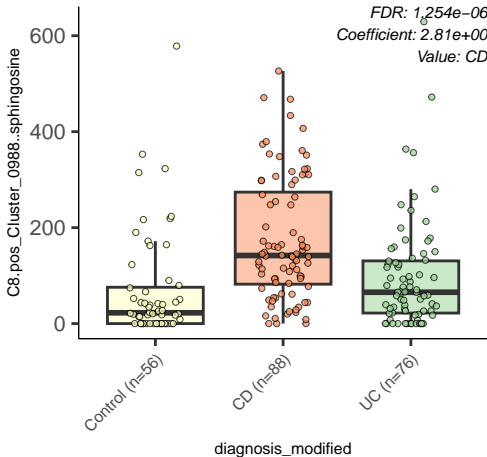
FDR: 1.254e-06  
Coefficient: 2.81e+00  
Value: CD

Control (n=56)

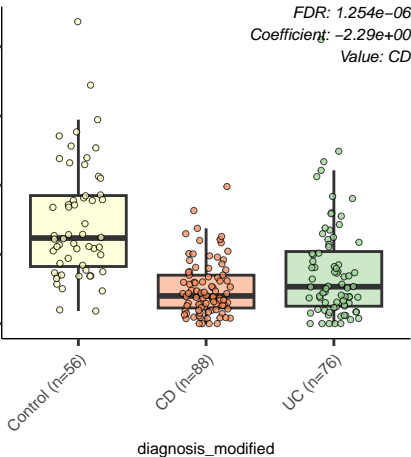
CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.pos\_Cluster\_0521..L.1.2.3.4.tetrahydro.beta.carboline.3.ca





HILIC\_pos\_Cluster\_1580..C18.2.carnitine

*FDR: 1.254e-06*  
*Coefficient: 4.01e+00*  
*Value: CD*

2000

1000

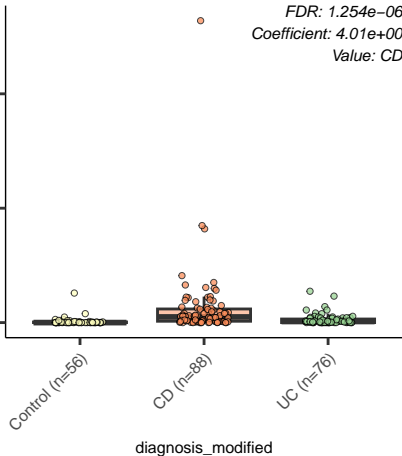
0

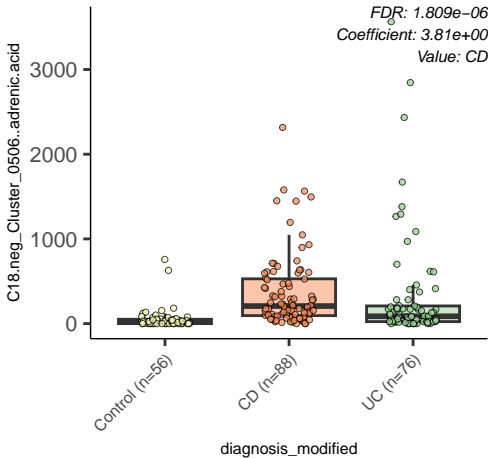
Control (n=56)

CD (n=88)

UC (n=76)

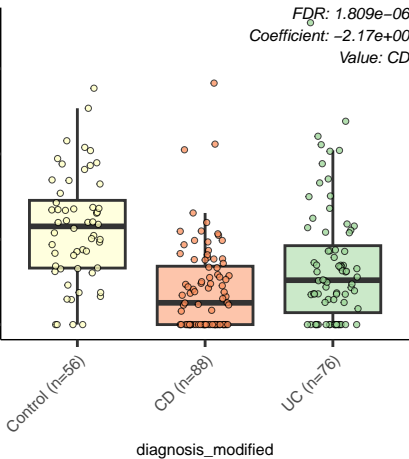
diagnosis\_modified

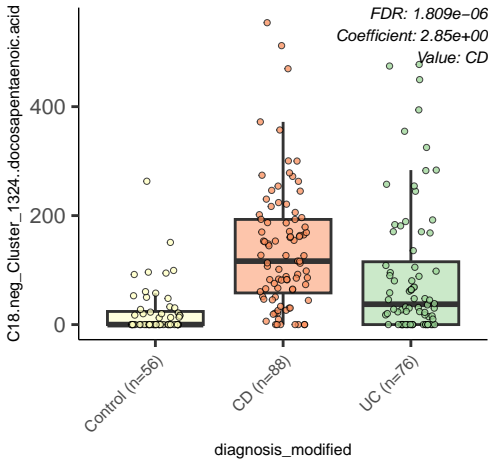




C18.neg\_Cluster\_0901..7.ketodeoxycholate

FDR: 1.809e-06  
Coefficient: -2.17e+00  
Value: CD





HILIC.neg\_Cluster\_0441...sebacate

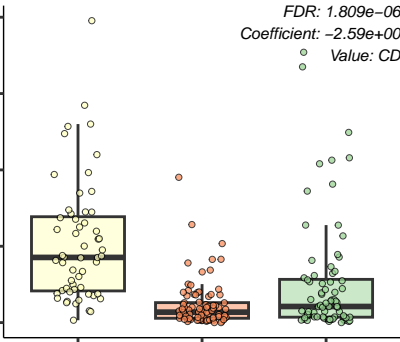
FDR: 1.809e-06  
Coefficient: -2.59e+00  
Value: CD

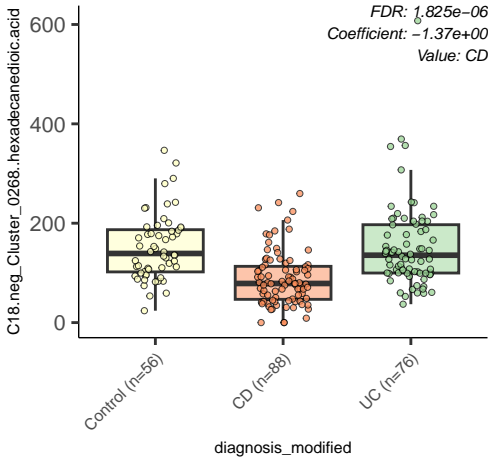
Control (n=56)

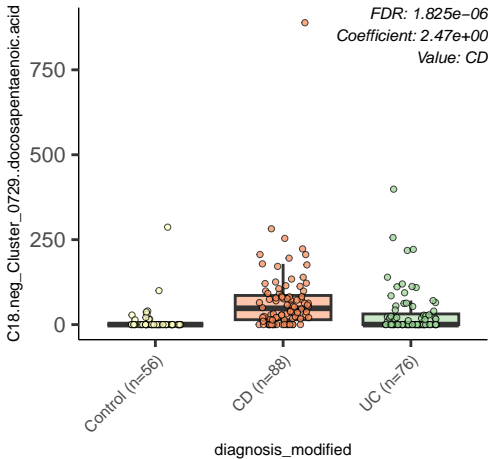
CD (n=88)

UC (n=76)

diagnosis\_modified







C18.neg\_Cluster\_0591..eicosatrienoic.acid

FDR: 2.047e-06  
Coefficient: 2.65e+00  
Value: CD

400

200

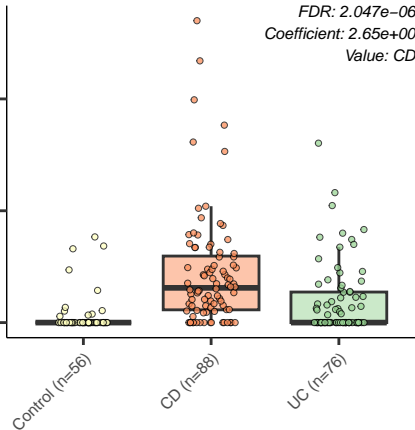
0

Control (n=56)

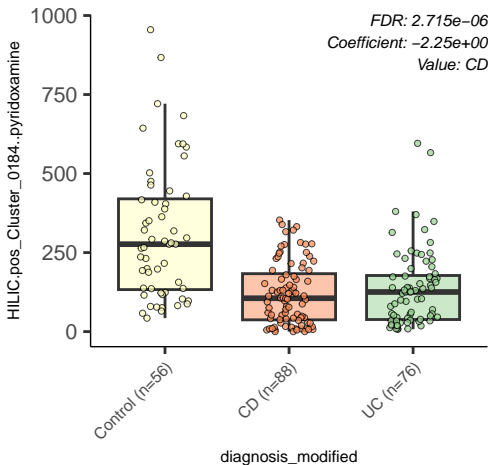
CD (n=88)

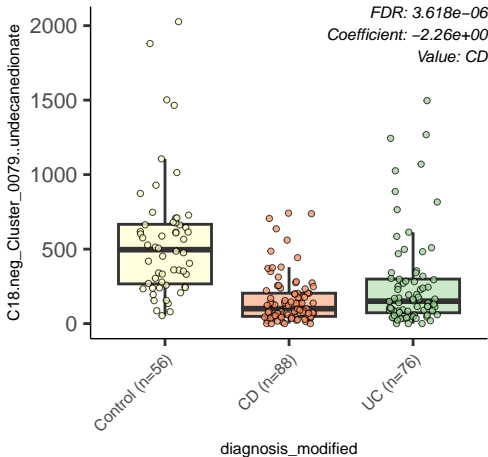
UC (n=76)

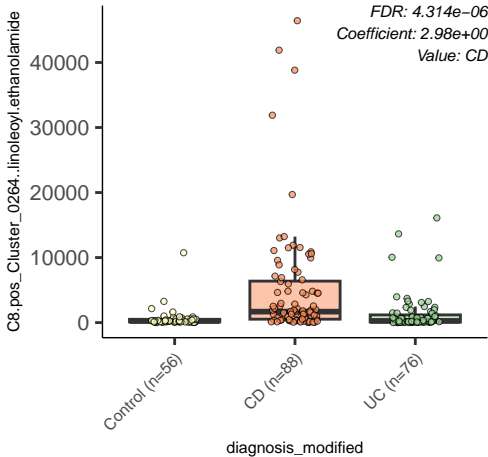
diagnosis\_modified

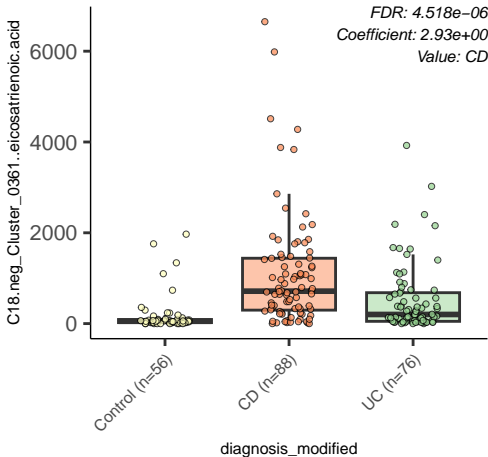












C8.pos\_Cluster\_0253..sphingosine

FDR: 1.050e-05

Coefficient: 2.17e+00

Value: CD

15000

10000

5000

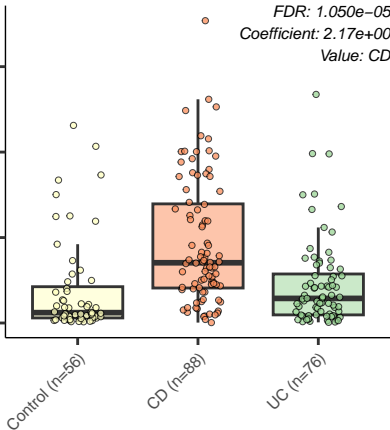
0

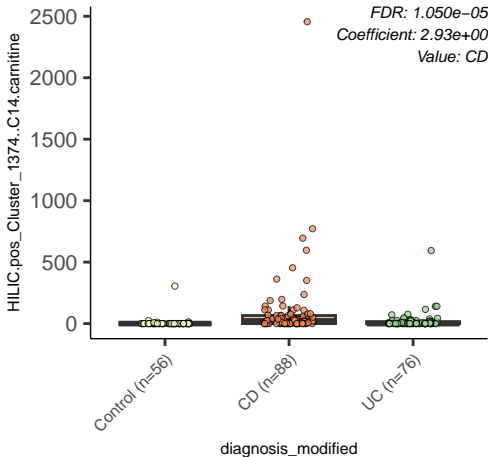
Control (n=56)

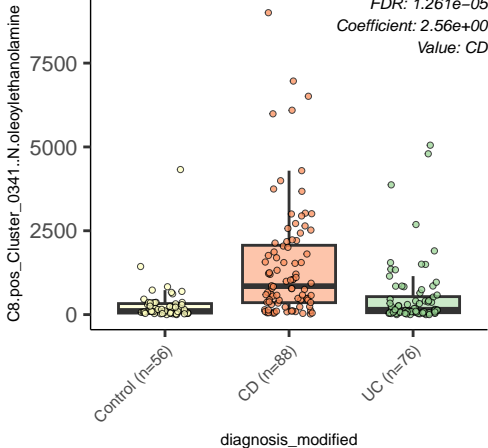
CD (n=88)

UC (n=76)

diagnosis\_modified

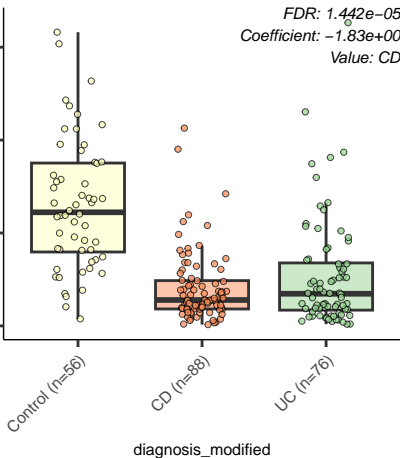






HILIC.pos\_Cluster\_0384..N.acetylglutamic.acid

FDR:  $1.442e-05$   
Coefficient:  $-1.83e+00$   
Value: CD





C18.neg\_Cluster\_0045..azelate

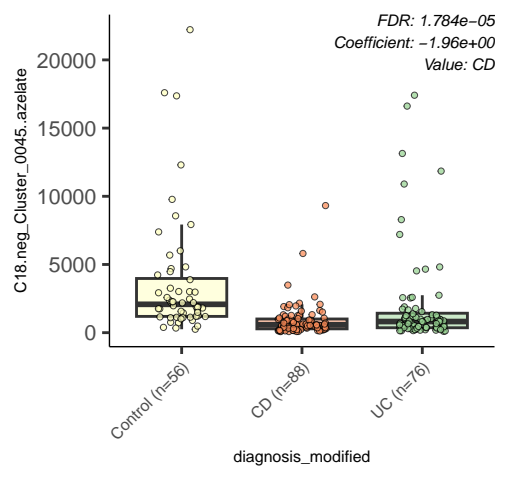
*FDR: 1.784e-05*  
*Coefficient: -1.96e+00*  
*Value: CD*

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.pos\_Cluster\_0540..pantothenate

*FDR: 1.829e-05*  
*Coefficient: -1.52e+00*  
*Value: CD*

10000

5000

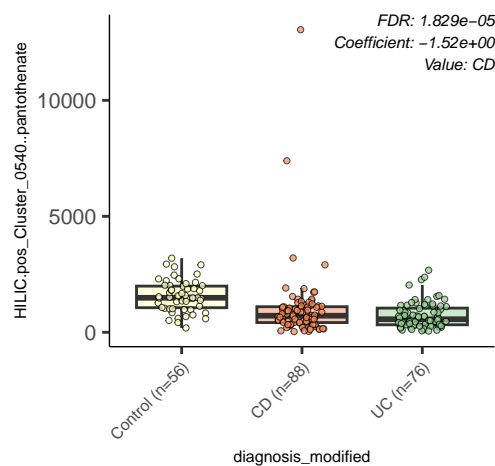
0

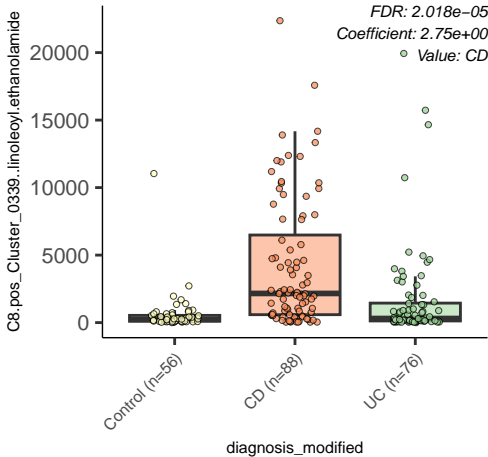
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.pos\_Cluster\_0524..N.acetyl.L.arginine

FDR: 2.041e-05  
Coefficient: -1.68e+00  
Value: CD

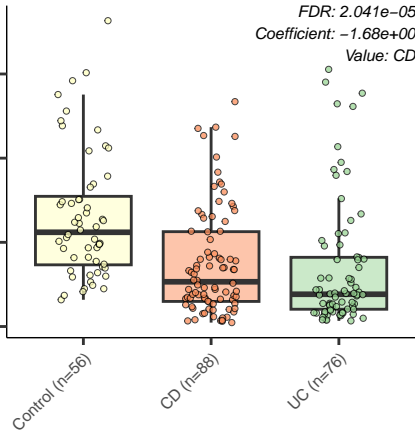
750  
500  
250  
0

Control (n=56)

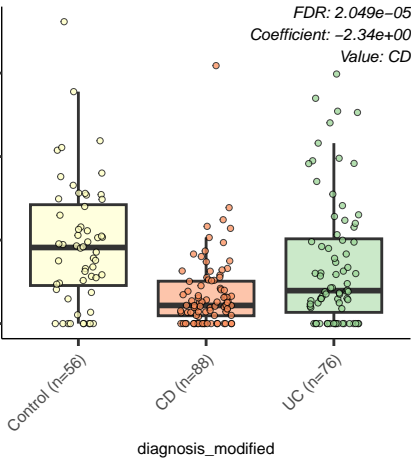
CD (n=88)

UC (n=76)

diagnosis\_modified



C18.neg\_Cluster\_0183...1.2.3.4.tetrahydro.b.carboline.1.3.dicar



C8.pos\_Cluster\_0166..sphingosine

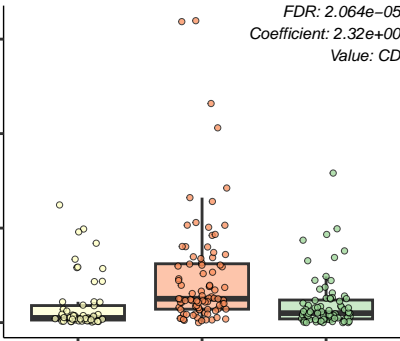
FDR: 2.064e-05  
Coefficient: 2.32e+00  
Value: CD

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC\_pos\_Cluster\_0177\_4.hydroxy.3.methylacetophen

FDR:  $2.064e-05$   
Coefficient:  $-2.14e+00$   
Value: CD

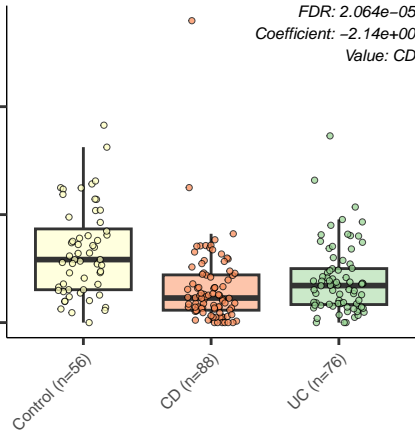
400  
200  
0

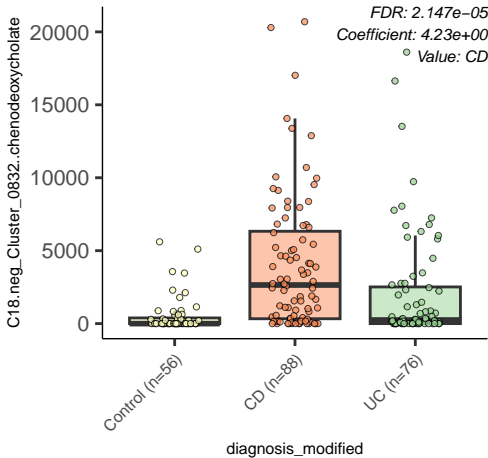
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified







HILIC.neg\_Cluster\_0288..suberate

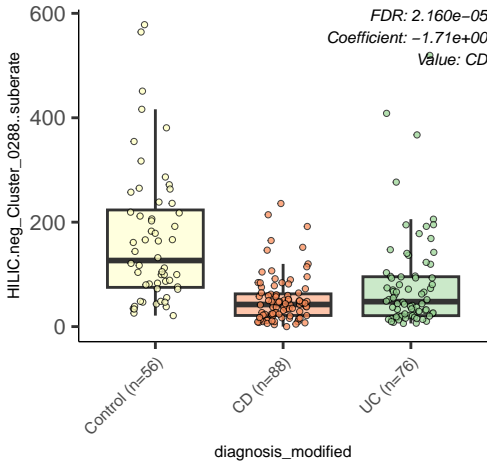
FDR: 2.160e-05  
Coefficient: -1.71e+00  
Value: CD

Control (n=56)

CD (n=88)

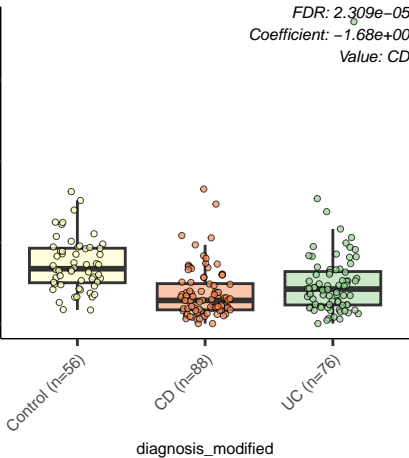
UC (n=76)

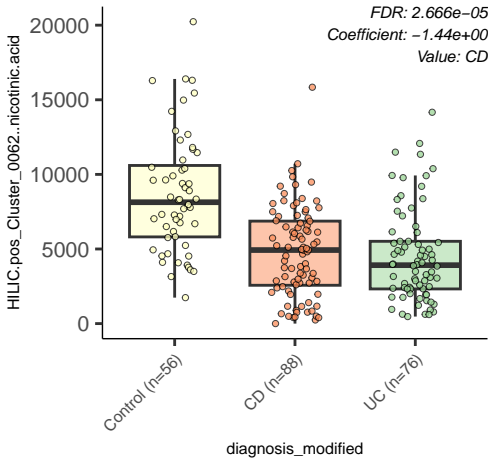
diagnosis\_modified



HILIC.pos\_Cluster\_0658..geranyl.acetoacetate.

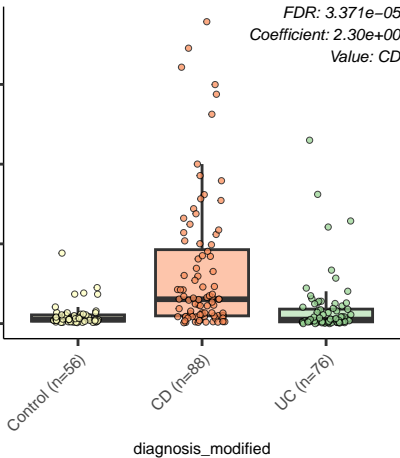
FDR:  $2.309e-05$   
Coefficient:  $-1.68e+00$   
Value: CD





HILIC.neg\_Cluster\_1088...linoleoyl.ethanolamide

FDR:  $3.371e-05$   
Coefficient:  $2.30e+00$   
Value: CD



HILIC.neg\_Cluster\_1325...linoleoyl.ethanolamide

FDR:  $3.587e-05$

Coefficient:  $2.45e+00$

Value: CD

15000

10000

5000

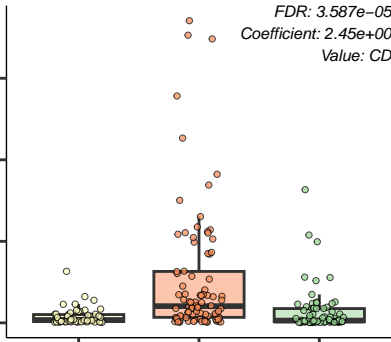
0

Control (n=56)

CD (n=88)

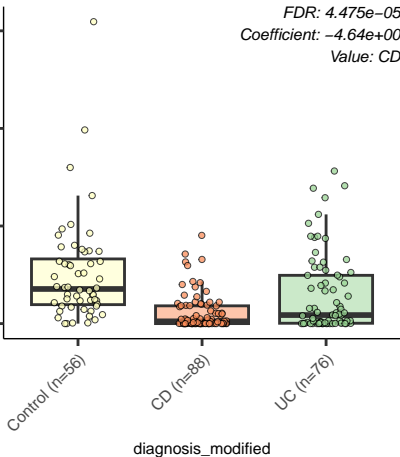
UC (n=76)

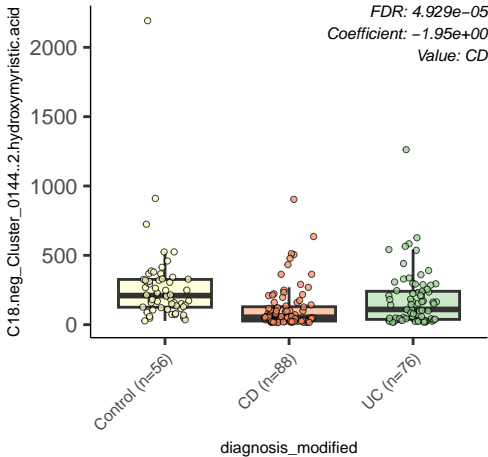
diagnosis\_modified



HILIC.neg\_Cluster\_0220..3.methyladipate.pimelate

FDR:  $4.475e-05$   
Coefficient:  $-4.64e+00$   
Value: CD





C18.neg\_Cluster\_0486..carnosol

FDR:  $4.929e-05$   
Coefficient:  $-3.55e+00$   
Value: CD

7500

5000

2500

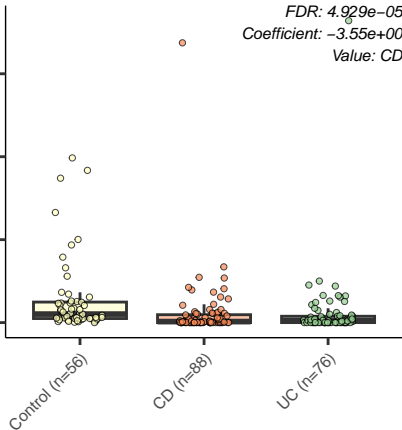
0

Control (n=56)

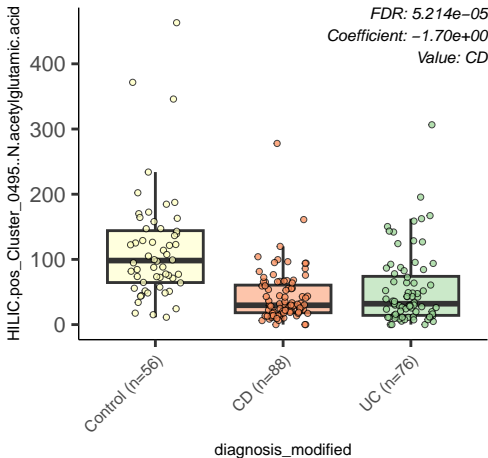
CD (n=88)

UC (n=76)

diagnosis\_modified







HILIC.pos\_Cluster\_0540..pantothenate

*FDR: 6.046e-05*  
*Coefficient: -1.49e+00*  
*Value: UC*

10000

5000

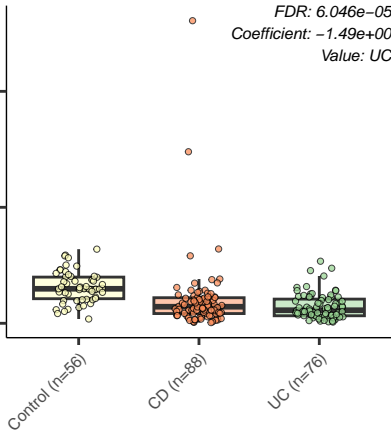
0

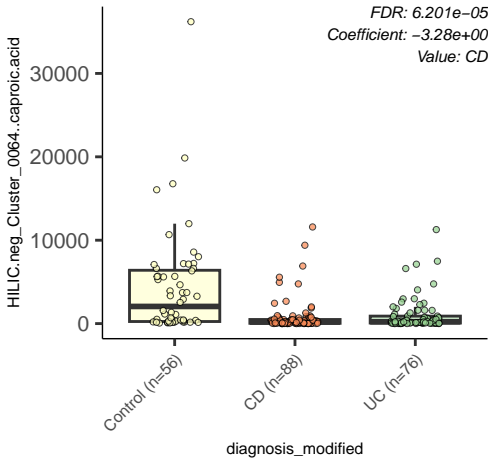
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





C8\_pos\_Cluster\_0629..cholestenone

FDR:  $7.785e-05$   
Coefficient:  $-2.38e+00$   
Value: CD

200

100

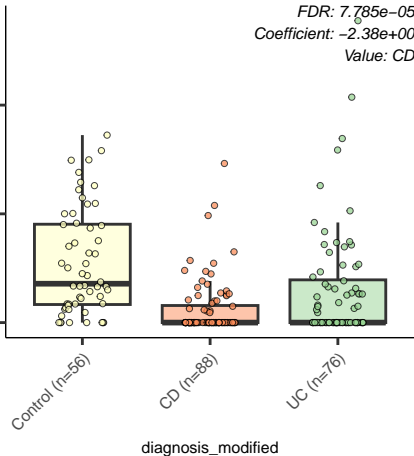
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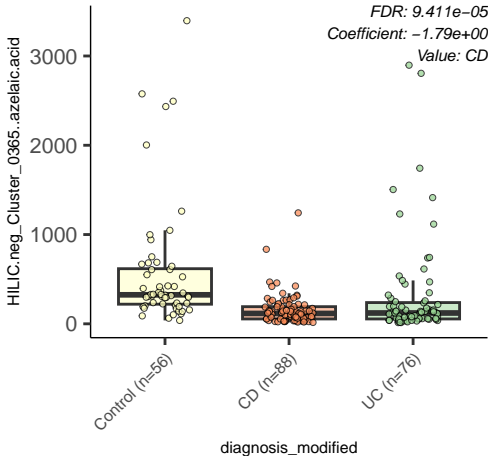
Control (n=56)

CD (n=88)

UC (n=76)

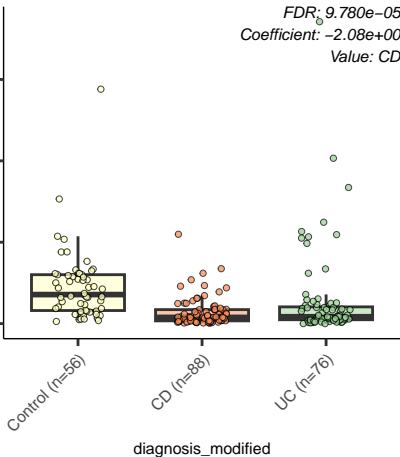
diagnosis\_modified





C18.neg\_Cluster\_0064..sebacate

FDR:  $9.780e-05$   
Coefficient:  $-2.08e+00$   
Value: CD



C18.neg\_Cluster\_01111..dodecanedioic.acid

FDR: 1.047e-04  
Coefficient: -1.75e+00  
Value: CD

4000

2000

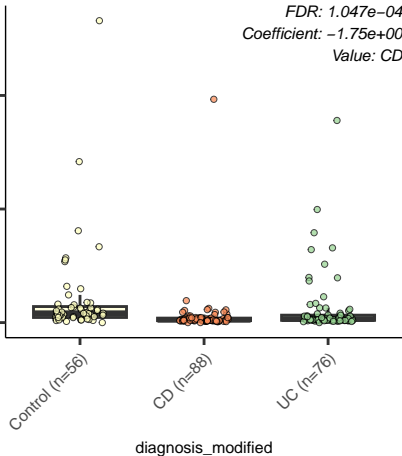
0

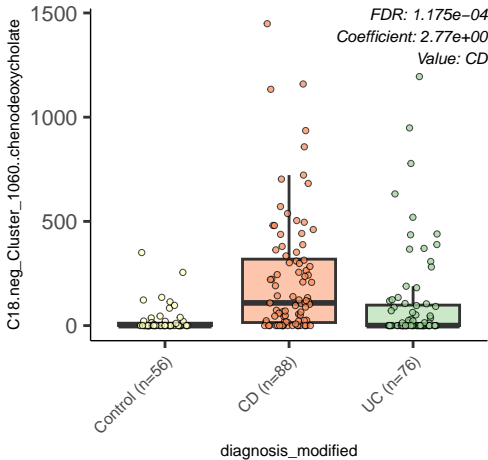
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified

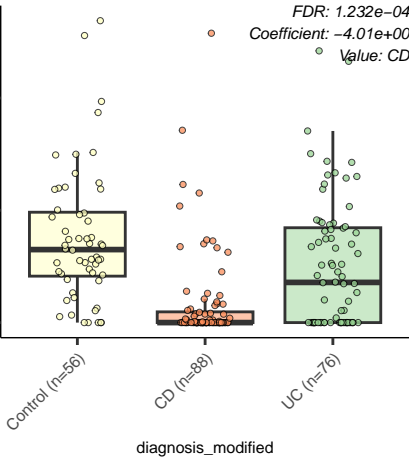


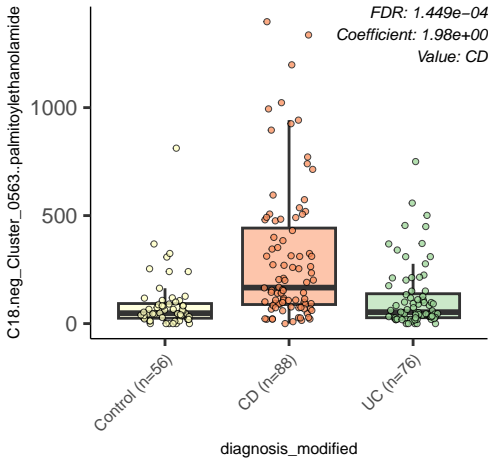


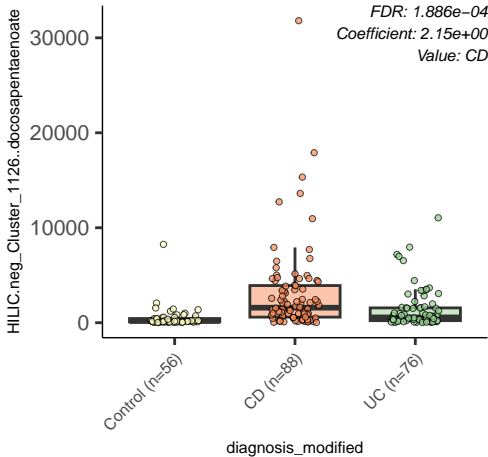


HILIC.pos\_Cluster\_1370..5alpha.cholestanol

FDR: 1.232e-04  
Coefficient: -4.01e+00  
Value: CD







C8.pos\_Cluster\_0123..sphingosine

FDR: 2.063e-04

Coefficient: 1.78e+00

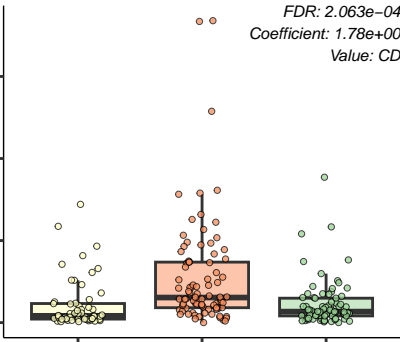
Value: CD

Control (n=56)

CD (n=88)

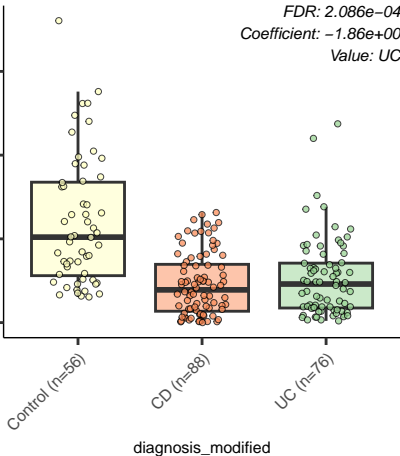
UC (n=76)

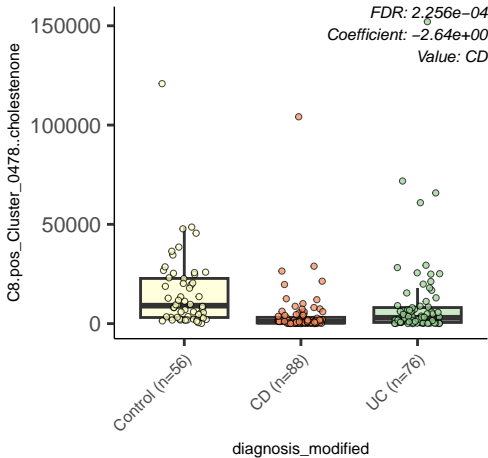
diagnosis\_modified

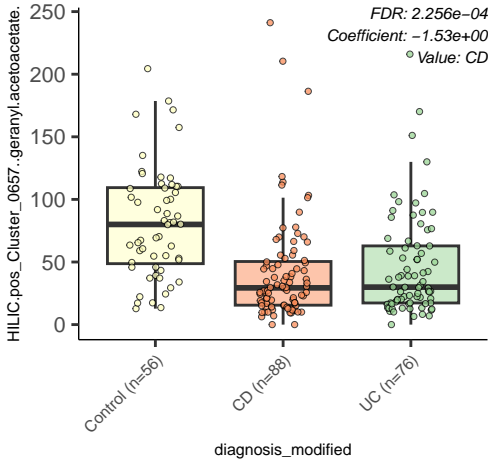


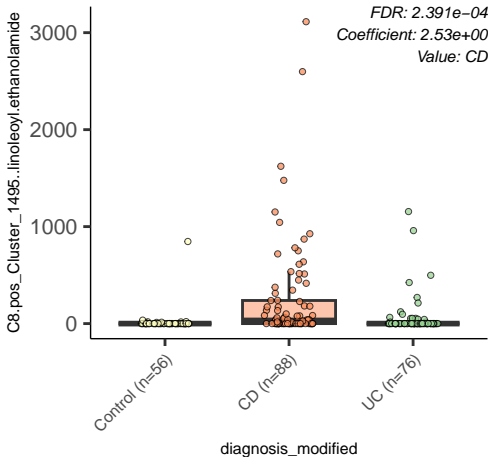
HILIC\_pos\_Cluster\_0268..pyridoxamine

FDR: 2.086e-04  
Coefficient: -1.86e+00  
Value: UC

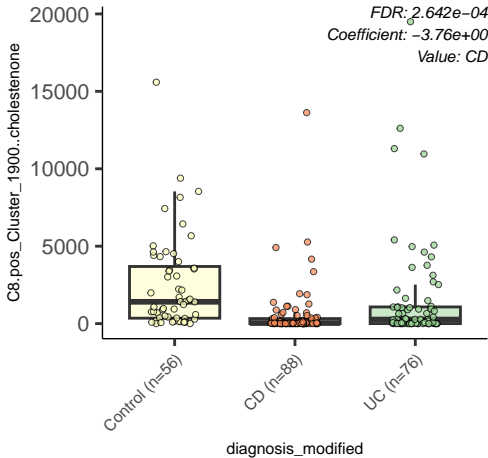






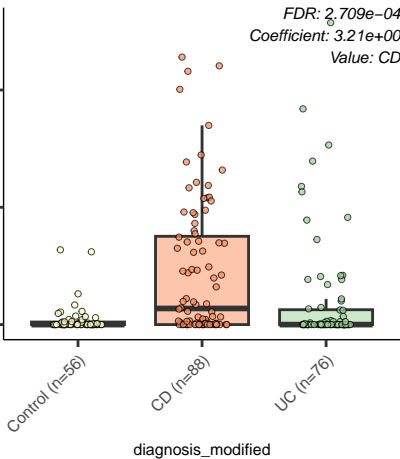


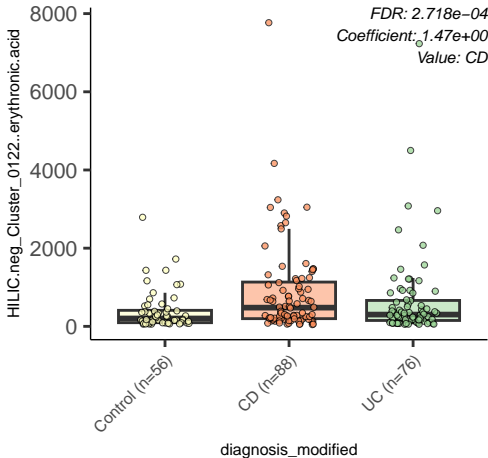




C18.neg\_Cluster\_1372..cholate

FDR:  $2.709 \times 10^{-4}$   
Coefficient:  $3.21 \times 10^0$   
Value: CD





C8\_pos\_Cluster\_0554..cholestenone

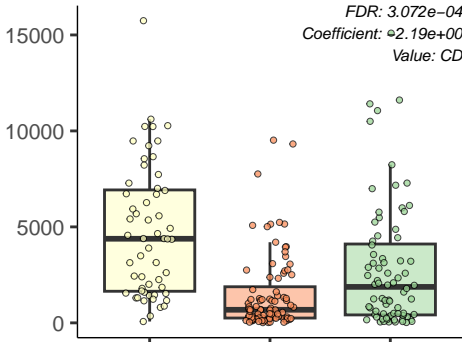
FDR:  $3.072 \times 10^{-4}$   
Coefficient:  $2.19 \times 10^0$   
Value: CD

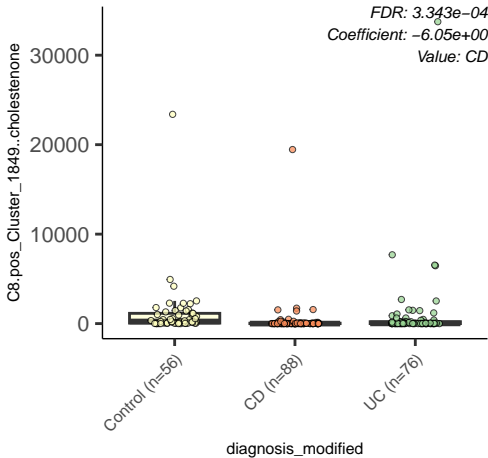
Control (n=56)

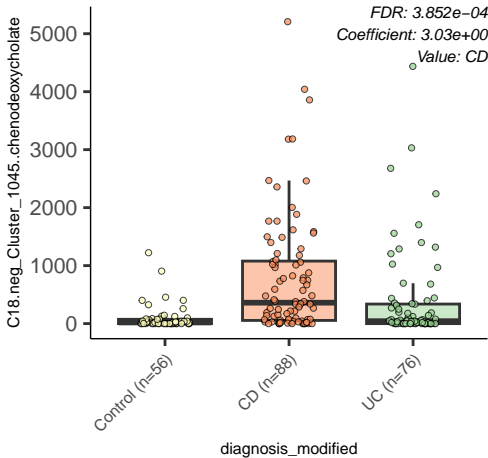
CD (n=88)

UC (n=76)

diagnosis\_modified

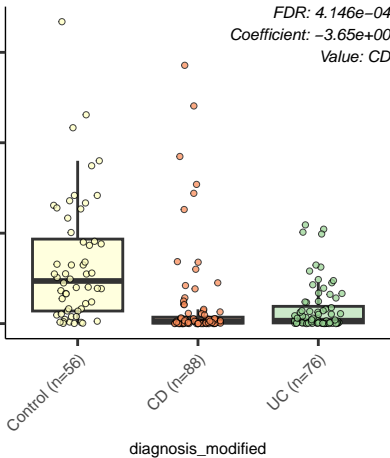






HILIC.neg\_Cluster\_0181..hydrocinnamic.acid

FDR:  $4.146e-04$   
Coefficient:  $-3.65e+00$   
Value: CD



C18.neg\_Cluster\_1722...cholate

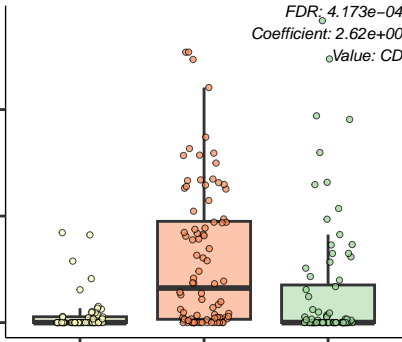
FDR:  $4.173e-04$   
Coefficient:  $2.62e+00$   
Value: CD

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.neg\_Cluster\_0082...nicotinate

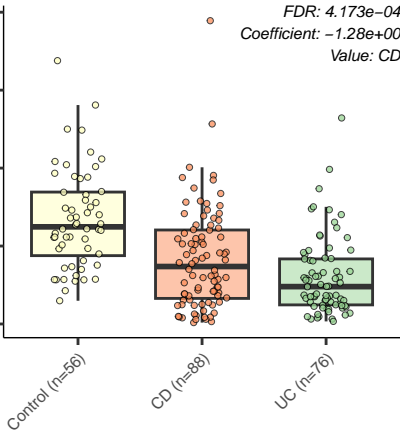
FDR:  $4.173e-04$   
Coefficient:  $-1.28e+00$   
Value: CD

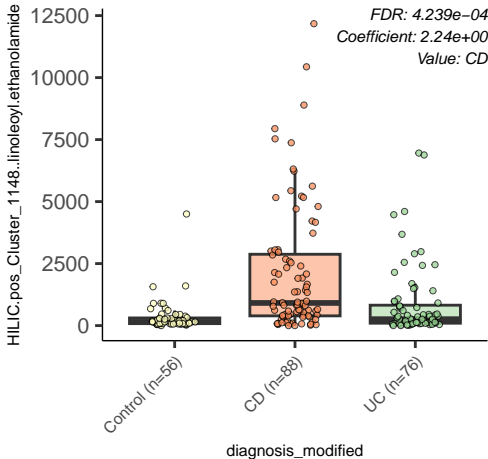
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.pos\_Cluster\_0524...N.acetyl.L.arginine

FDR: 4.716e-04  
Coefficient: -1.46e+00  
Value: UC

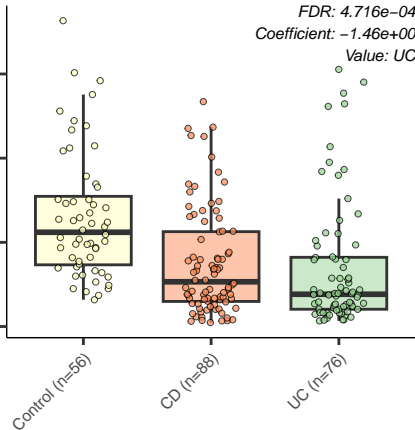
750  
500  
250  
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0082...nicotinate

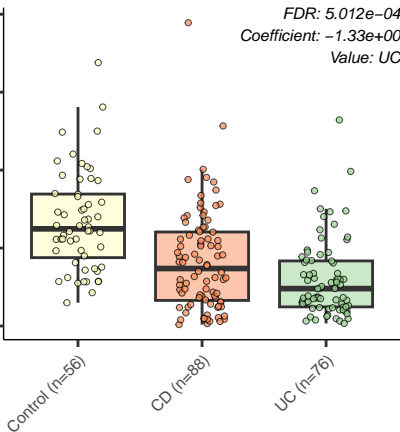
FDR: 5.012e-04  
Coefficient: -1.33e+00  
Value: UC

Control (n=56)

CD (n=88)

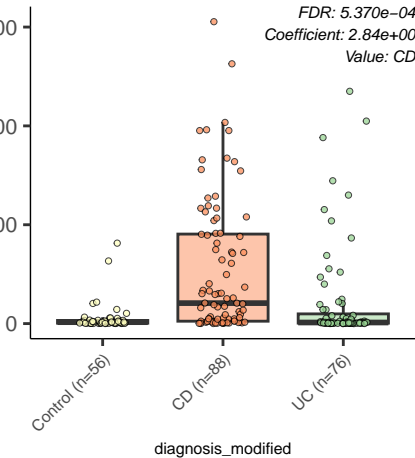
UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_1403..cholate

FDR: 5.370e-04  
Coefficient: 2.84e+00  
Value: CD



C18.neg\_Cluster\_1941..arachidonic.acid

*FDR: 5.404e-04*  
*Coefficient: 1.47e+00*  
*Value: UC*

400

200

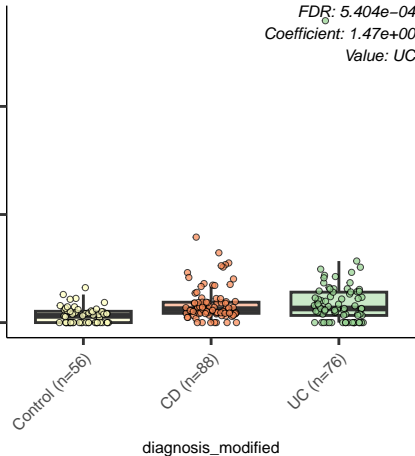
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



C18.neg\_Cluster\_1621..cholate

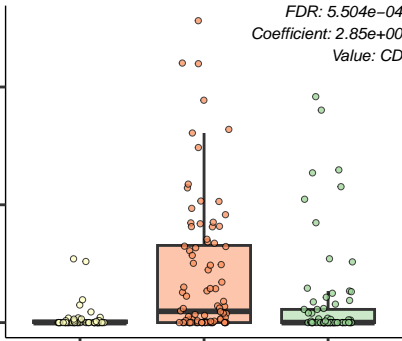
FDR: 5.504e-04  
Coefficient: 2.85e+00  
Value: CD

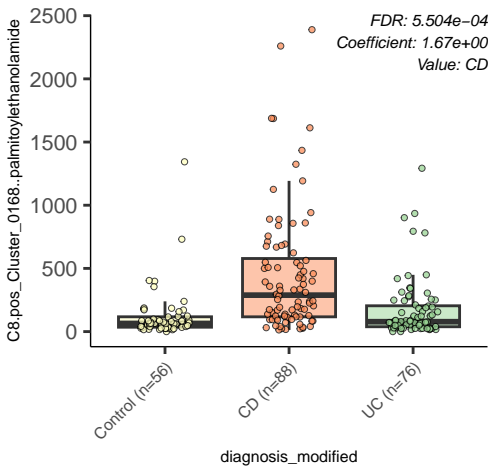
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified

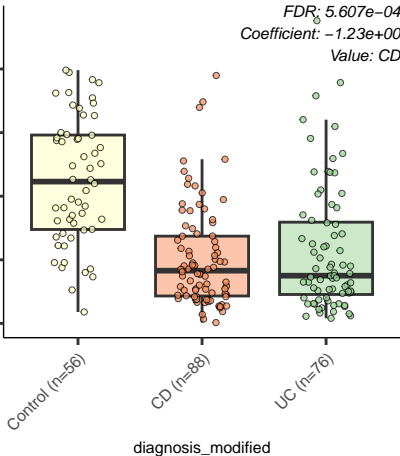




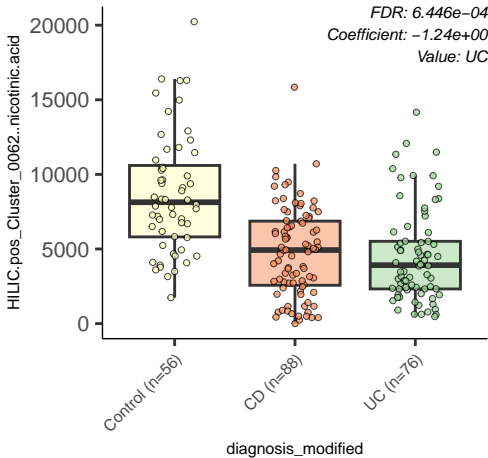


HILIC.neg\_Cluster\_0372..N.acetylglutamate

FDR:  $5.607e-04$   
Coefficient:  $-1.23e+00$   
Value: CD



diagnosis\_modified



C18.neg\_Cluster\_0486..carnosol

FDR:  $6.741e-04$   
Coefficient:  $-3.15e+00$   
Value: UC

7500

5000

2500

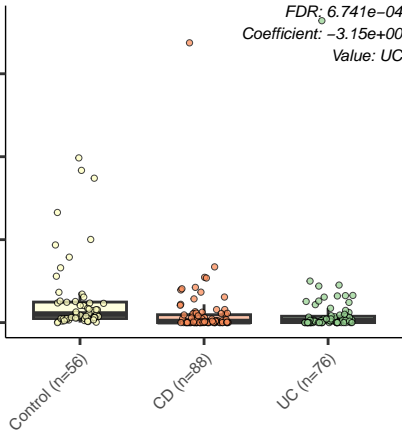
0

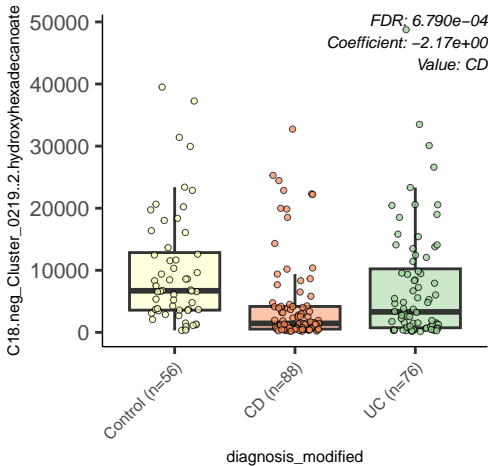
Control (n=56)

CD (n=88)

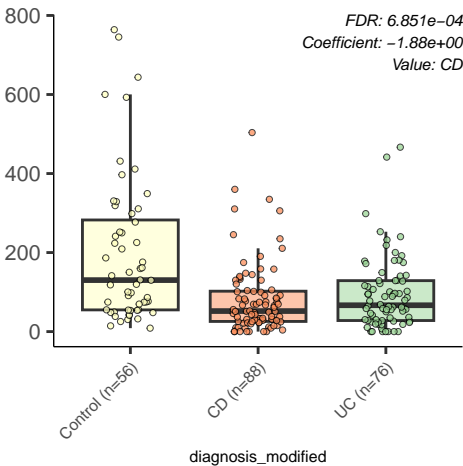
UC (n=76)

diagnosis\_modified



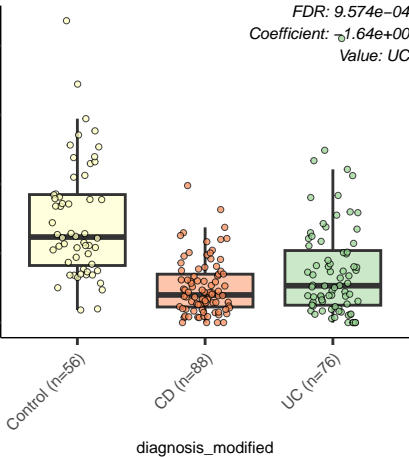


HILIC.neg.Cluster\_0622..1.2.3.4.tetrahydro.1.methyl.beta.carboline



HILIC\_pos\_Cluster\_0521..L.1.2.3.4.tetrahydro.beta.carboline.3.ca

FDR:  $9.574e-04$   
Coefficient:  $-1.64e+00$   
Value: UC



HILIC\_pos\_Cluster\_0081..pipecolic.acid

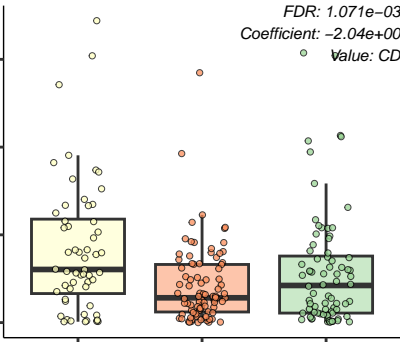
FDR:  $1.071\text{e-}03$   
Coefficient:  $-2.04\text{e}+00$   
Value: CD

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0677..cystine

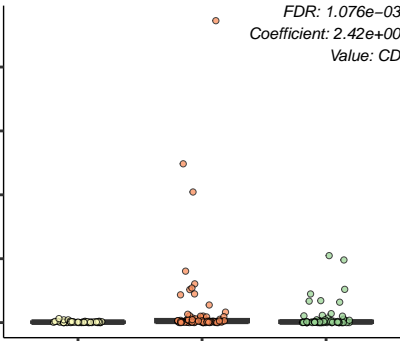
*FDR: 1.076e-03*  
*Coefficient: 2.42e+00*  
*Value: CD*

Control (n=56)

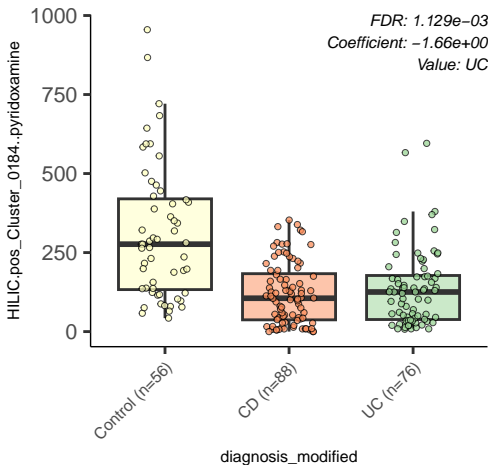
CD (n=88)

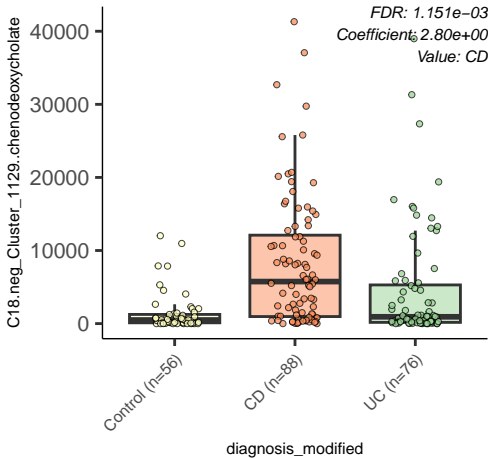
UC (n=76)

diagnosis\_modified









C18.neg\_Cluster\_1273..cholate

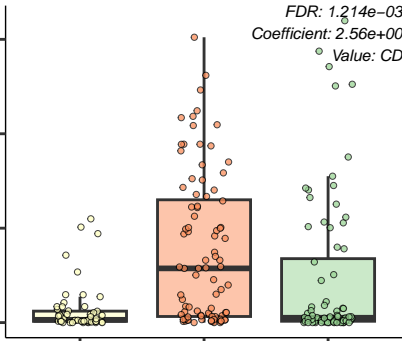
FDR: 1.214e-03  
Coefficient: 2.56e+00  
Value: CD

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC\_pos\_Cluster\_2093..urobilin.

FDR:  $1.310e-03$   
Coefficient:  $-4.61e+00$   
Value: UC

30000

20000

10000

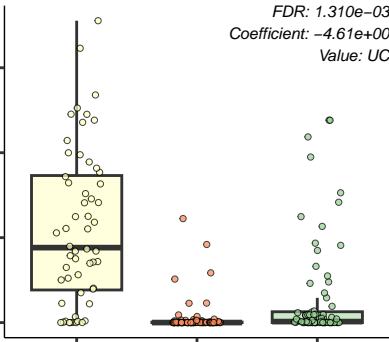
0

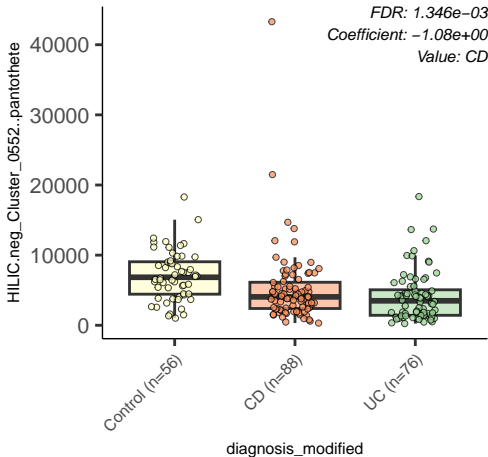
Control (n=56)

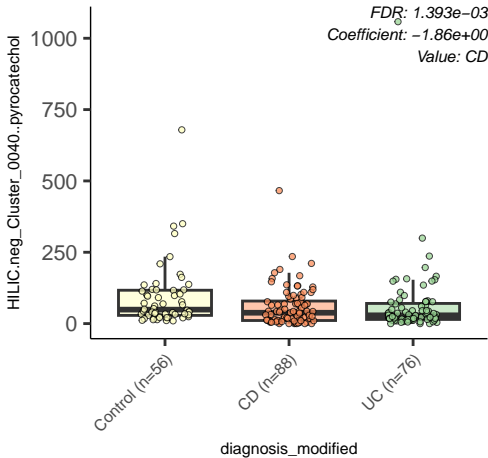
CD (n=88)

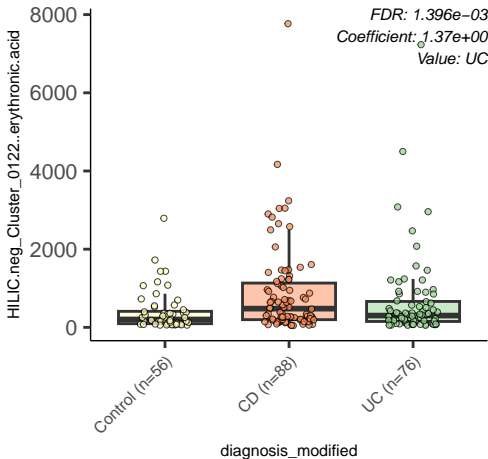
UC (n=76)

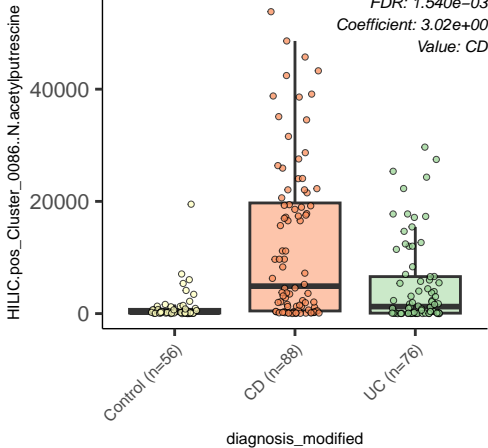
diagnosis\_modified













C18.neg\_Cluster\_1258..cholate

1e+05

5e+04

0e+00

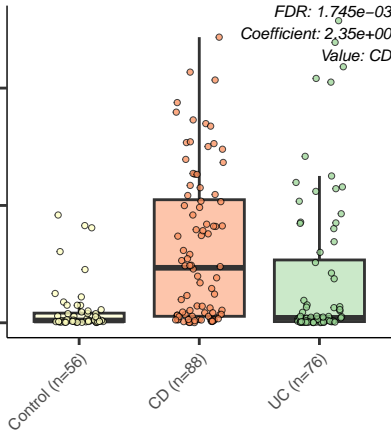
Control (n=56)

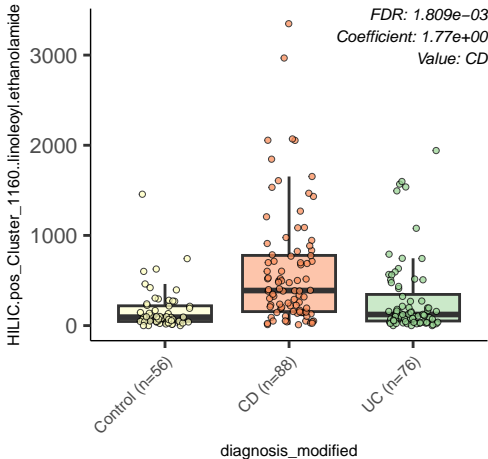
CD (n=88)

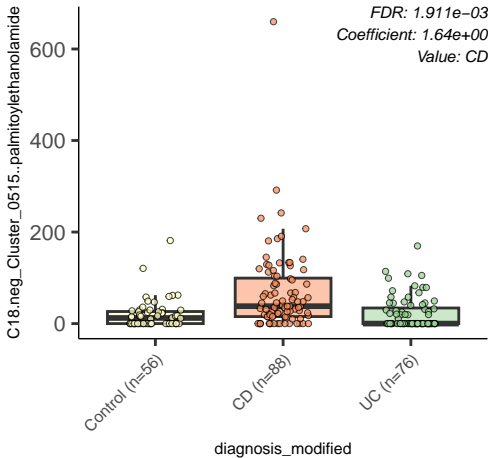
UC (n=76)

diagnosis\_modified

FDR: 1.745e-03  
Coefficient: 2.35e+00  
Value: CD

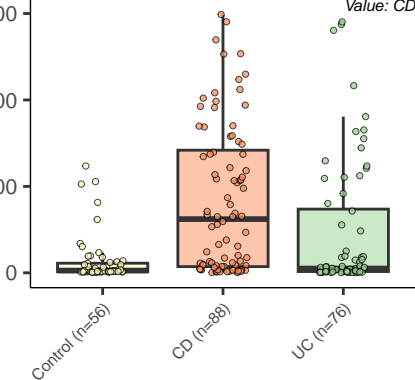




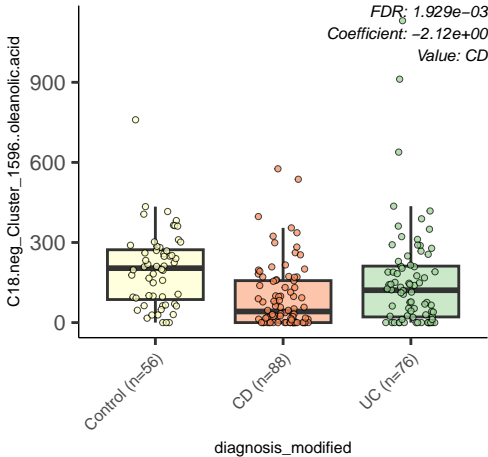


C18.neg\_Cluster\_0930..cholate

FDR: 1.911e-03  
Coefficient: 2.29e+00  
Value: CD



diagnosis\_modified



C18.neg\_Cluster\_1178..cholate

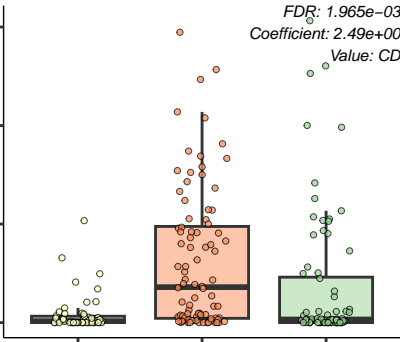
*FDR: 1.965e-03*  
*Coefficient: 2.49e+00*  
*Value: CD*

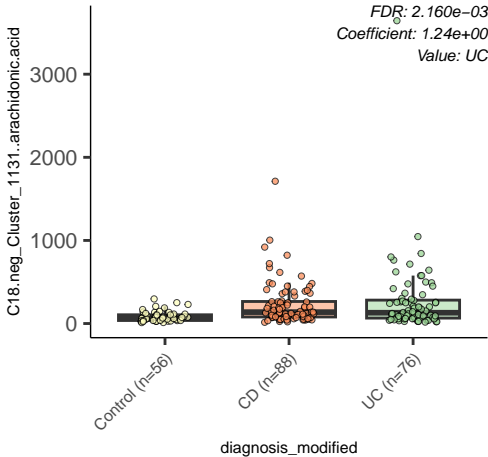
Control (n=56)

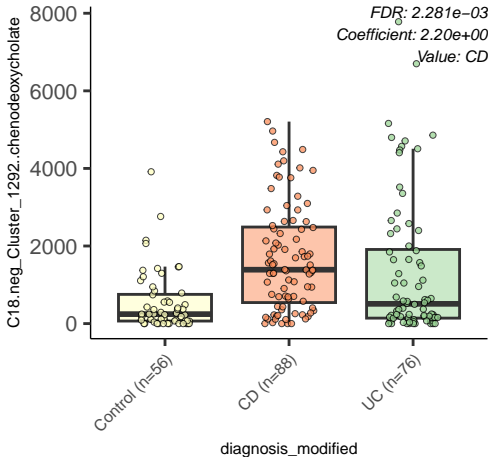
CD (n=88)

UC (n=76)

diagnosis\_modified









C18.neg\_Cluster\_1941..arachidonic.acid

*FDR: 2.466e-03*  
*Coefficient: 1.24e+00*  
*Value: CD*

400

200

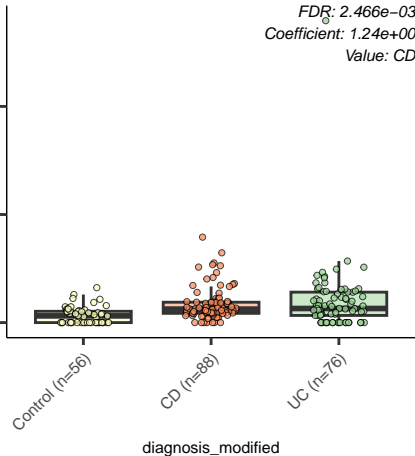
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0182..guanine

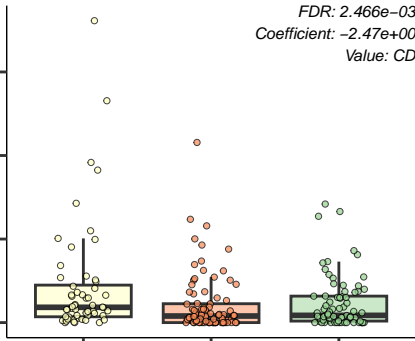
FDR:  $2.466e-03$   
Coefficient:  $-2.47e+00$   
Value: CD

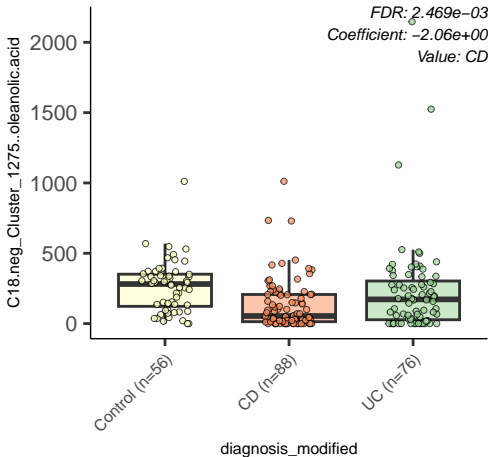
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC\_neg\_Cluster\_0697..pentadecanoate

FDR:  $2.724e-03$   
Coefficient:  $-1.70e+00$   
Value: CD

60000

40000

20000

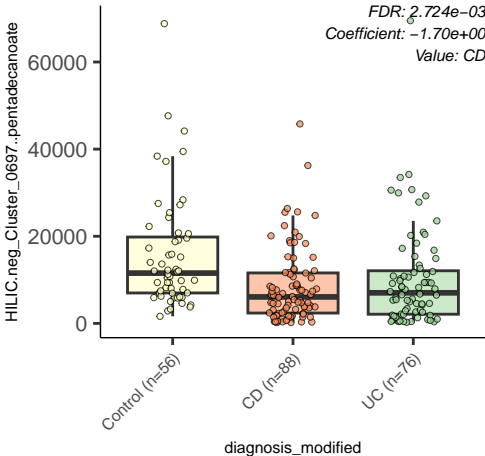
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



C18.neg\_Cluster\_0177...tetradecanedioate

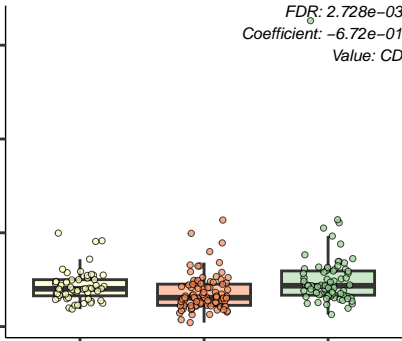
FDR:  $2.728e-03$   
Coefficient:  $-6.72e-01$   
Value: CD

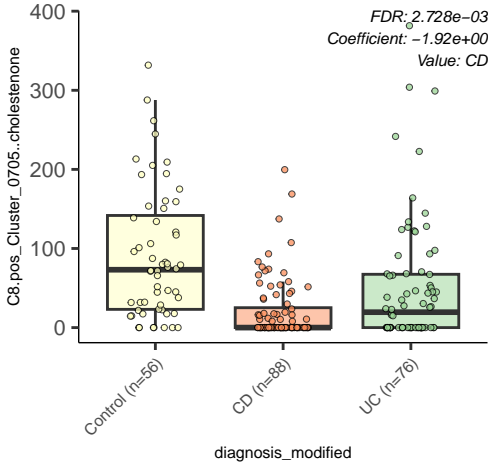
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.neg\_Cluster\_0120..adenine

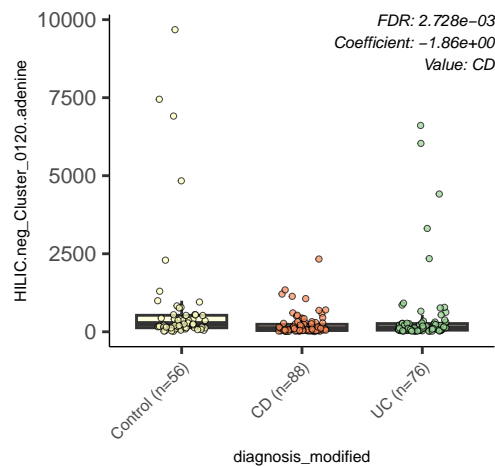
*FDR: 2.728e-03*  
*Coefficient: -1.86e+00*  
*Value: CD*

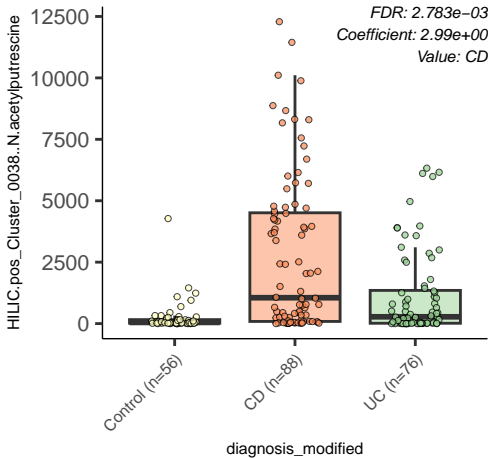
Control (n=56)

CD (n=88)

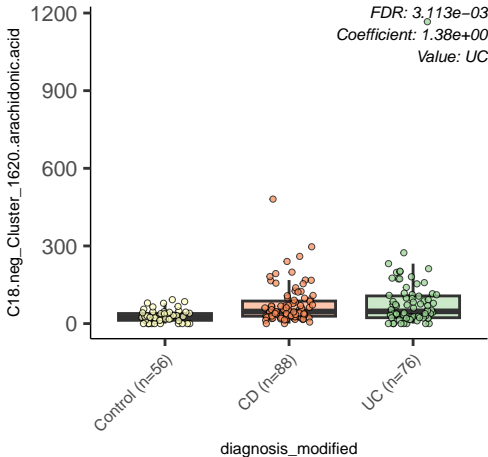
UC (n=76)

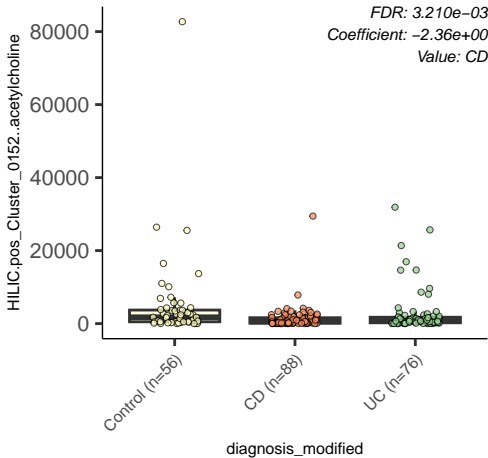
diagnosis\_modified

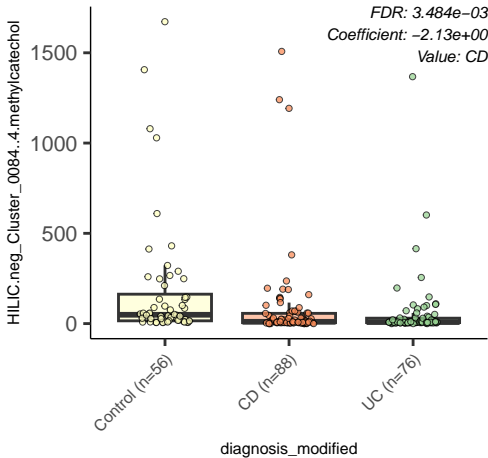












C18.neg\_Cluster\_0506..adrenic.acid

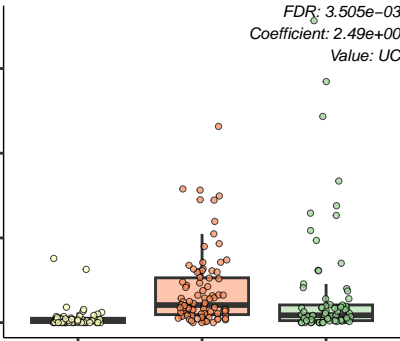
FDR: 3.505e-03  
Coefficient: 2.49e+00  
Value: UC

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



C18.neg\_Cluster\_0731..lithocholic.acid

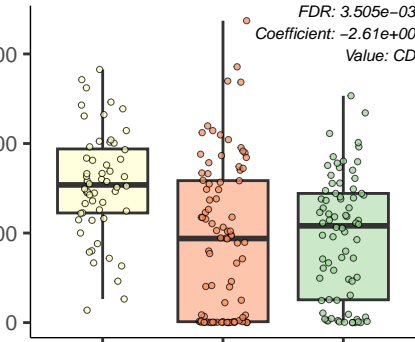
FDR:  $3.505e-03$   
Coefficient:  $-2.61e+00$   
Value: CD

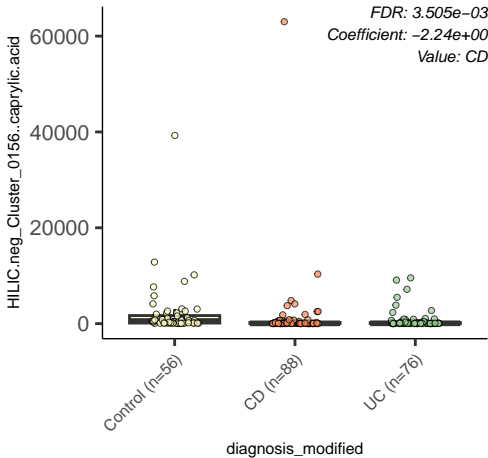
Control (n=56)

CD (n=88)

UC (n=76)

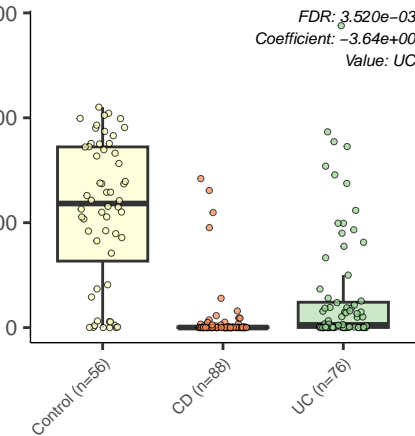
diagnosis\_modified



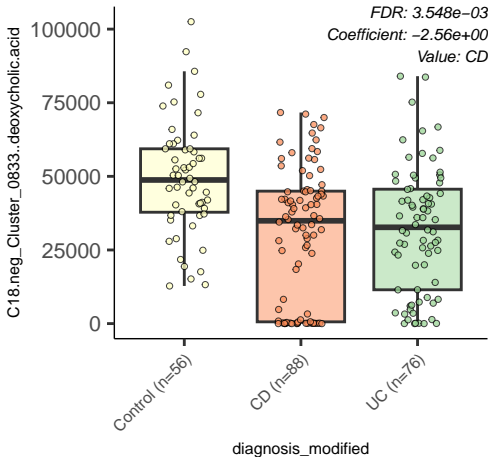


C18.neg\_Cluster\_2021...urobilin

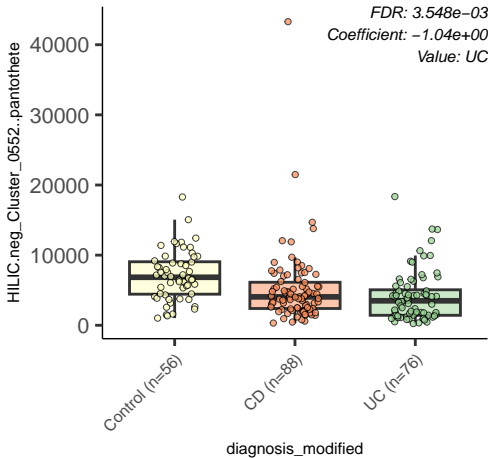
*FDR: 3.520e-03*  
*Coefficient: -3.64e+00*  
*Value: UC*

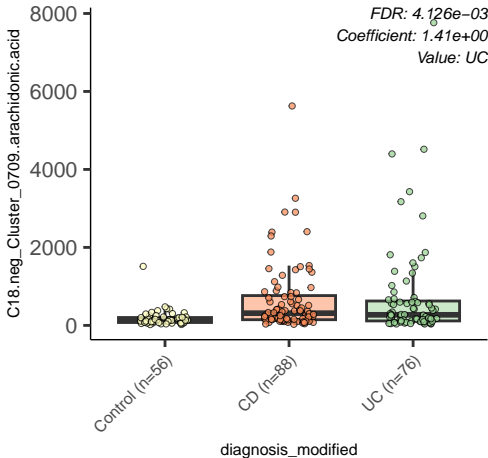


diagnosis\_modified



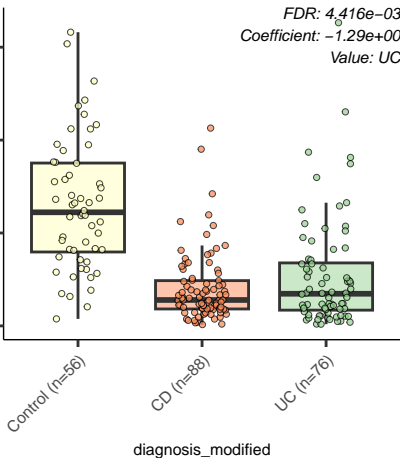


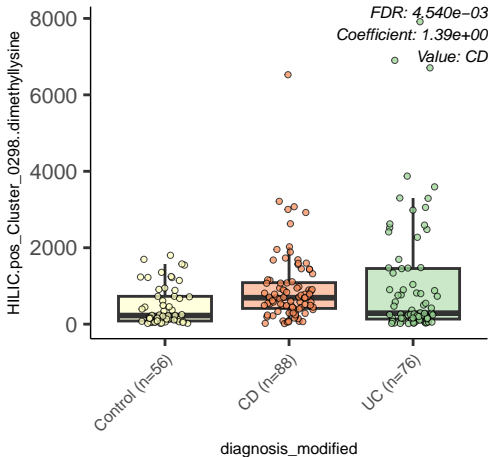


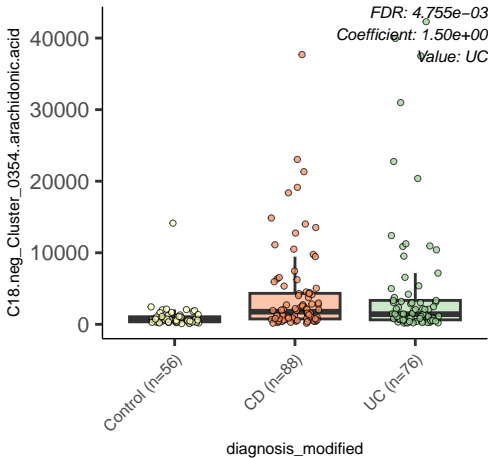


HILIC.pos\_Cluster\_0384..N.acetylglutamic.acid

FDR: 4.416e-03  
Coefficient: -1.29e+00  
Value: UC







HILIC\_pos\_Cluster\_0081..pipecolic.acid

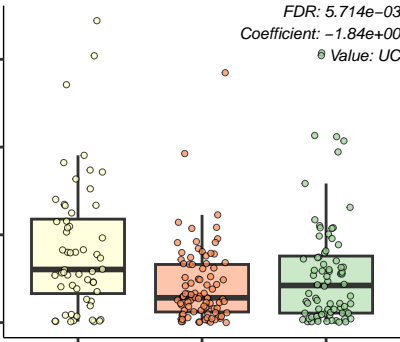
FDR:  $5.714e-03$   
Coefficient:  $-1.84e+00$   
Value: UC

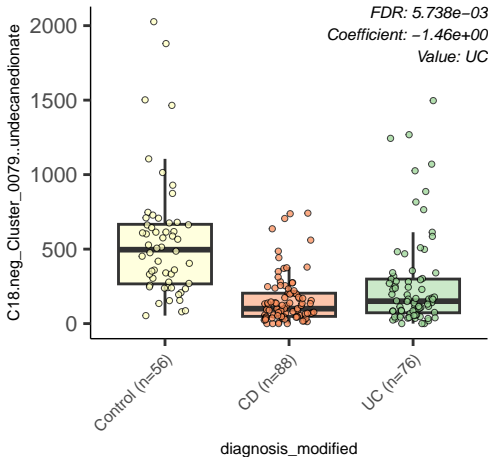
Control (n=56)

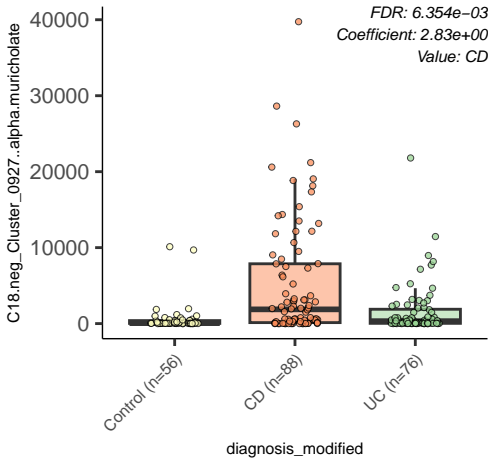
CD (n=88)

UC (n=76)

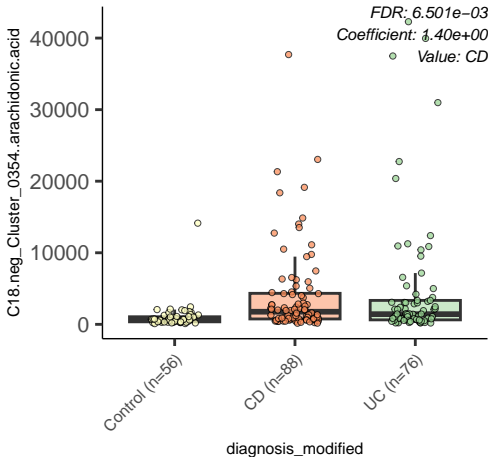
diagnosis\_modified











C18.neg\_Cluster\_1680...maslinic.acid

FDR:  $7.846e-03$   
Coefficient:  $-2.10e+00$   
Value: CD

4000

2000

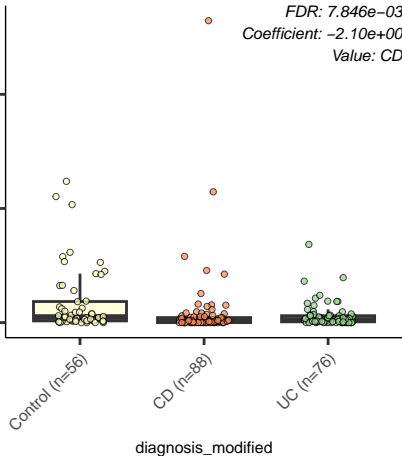
0

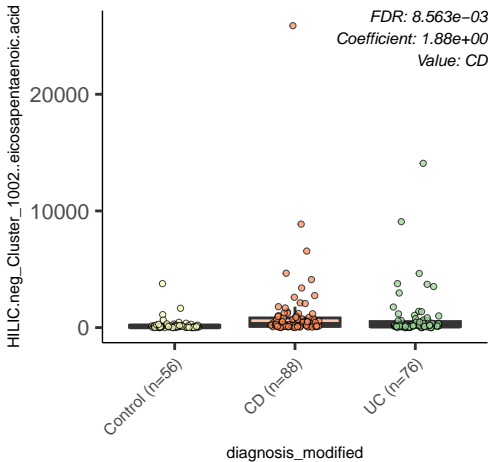
Control (n=56)

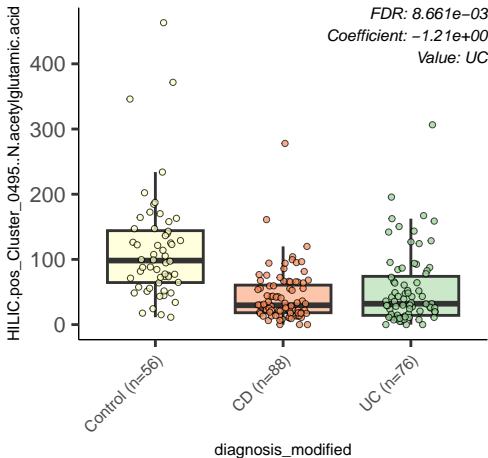
CD (n=88)

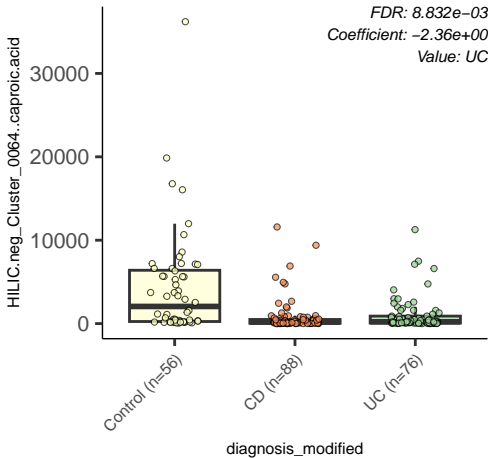
UC (n=76)

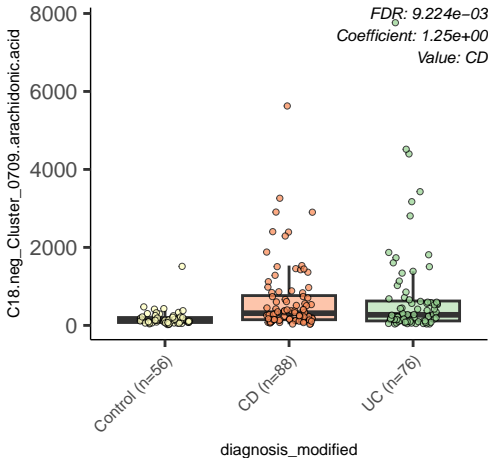
diagnosis\_modified

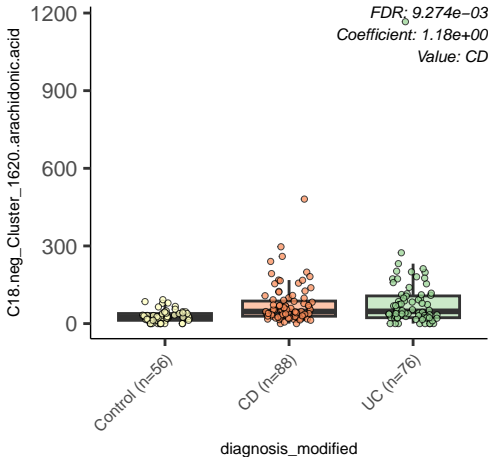


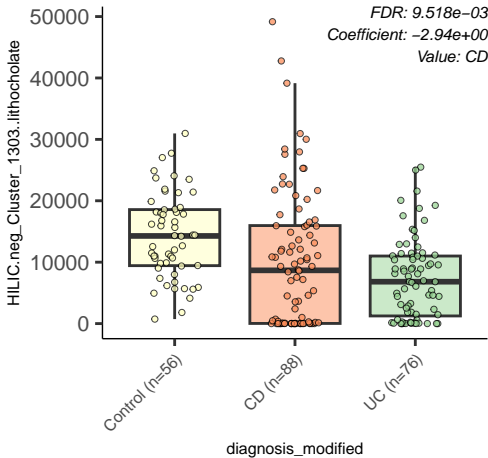














HILIC.pos\_Cluster\_1486..C16.carnitine

*FDR: 9.666e-03*  
*Coefficient: 2.28e+00*  
*Value: UC*

4000

2000

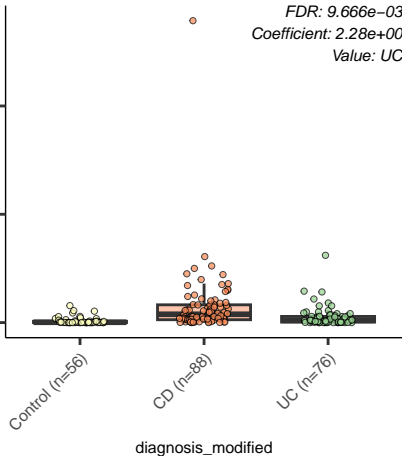
0

Control (n=56)

CD (n=88)

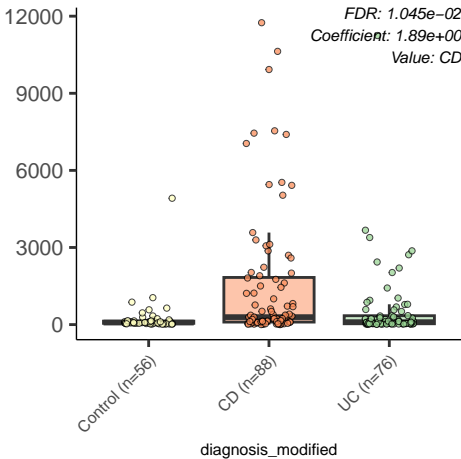
UC (n=76)

diagnosis\_modified

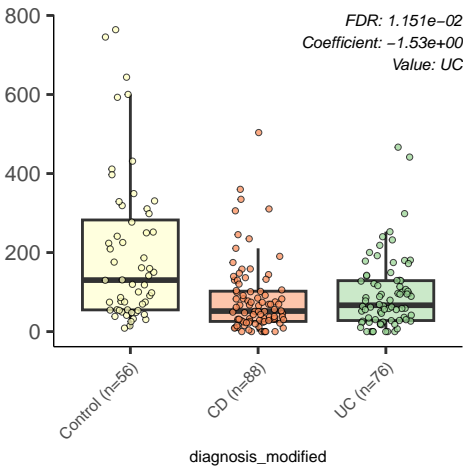


HILIC.pos\_Cluster\_0114..2.hydroxyphenethylamine

FDR:  $1.045e-02$   
Coefficient:  $1.89e+00$   
Value: CD



HILIC.neg\_Cluster\_0622..1.2.3.4.tetrahydro.1.methyl.beta.carboline



HILIC.pos\_Cluster\_0447..ADMA

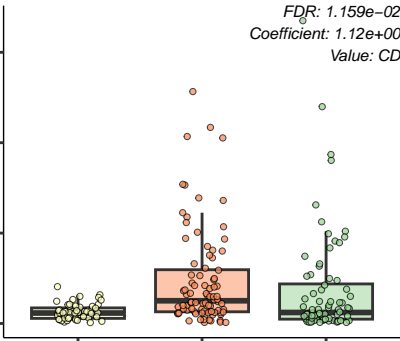
FDR: 1.159e-02  
Coefficient: 1.12e+00  
Value: CD

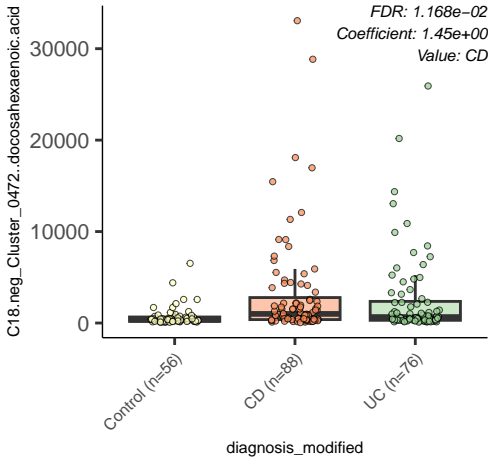
Control (n=56)

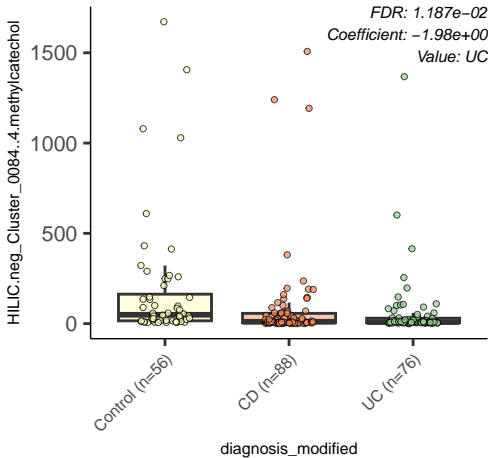
CD (n=88)

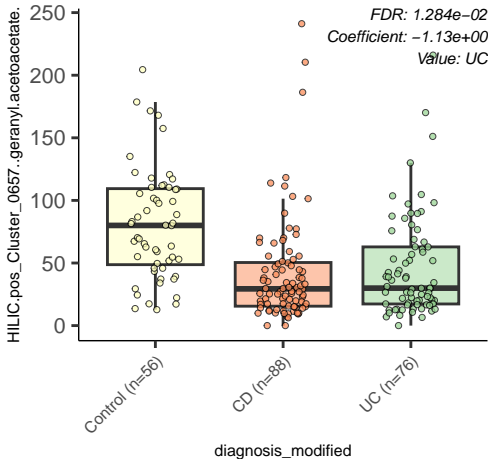
UC (n=76)

diagnosis\_modified



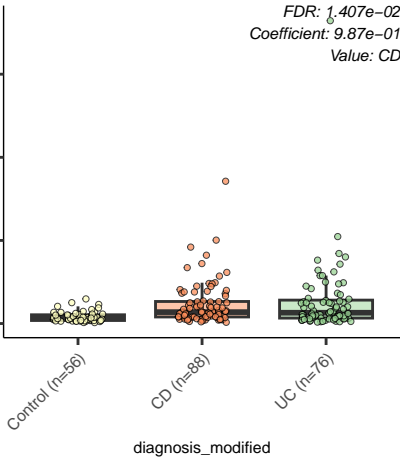




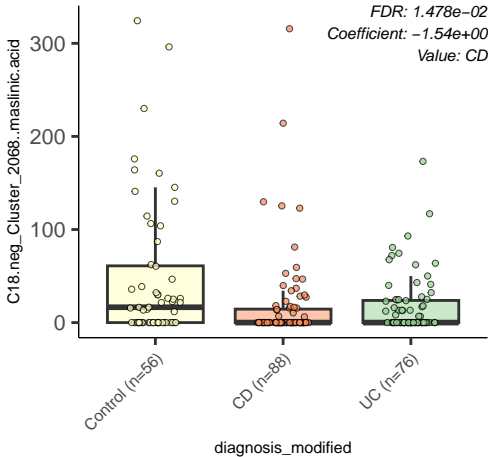


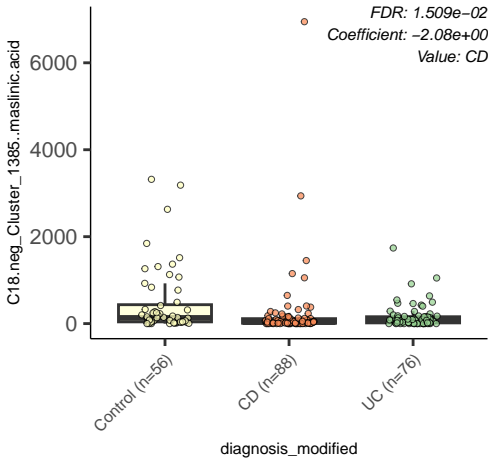
C18.neg\_Cluster\_1131..arachidonic.acid

FDR:  $1.407e-02$   
Coefficient:  $9.87e-01$   
Value: CD









HILIC.neg\_Cluster\_0335..4.pyridoxate

FDR:  $1.588e-02$   
Coefficient:  $-1.26e+00$   
Value: CD

20000

10000

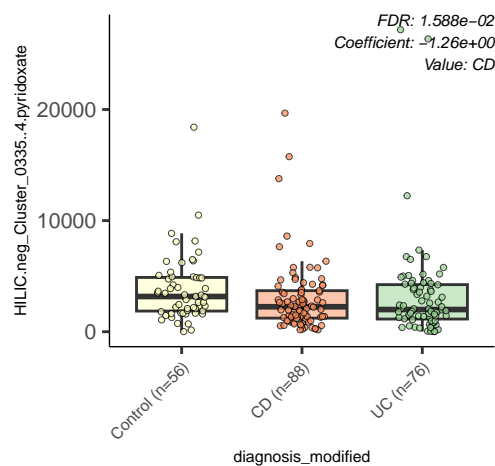
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0441...sebacate

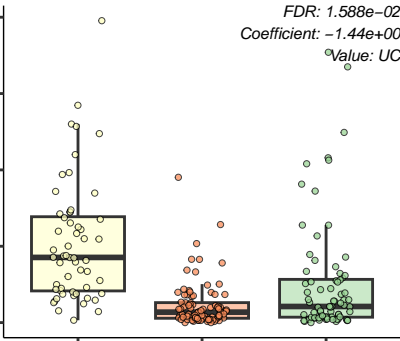
FDR: 1.588e-02  
Coefficient: -1.44e+00  
Value: UC

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



C18.neg\_Cluster\_0901..7.ketodeoxycholate

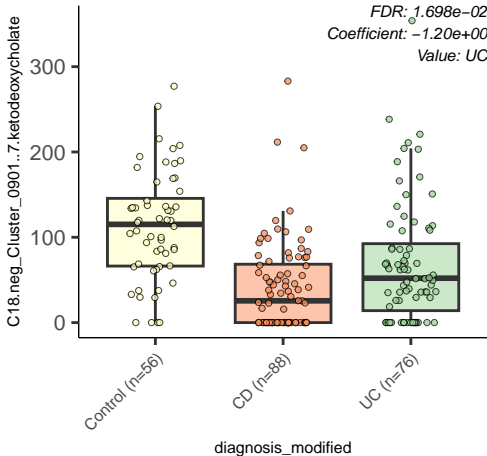
FDR:  $1.698e-02$   
Coefficient:  $-1.20e+00$   
Value: UC

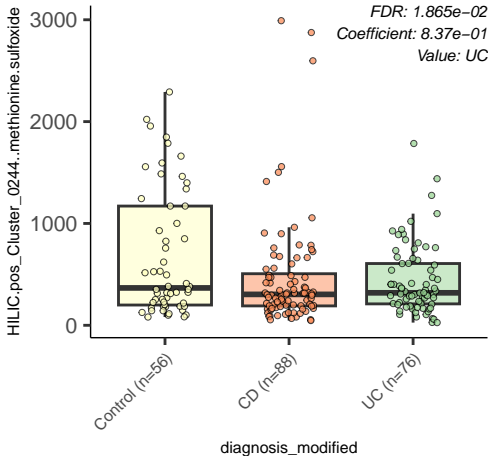
Control (n=56)

CD (n=88)

UC (n=76)

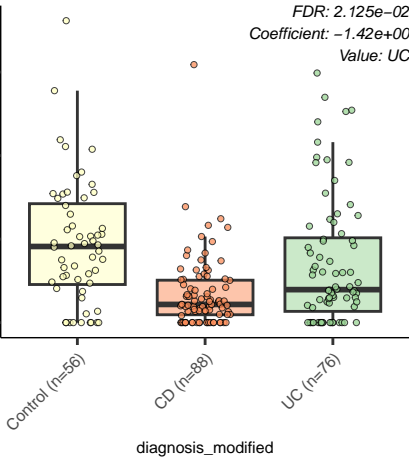
diagnosis\_modified

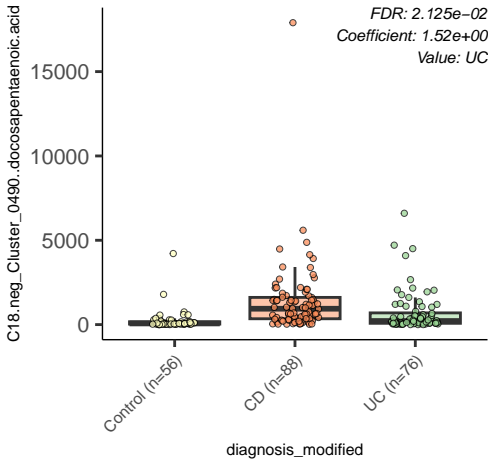




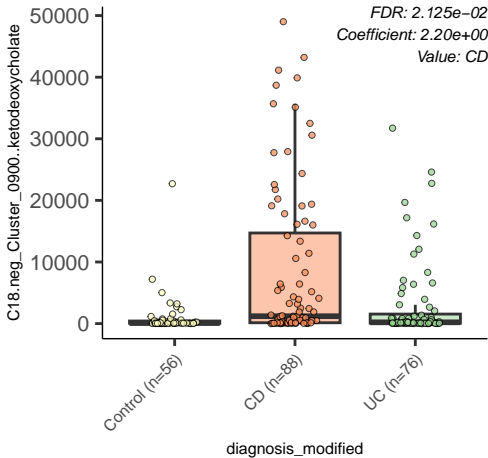
C18.neg.Cluster\_0183...1.2.3.4.tetrahydro.b.carboline.1.3.dicar

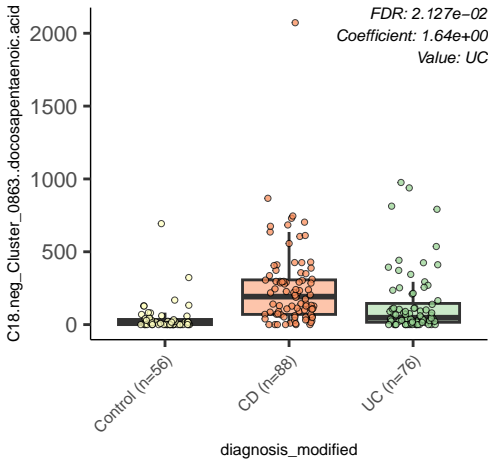
FDR:  $2.125e-02$   
Coefficient:  $-1.42e+00$   
Value: UC

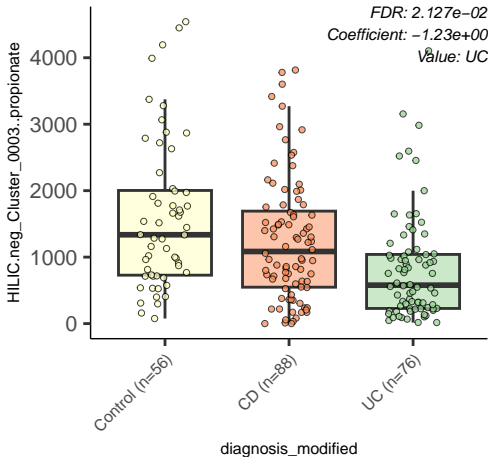


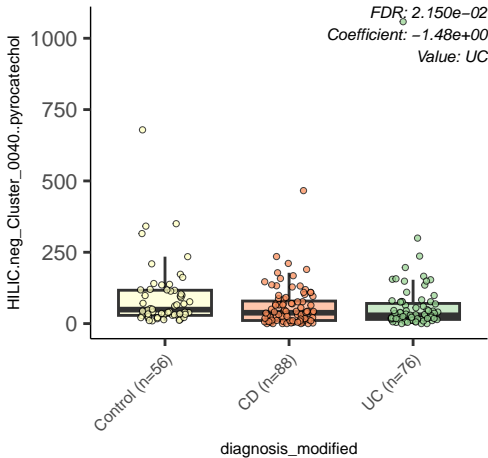












HILIC.neg\_Cluster\_0085..taurine

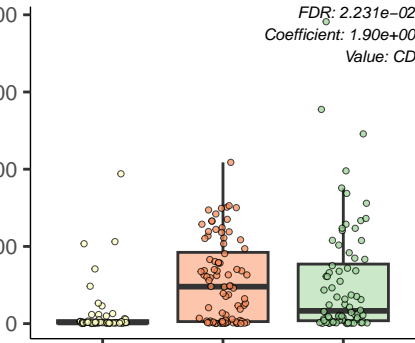
FDR: 2.231e-02  
Coefficient: 1.90e+00  
Value: CD

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC\_pos\_Cluster\_0295..arginine

FDR:  $2.652e-02$   
Coefficient:  $-1.37e+00$   
Value: CD

20000

10000

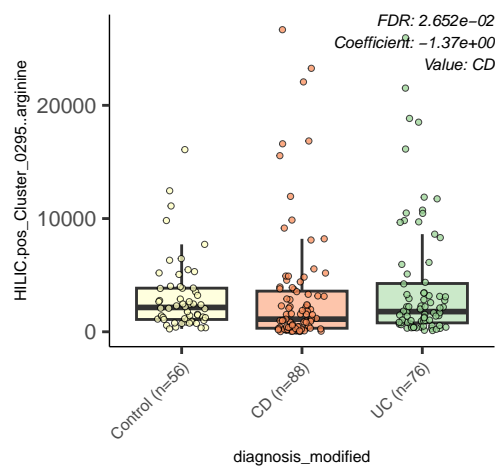
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.pos\_Cluster\_0033..histamine

*FDR: 2.714e-02*  
*Coefficient: 1.88e+00*  
*Value: CD*

30000

20000

10000

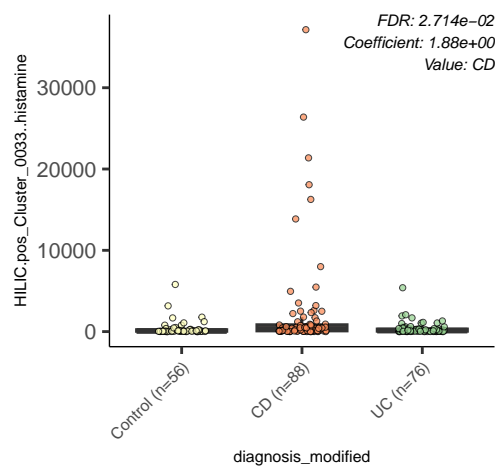
0

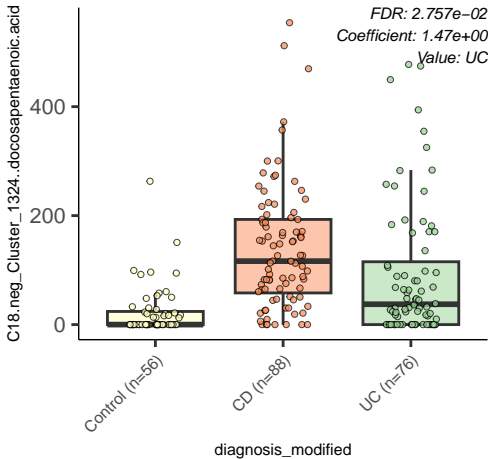
Control (n=56)

CD (n=88)

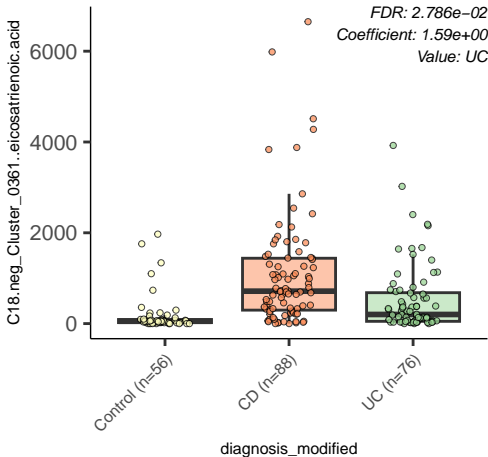
UC (n=76)

diagnosis\_modified









HILIC\_neg\_Cluster\_0697..pentadecanoate

FDR:  $2.813e-02$   
Coefficient:  $-1.38e+00$   
Value: UC

60000

40000

20000

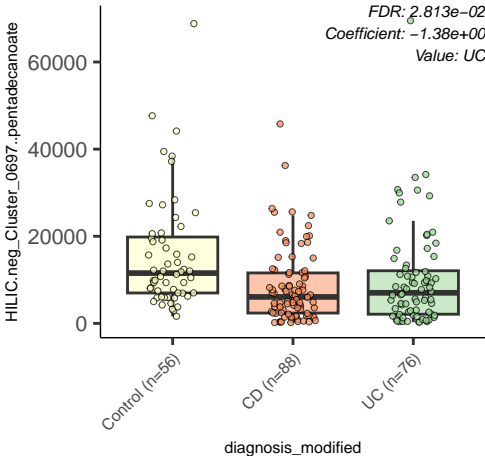
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0335..4.pyridoxate

FDR:  $2.837e-02$   
Coefficient:  $-1.22e+00$   
Value: UC

20000

10000

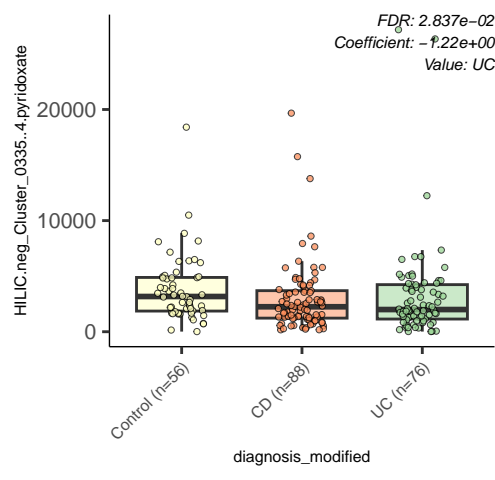
0

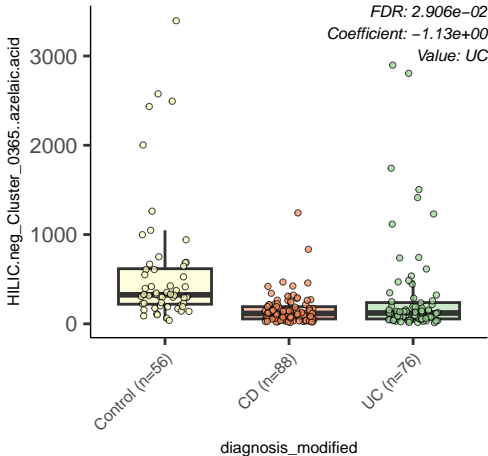
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





C8.pos\_Cluster\_0988...sphingosine

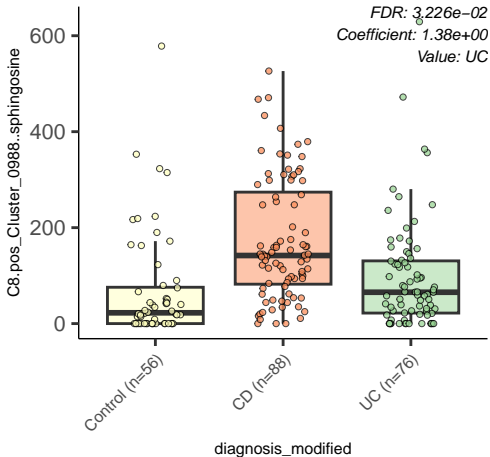
FDR:  $3.226e-02$   
Coefficient:  $1.38e+00$   
Value: UC

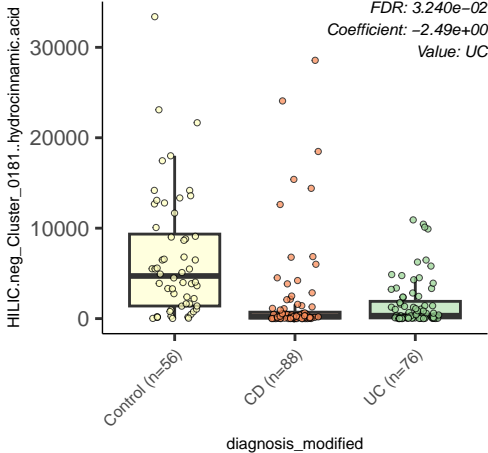
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC\_pos\_Cluster\_0177\_4.hydroxy.3.methylacetophen

FDR:  $3.370e-02$   
Coefficient:  $-1.22e+00$   
Value: UC

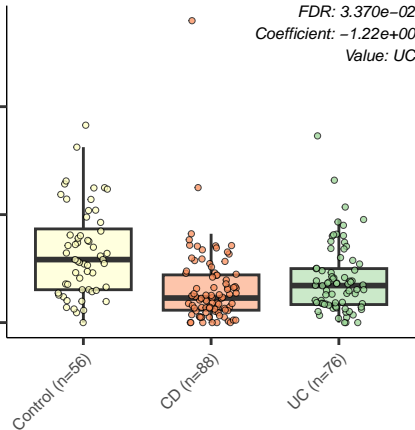
400  
200  
0

Control (n=56)

CD (n=88)

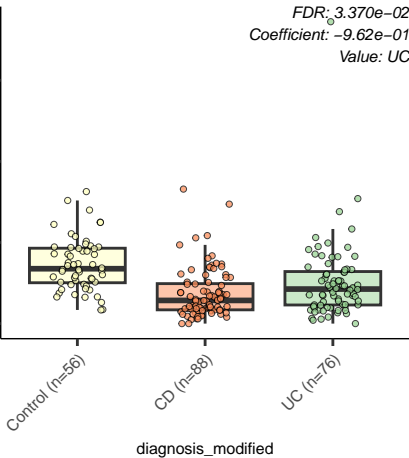
UC (n=76)

diagnosis\_modified

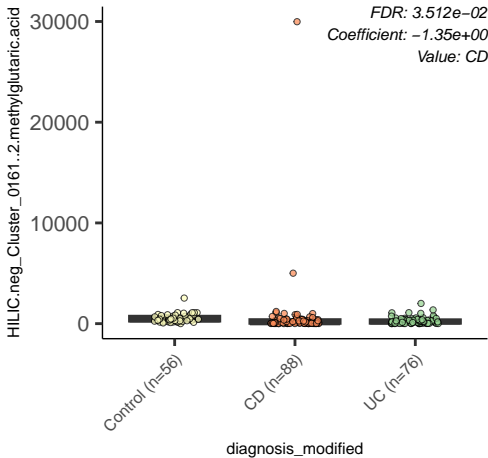


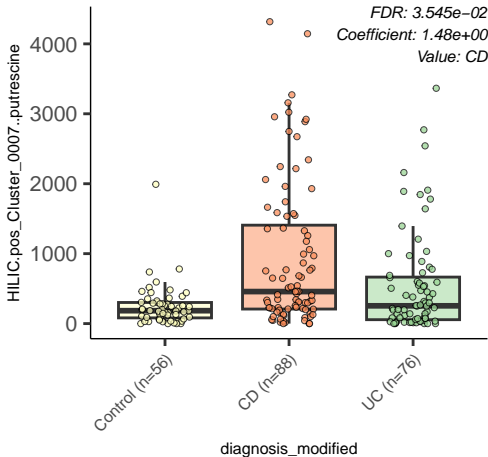
HILIC.pos\_Cluster\_0658..geranyl.acetoacetate.

FDR:  $3.370e-02$   
Coefficient:  $-9.62e-01$   
Value: UC



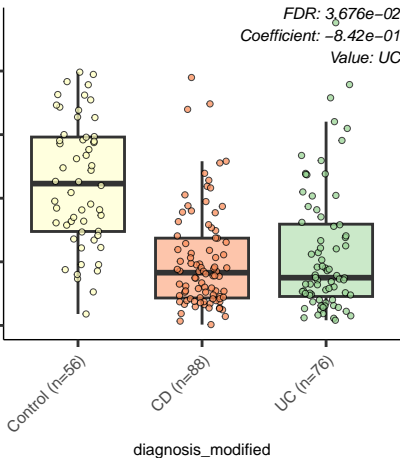




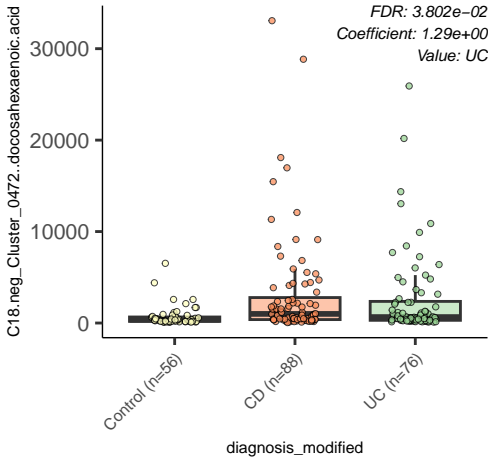


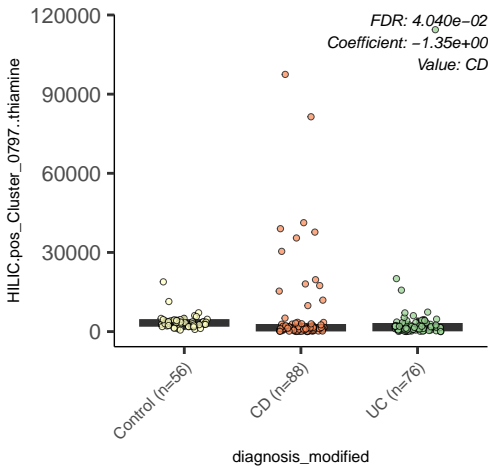
HILIC.neg\_Cluster\_0372..N.acetylglutamate

FDR:  $3.676e-02$   
Coefficient:  $-8.42e-01$   
Value: UC



diagnosis\_modified





HILIC.neg\_Cluster\_0288..suberate

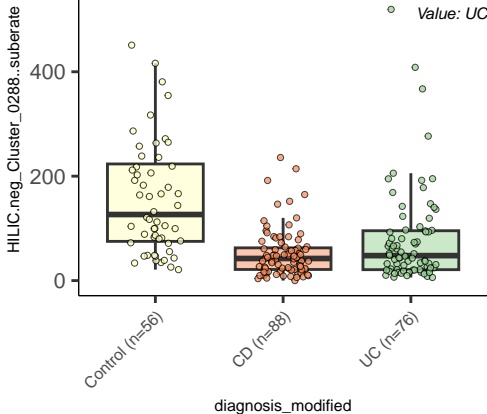
FDR: 4.142e-02  
Coefficient: -9.49e-01  
Value: UC

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC\_pos\_Cluster\_0160..glutamate

FDR:  $4.162e-02$   
Coefficient:  $-7.31e-01$   
Value: CD

10000

5000

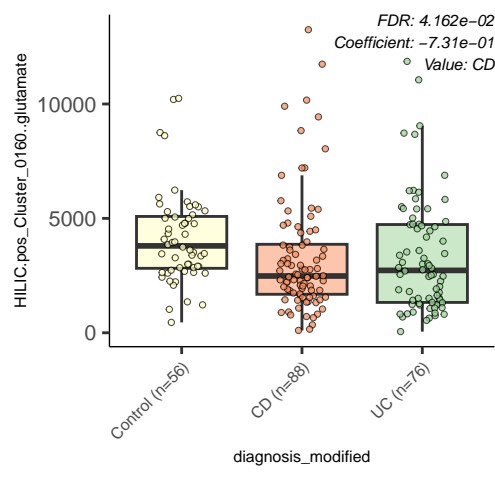
0

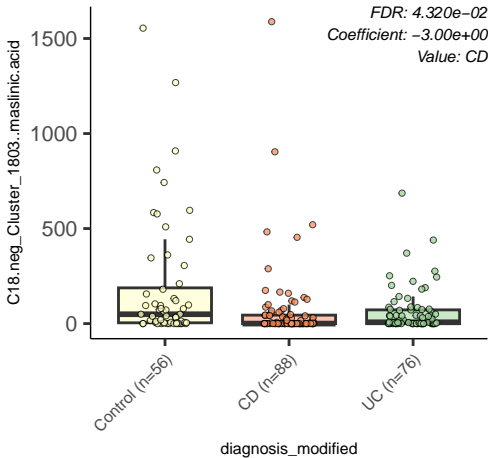
Control (n=56)

CD (n=88)

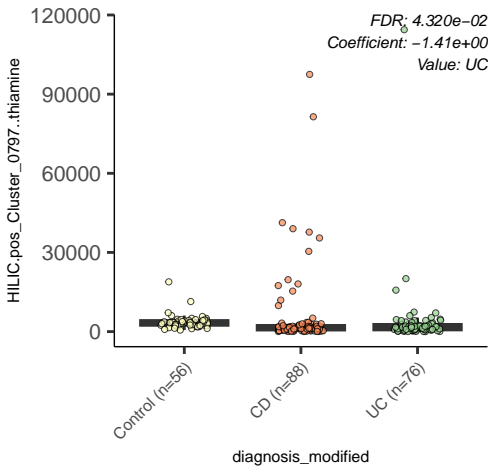
UC (n=76)

diagnosis\_modified



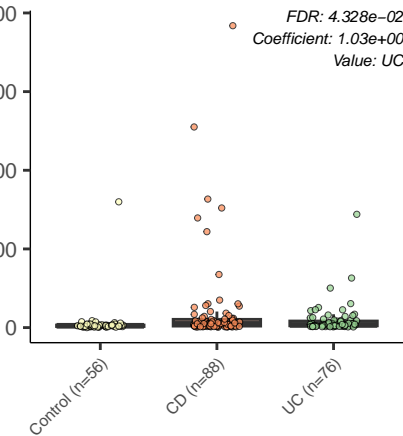






HILIC.pos\_Cluster\_0230..carnitine

*FDR: 4.328e-02*  
*Coefficient: 1.03e+00*  
*Value: UC*



diagnosis\_modified

C8\_pos\_Cluster\_0629..cholestenone

FDR:  $4.436e-02$   
Coefficient:  $-1.39e+00$   
Value: UC

200

100

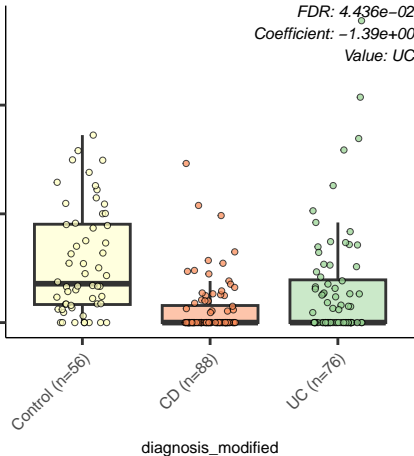
0

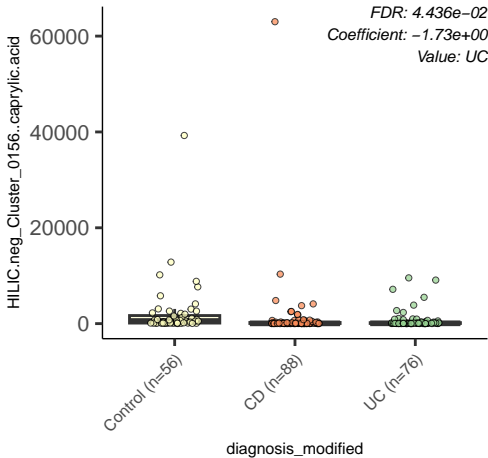
Control (n=56)

CD (n=88)

UC (n=76)

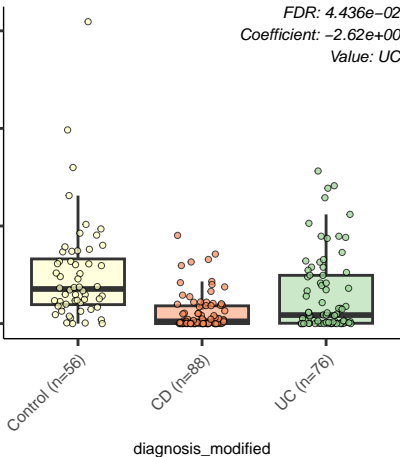
diagnosis\_modified





HILIC.neg\_Cluster\_0220..3.methyladipate.pimelate

FDR:  $4.436e-02$   
Coefficient:  $-2.62e+00$   
Value: UC



HILIC.neg\_Cluster\_0036..glycerate

6000

4000

2000

0

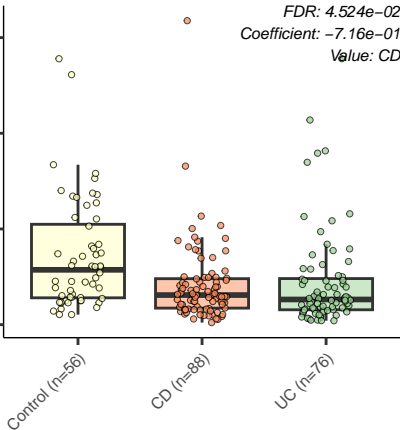
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified

FDR:  $4.524e-02$   
Coefficient:  $-7.16e-01$   
Value: CD



HILIC\_pos\_Cluster\_0022...choline

FDR:  $4.604e-02$   
Coefficient:  $7.93e-01$   
Value: UC

75000

50000

25000

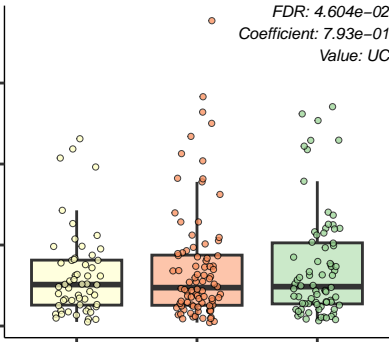
0

Control (n=56)

CD (n=88)

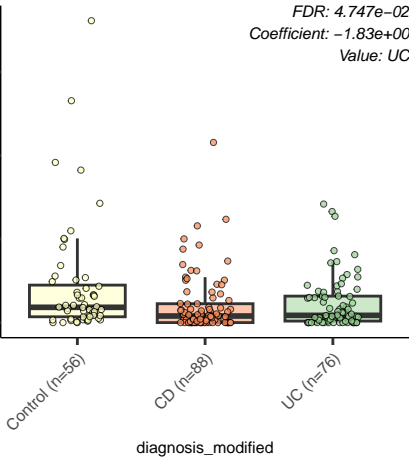
UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0182..guanine

FDR:  $4.747e-02$   
Coefficient:  $-1.83e+00$   
Value: UC



diagnosis\_modified



C18.neg\_Cluster\_0064..sebacate

*FDR: 5.550e-02*  
*Coefficient: -1.19e+00*  
*Value: UC*

7500

5000

2500

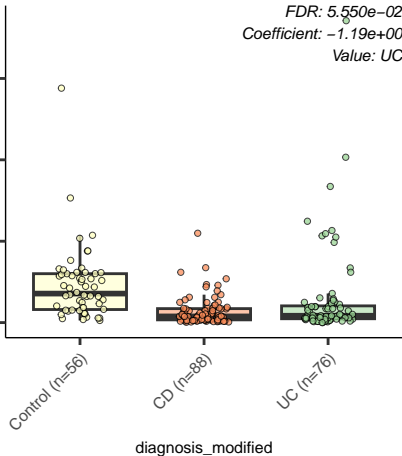
0

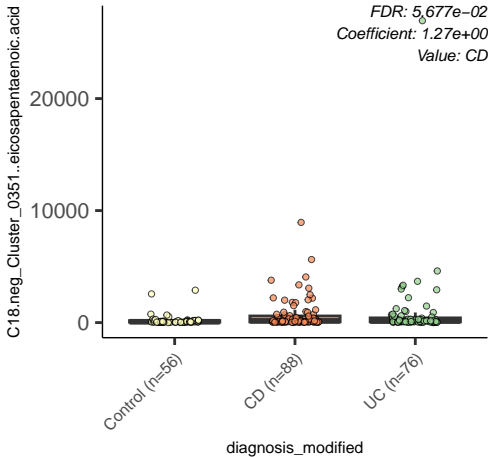
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





C8.pos\_Cluster\_0277..stearoyl.ethanolamide

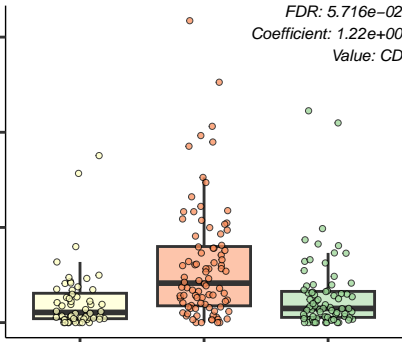
FDR: 5.716e-02  
Coefficient: 1.22e+00  
Value: CD

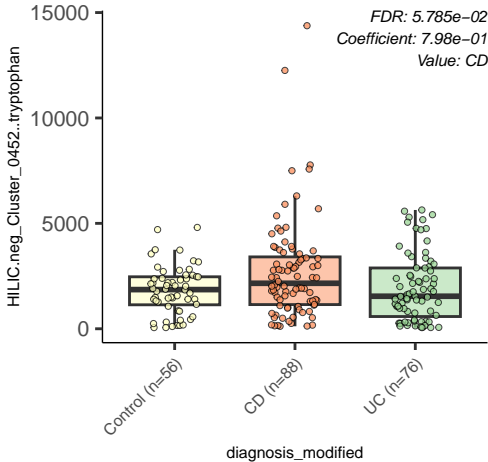
Control (n=56)

CD (n=88)

UC (n=76)

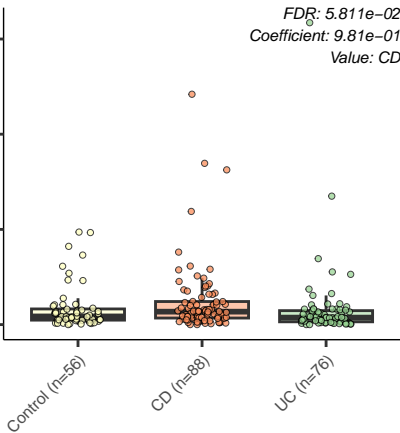
diagnosis\_modified





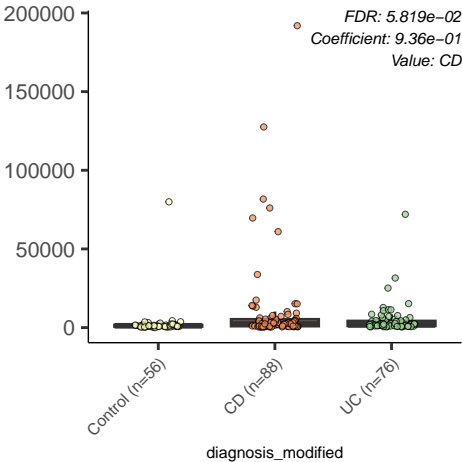
HILIC.neg\_Cluster\_1170..lactose

*FDR: 5.811e-02*  
*Coefficient: 9.81e-01*  
*Value: CD*



diagnosis\_modified

HILIC.pos\_Cluster\_0230..carnitine



C18.neg\_Cluster\_0045..azelate

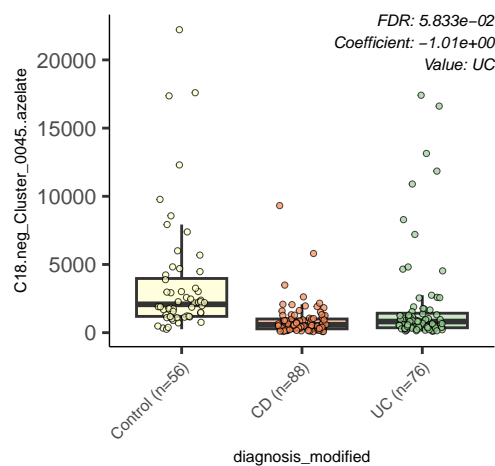
*FDR: 5.833e-02*  
*Coefficient: -1.01e+00*  
*Value: UC*

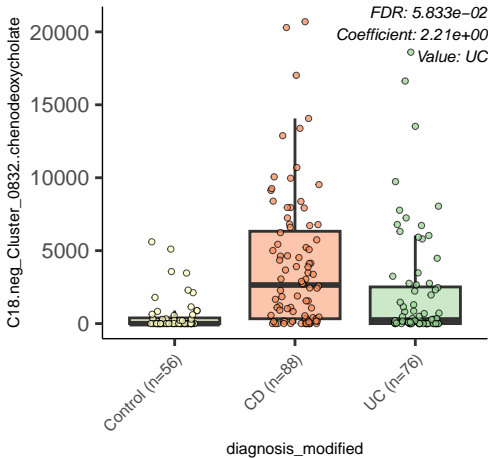
Control (n=56)

CD (n=88)

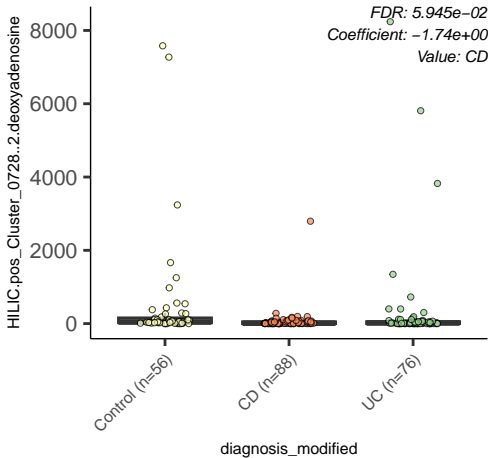
UC (n=76)

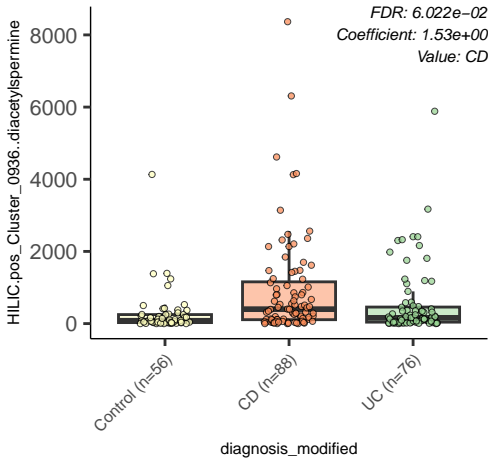
diagnosis\_modified

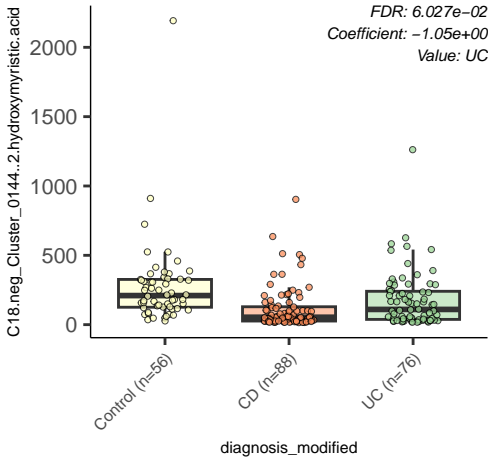












HILIC.pos\_Cluster\_0254...3.methylxanthine

FDR: 6.033e-02  
Coefficient: 1.79e+00  
Value: CD

1000

500

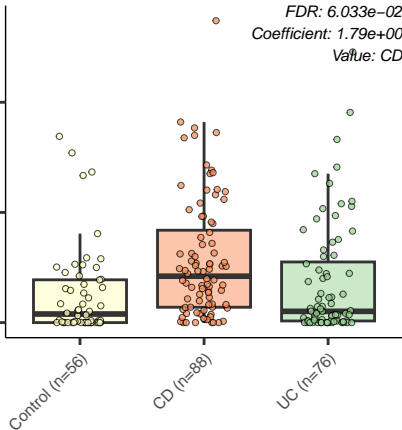
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0066..valine

FDR: 6.756e-02  
Coefficient: 8.90e-01  
Value: CD

60000

40000

20000

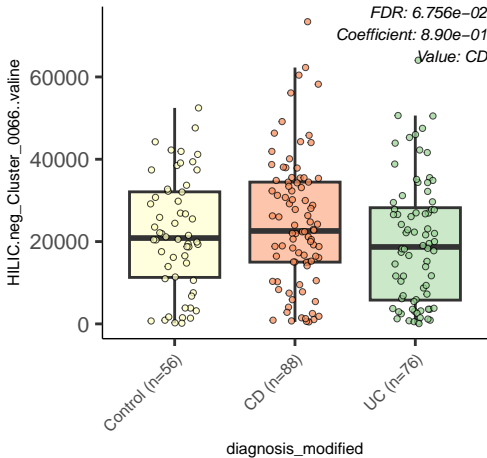
0

Control (n=56)

CD (n=88)

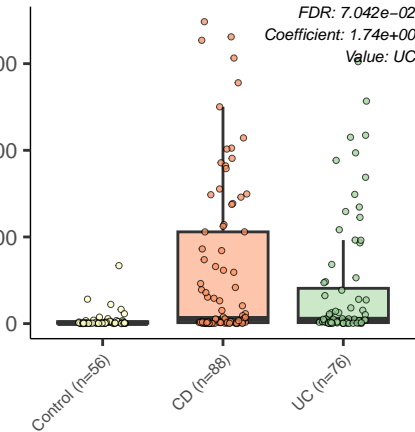
UC (n=76)

diagnosis\_modified

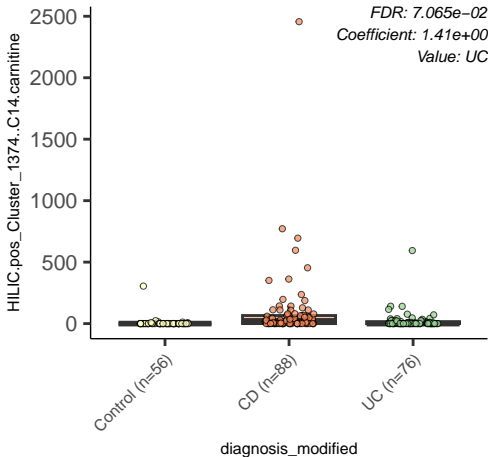


HILIC\_pos\_Cluster\_0090..creatine

FDR: 7.042e-02  
Coefficient: 1.74e+00  
Value: UC

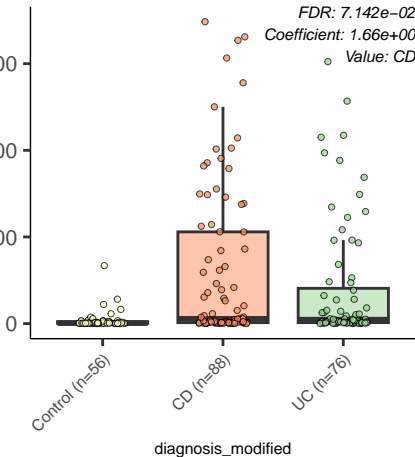


diagnosis\_modified

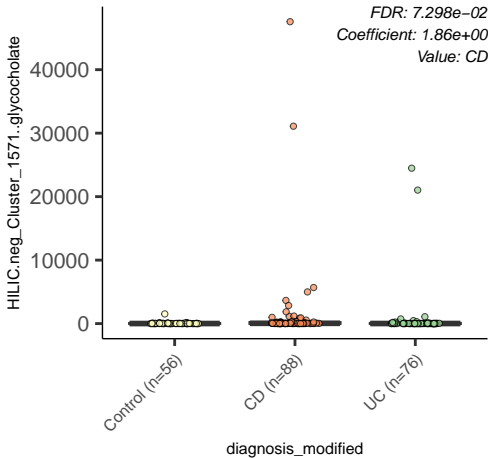


HILIC\_pos\_Cluster\_0090..creatine

FDR:  $7.142e-02$   
Coefficient:  $1.66e+00$   
Value: CD

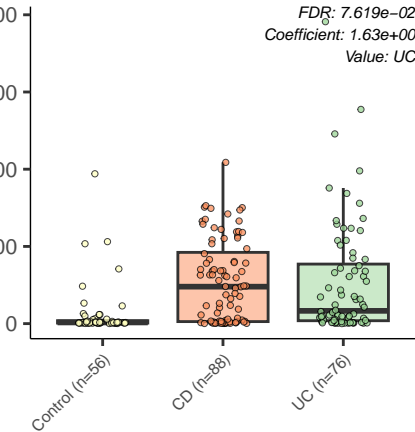




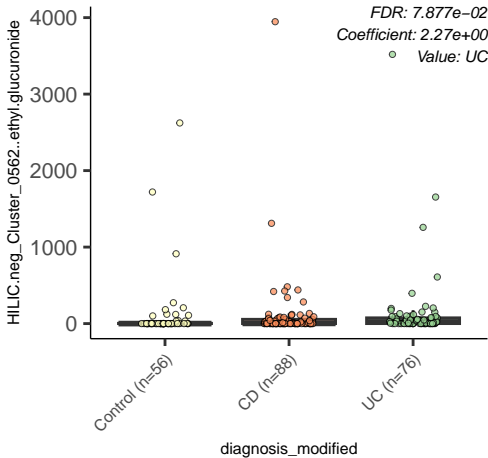


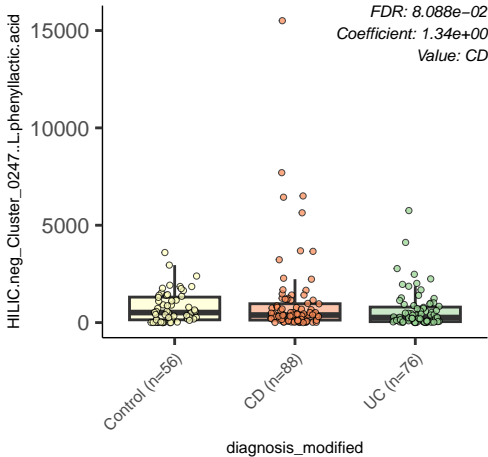
HILIC.neg\_Cluster\_0085..taurine

FDR: 7.619e-02  
Coefficient: 1.63e+00  
Value: UC



diagnosis\_modified





HILIC.pos\_Cluster\_0066...taurine

*FDR: 8.491e-02*  
*Coefficient: 1.61e+00*  
*Value: CD*

30000

20000

10000

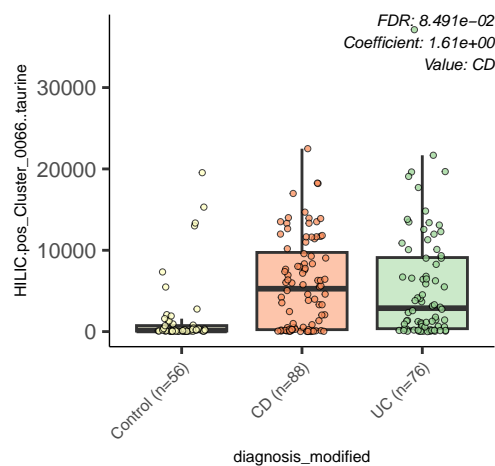
0

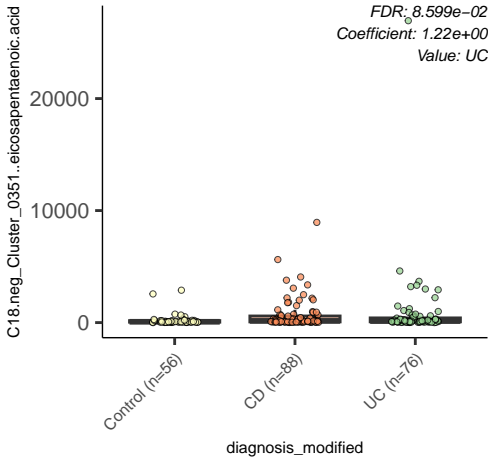
Control (n=56)

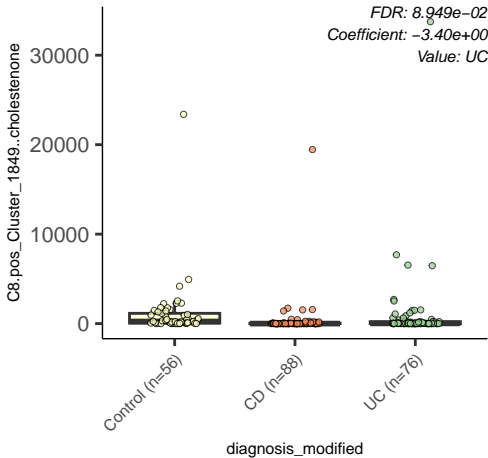
CD (n=88)

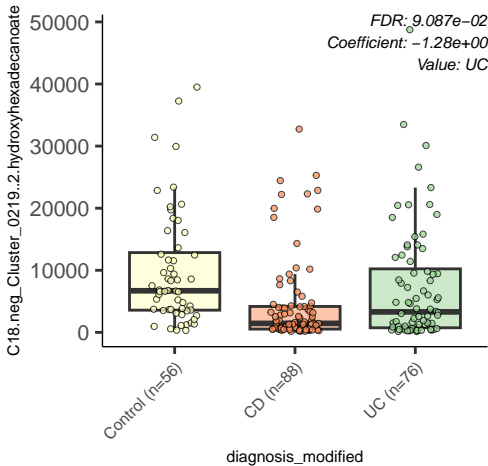
UC (n=76)

diagnosis\_modified

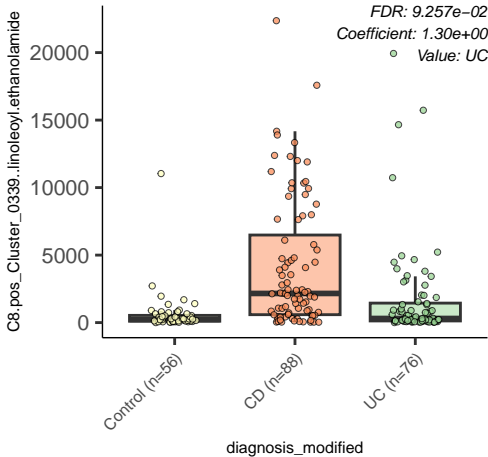






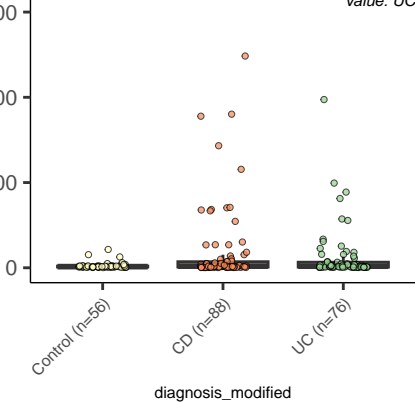






HILIC.neg\_Cluster\_0020...lactate

*FDR: 9.259e-02*  
*Coefficient: 1.22e+00*  
*Value: UC*



HILIC.neg\_Cluster\_0120..adenine

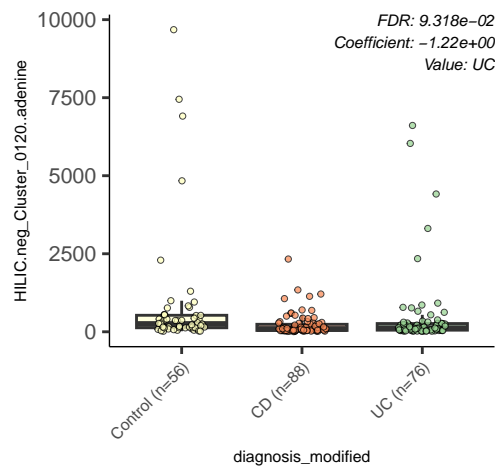
*FDR: 9.318e-02*  
*Coefficient: -1.22e+00*  
*Value: UC*

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0677..cystine

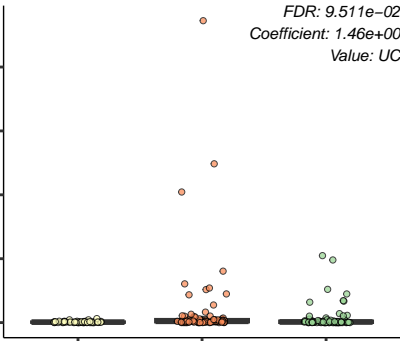
*FDR: 9.511e-02*  
*Coefficient: 1.46e+00*  
*Value: UC*

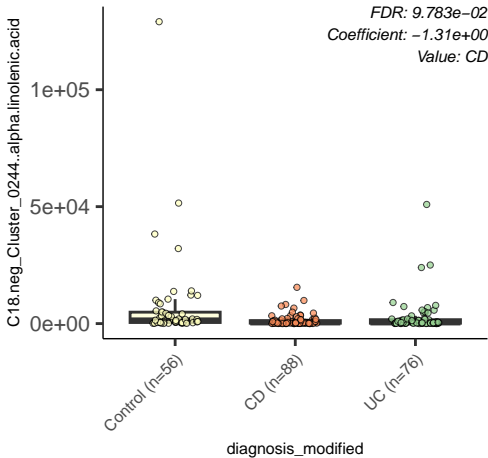
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.neg\_Cluster\_0299..ascorbate

FDR:  $9.783e-02$   
Coefficient:  $-1.35e+00$   
Value: CD

20000

10000

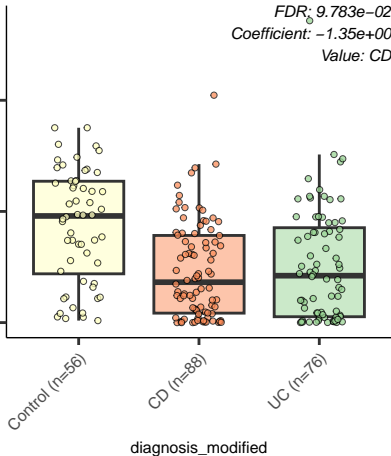
0

Control (n=56)

CD (n=88)

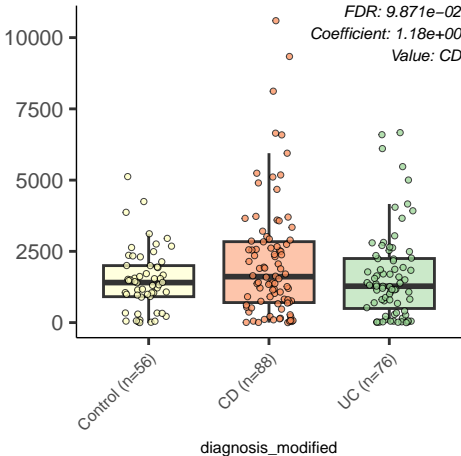
UC (n=76)

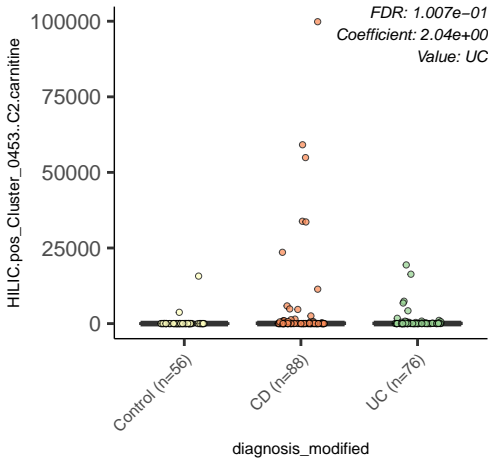
diagnosis\_modified



HILIC\_neg\_Cluster\_0162..glutamine

FDR:  $9.871e-02$   
Coefficient:  $1.18e+00$   
Value: CD







HILIC.neg\_Cluster\_0059..proline

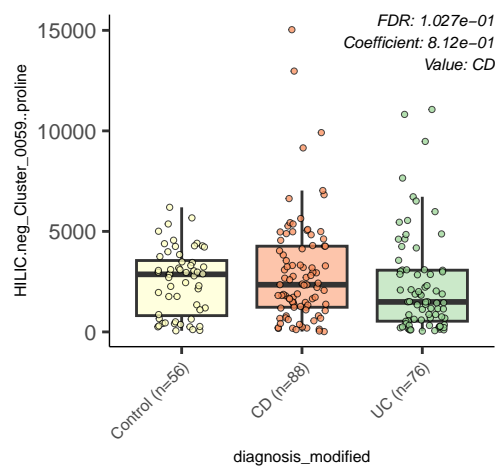
*FDR: 1.027e-01*  
*Coefficient: 8.12e-01*  
*Value: CD*

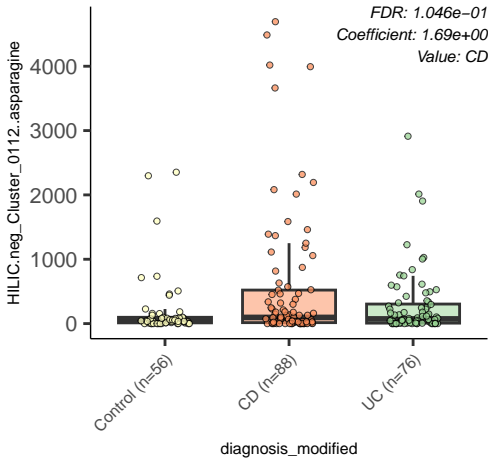
Control (n=56)

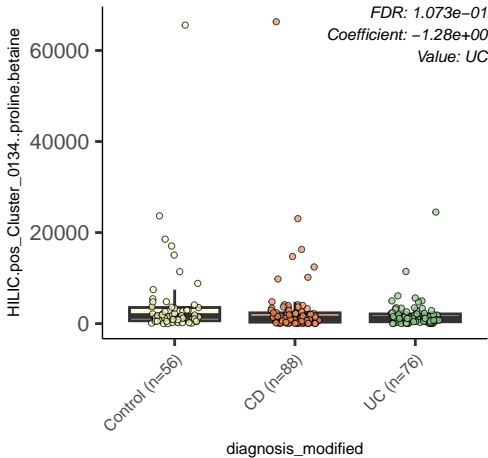
CD (n=88)

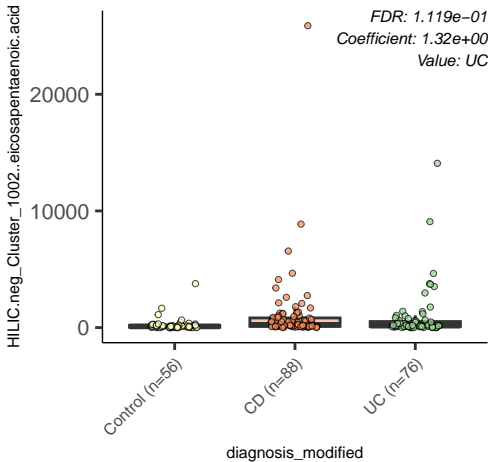
UC (n=76)

diagnosis\_modified









HILIC.pos\_Cluster\_0079..pyroglutamic.acid

*FDR: 1.119e-01*  
*Coefficient: 7.69e-01*  
*Value: UC*

10000

5000

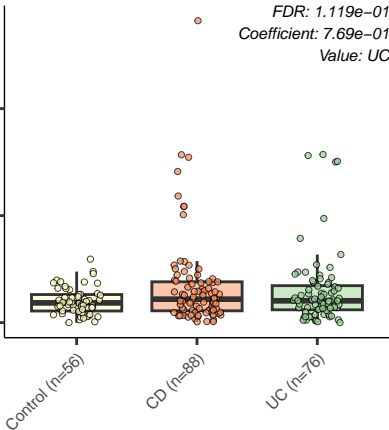
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC\_pos\_Cluster\_1580..C18.2.carnitine

*FDR: 1.119e-01*  
*Coefficient: 1.57e+00*  
*Value: UC*

2000

1000

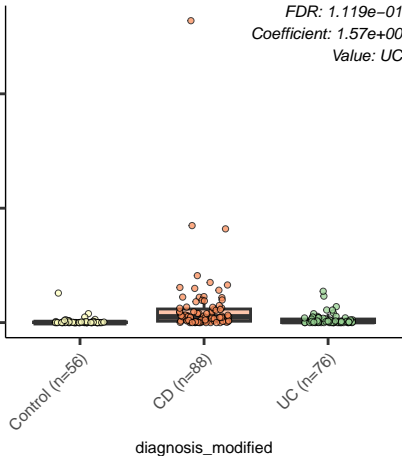
0

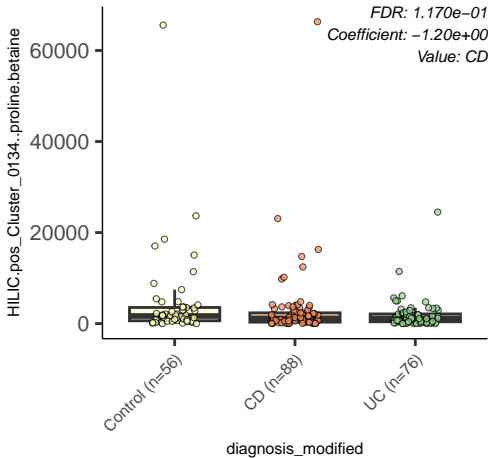
Control (n=56)

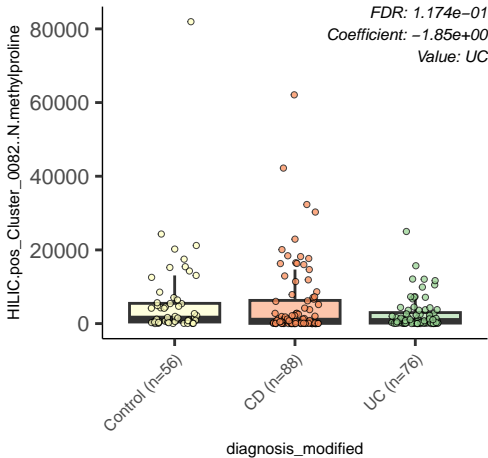
CD (n=88)

UC (n=76)

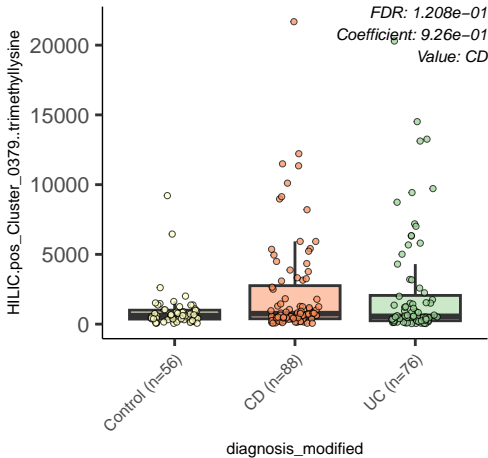
diagnosis\_modified











C18.neg\_Cluster\_1680...maslinic.acid

FDR: 1.226e-01  
Coefficient: -1.43e+00  
Value: UC

4000

2000

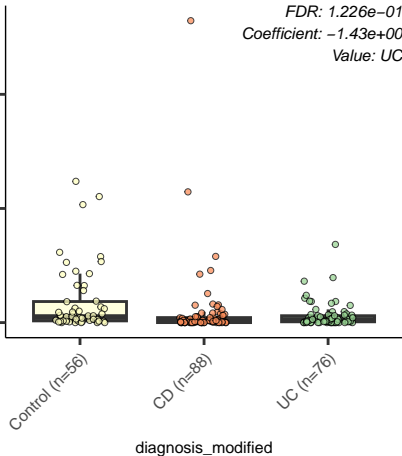
0

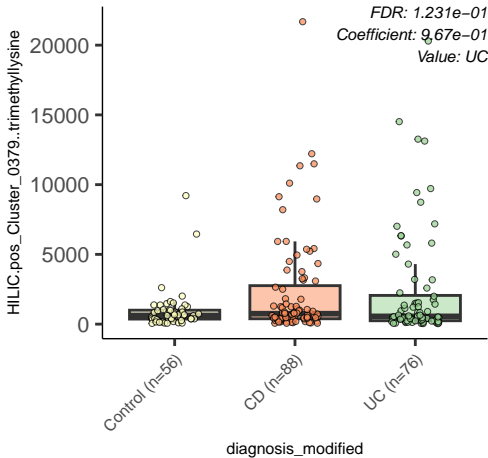
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





C8.pos\_Cluster\_0253..sphingosine

FDR: 1.233e-01  
Coefficient: 9.22e-01  
Value: UC

15000

10000

5000

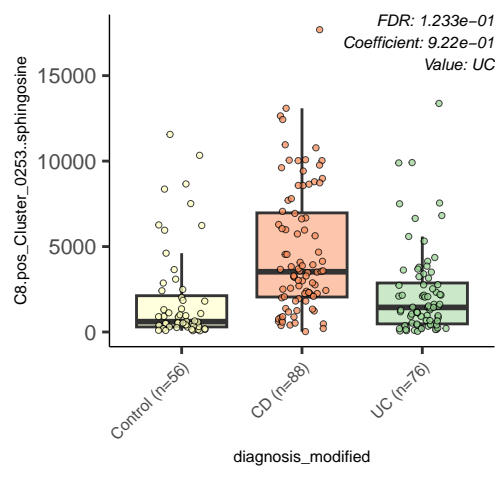
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC\_pos\_Cluster\_0306..citruiline

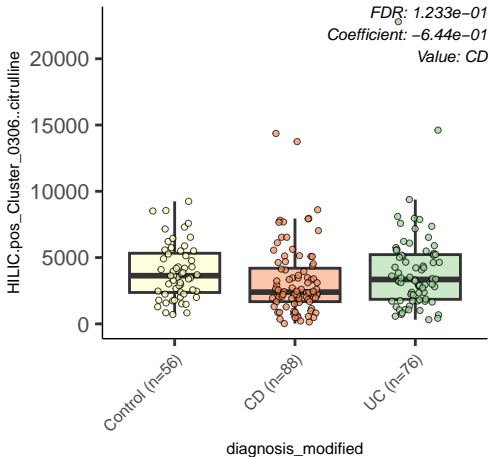
FDR:  $1.233\text{e-}01$   
Coefficient:  $-6.44\text{e-}01$   
Value: CD

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified



HILIC.pos\_Cluster\_0032...cytosine

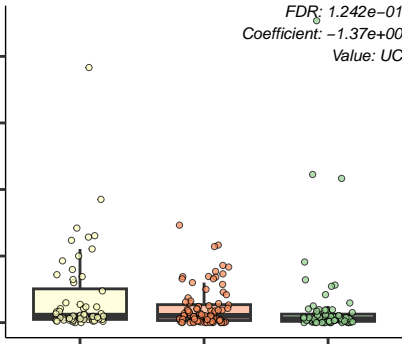
FDR: 1.242e-01  
Coefficient: -1.37e+00  
Value: UC

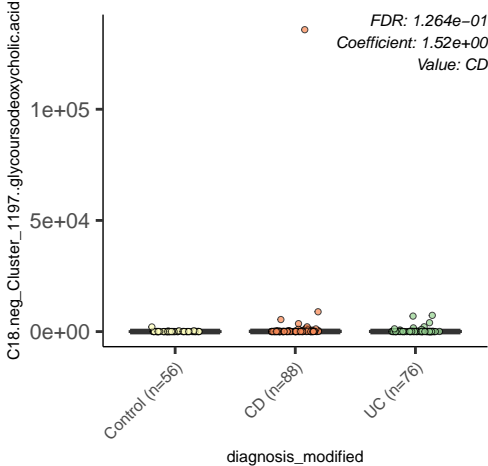
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.neg\_Cluster\_0105..leucine

60000

40000

20000

0

Control (n=56)

CD (n=88)

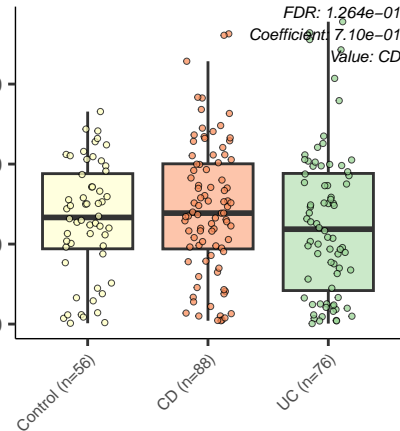
UC (n=76)

diagnosis\_modified

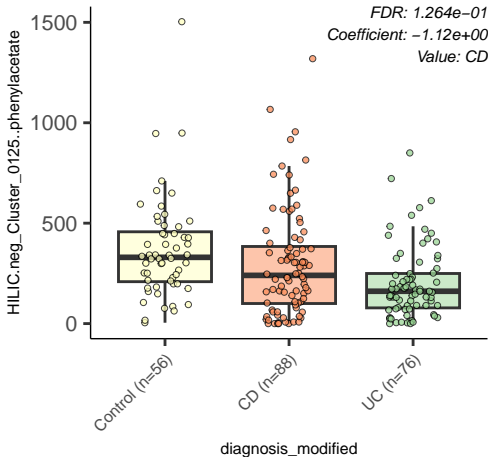
FDR: 1.264e-01

Coefficient: 7.10e-01

Value: CD







HILIC.neg\_Cluster\_0299..ascorbate

FDR:  $1.264e-01$   
Coefficient:  $-1.34e+00$   
Value: UC

20000

10000

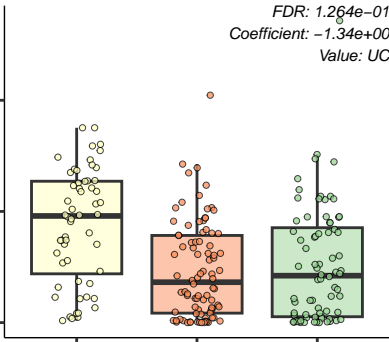
0

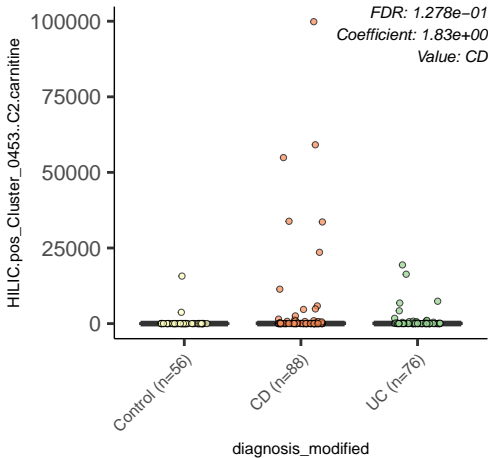
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.pos\_Cluster\_0113..trigonelline

FDR: 1.307e-01  
Coefficient: 1.25e+00  
Value: CD

20000

10000

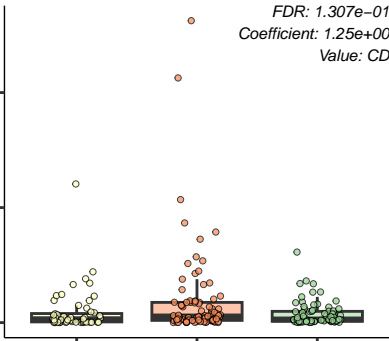
0

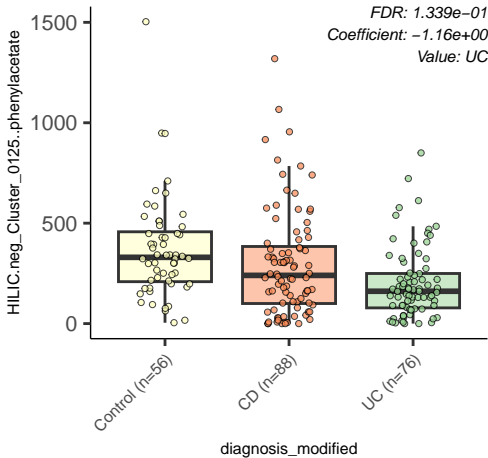
Control (n=56)

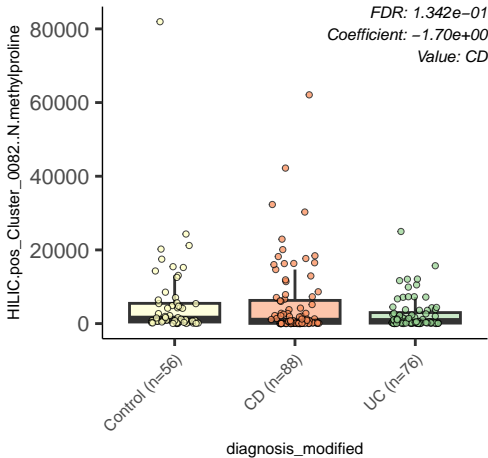
CD (n=88)

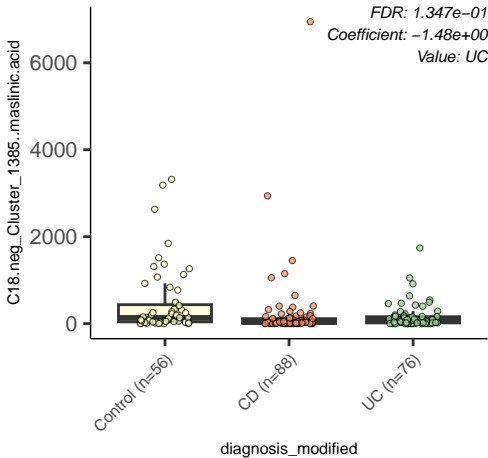
UC (n=76)

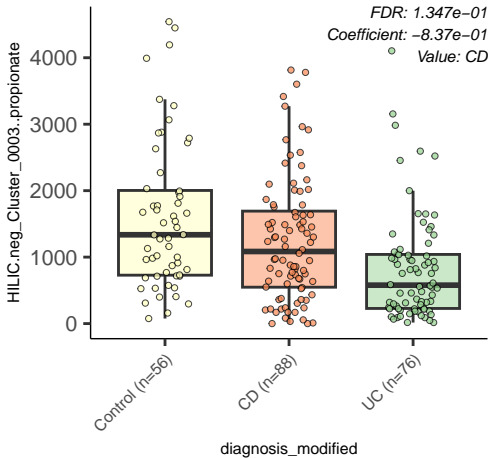
diagnosis\_modified







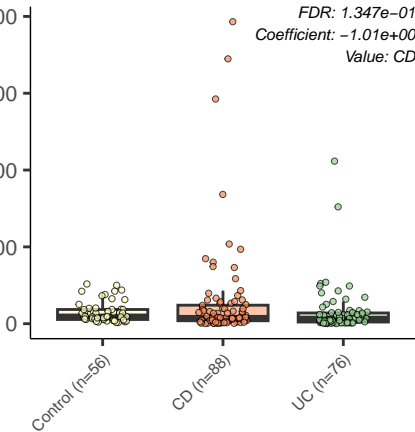






HILIC.neg\_Cluster\_0254..urate

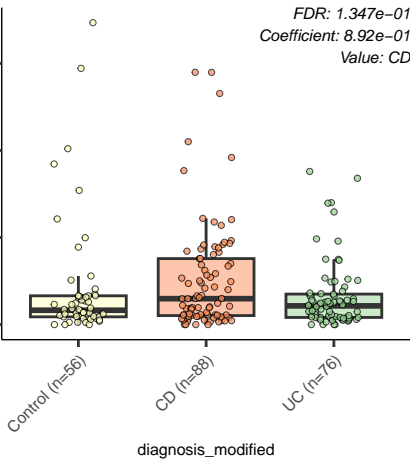
FDR:  $1.347e-01$   
Coefficient:  $-1.01e+00$   
Value: CD

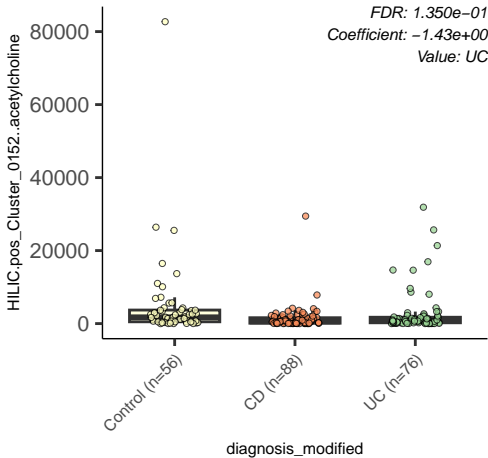


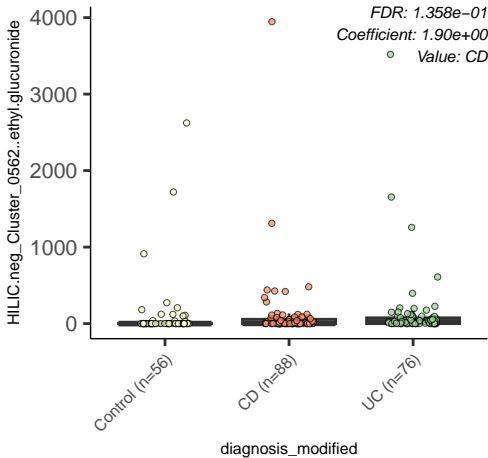
diagnosis\_modified

HILIC\_pos\_Cluster\_0150..4.guanidinobutanoic.acid

FDR: 1.347e-01  
Coefficient: 8.92e-01  
Value: CD







HILIC.neg\_Cluster\_0242..phenylalanine

FDR: 1.381e-01  
Coefficient: 5.99e-01  
Value: CD

60000

40000

20000

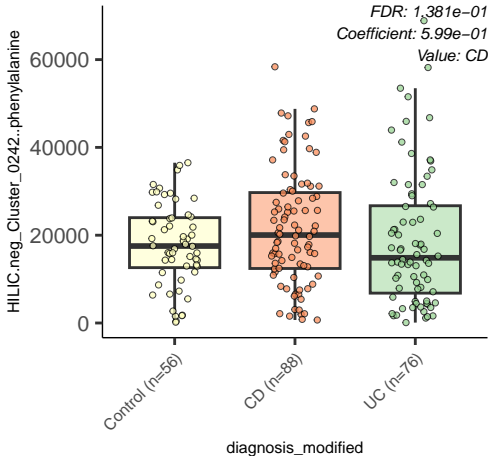
0

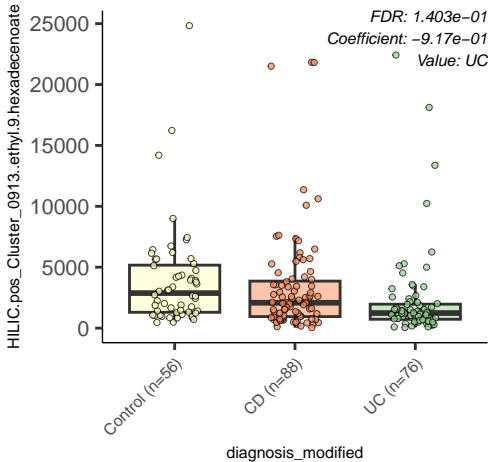
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.pos\_Cluster\_0066...taurine

*FDR: 1.405e-01*  
*Coefficient: 1.49e+00*  
*Value: UC*

30000

20000

10000

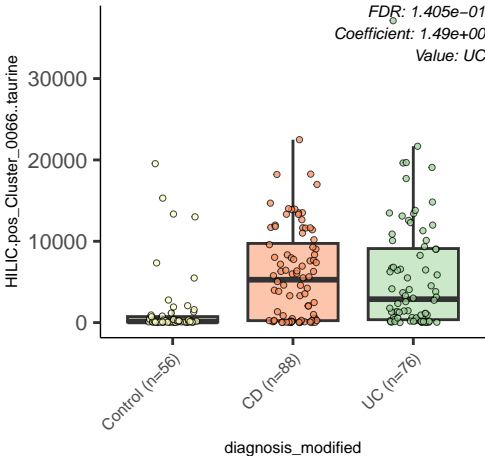
0

Control (n=56)

CD (n=88)

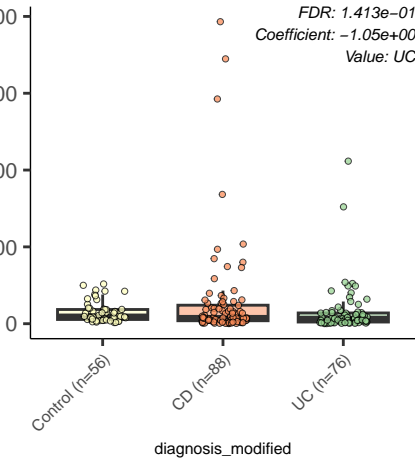
UC (n=76)

diagnosis\_modified



HILIC.neg\_Cluster\_0254..urate

FDR:  $1.413e-01$   
Coefficient:  $-1.05e+00$   
Value: UC





C8\_pos\_Cluster\_0554..cholestenone

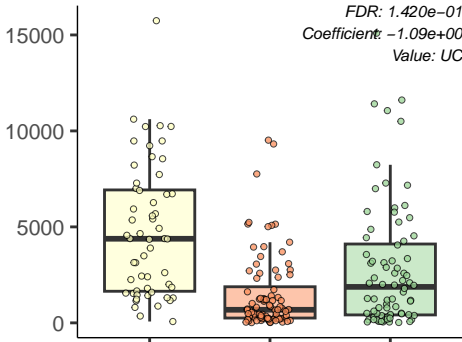
FDR: 1.420e-01  
Coefficient: -1.09e+00  
Value: UC

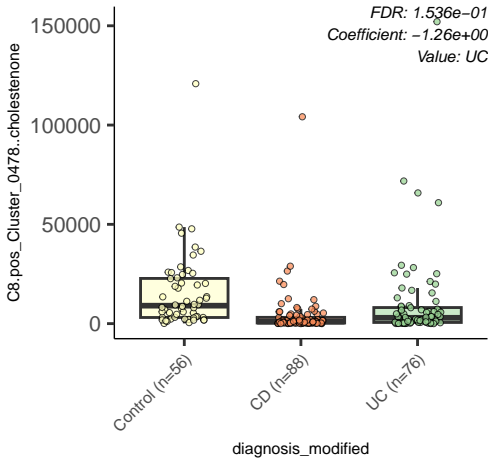
Control (n=56)

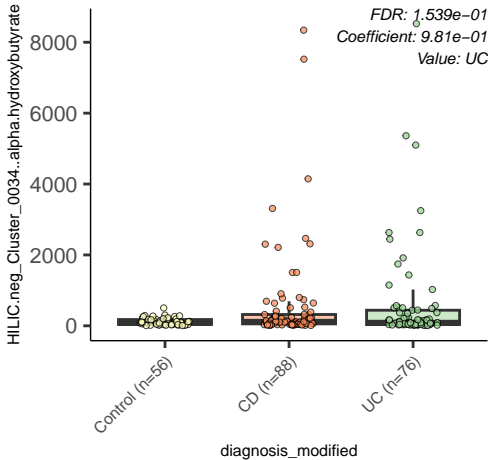
CD (n=88)

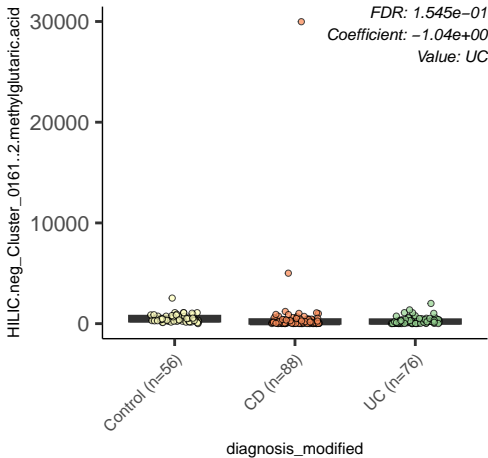
UC (n=76)

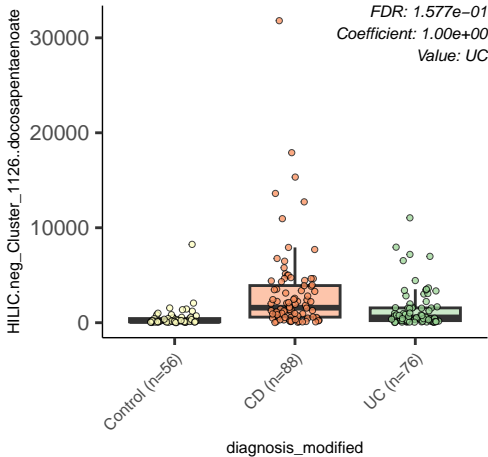
diagnosis\_modified

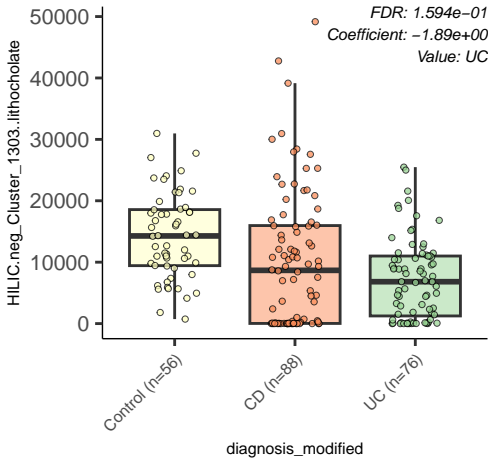


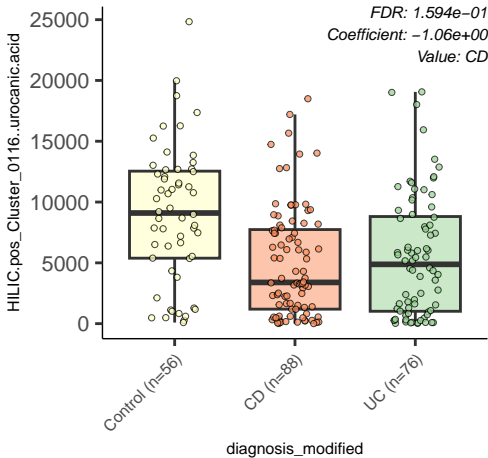


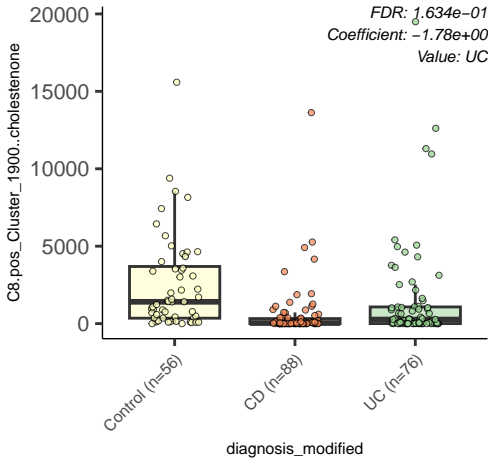




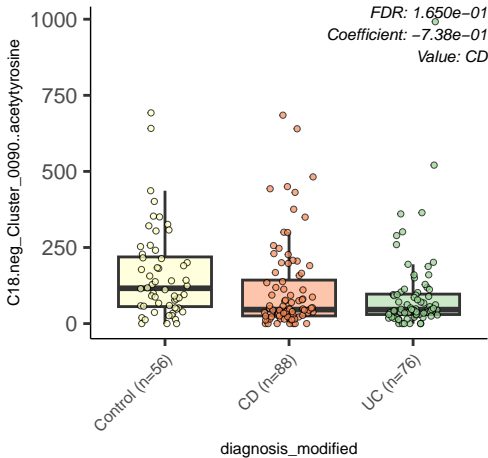


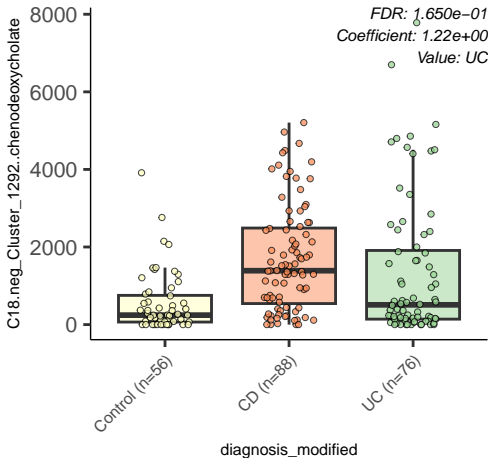












HILIC.pos\_Cluster\_0036..creatinine

*FDR: 1.661e-01*  
*Coefficient: 1.67e+00*  
*Value: CD*

60000

40000

20000

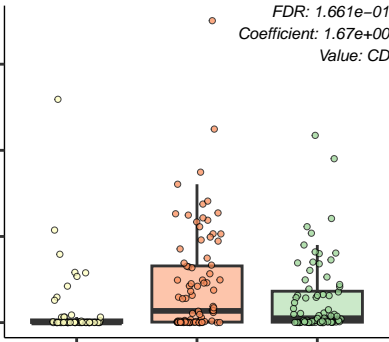
0

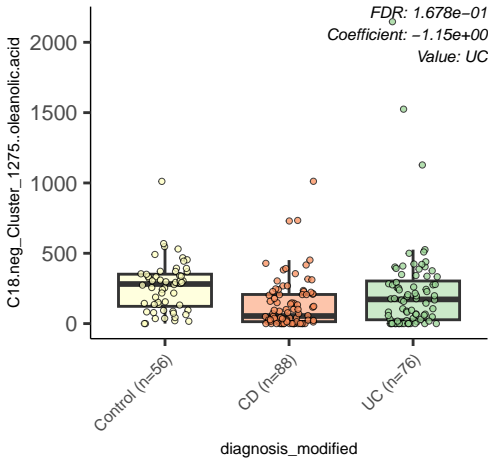
Control (n=56)

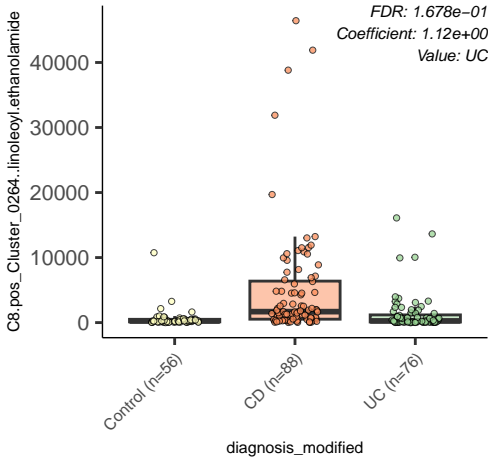
CD (n=88)

UC (n=76)

diagnosis\_modified







HILIC.neg\_Cluster\_0020...lactate

*FDR: 1.681e-01*  
*Coefficient: 9.95e-01*  
*Value: CD*

90000

60000

30000

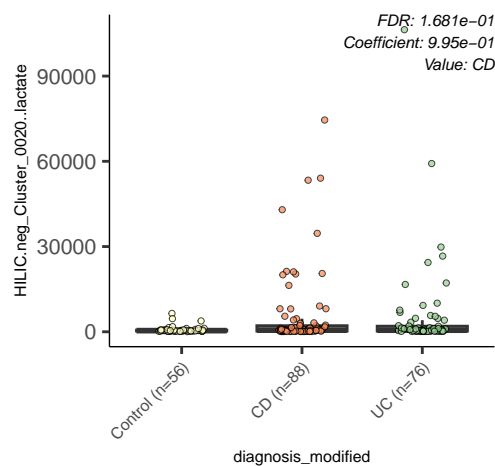
0

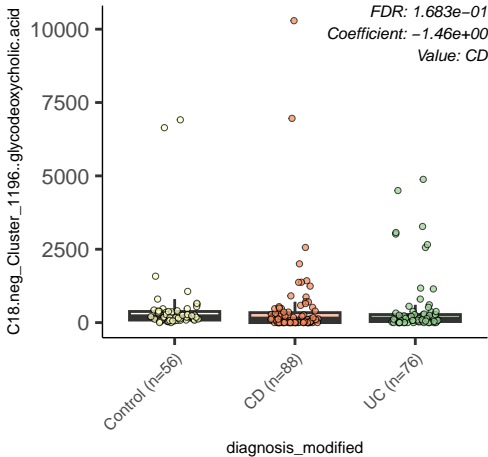
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.pos\_Cluster\_0156..glutamine

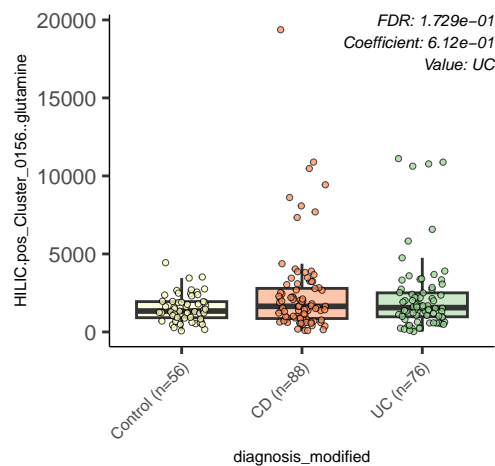
*FDR: 1.729e-01*  
*Coefficient: 6.12e-01*  
*Value: UC*

Control (n=56)

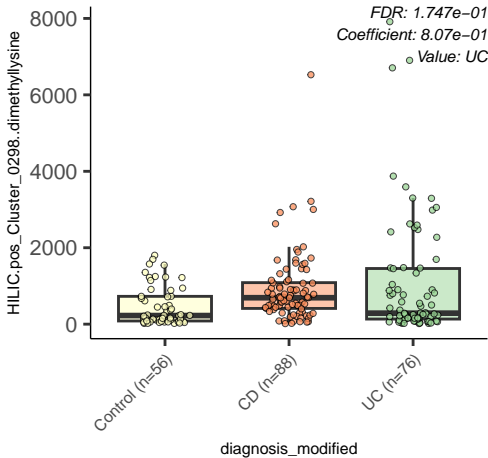
CD (n=88)

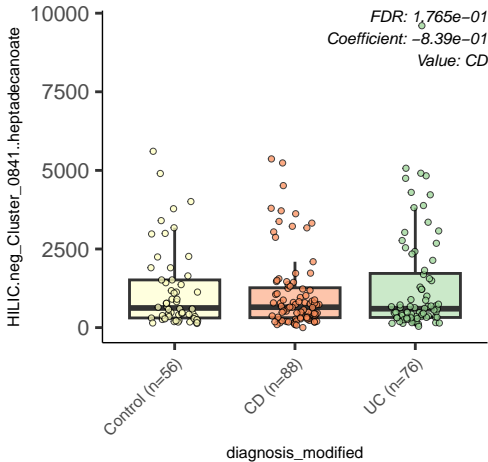
UC (n=76)

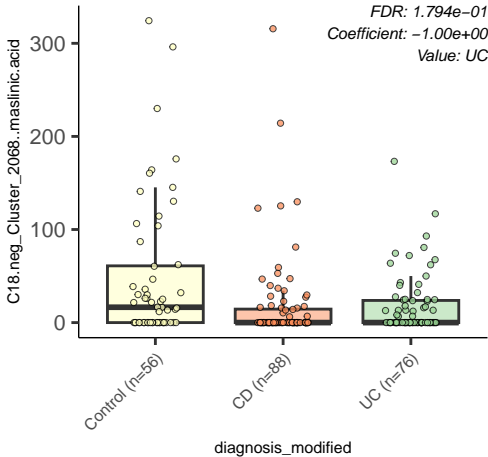
diagnosis\_modified

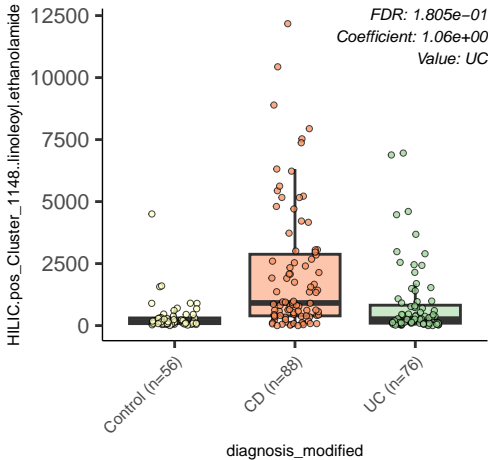


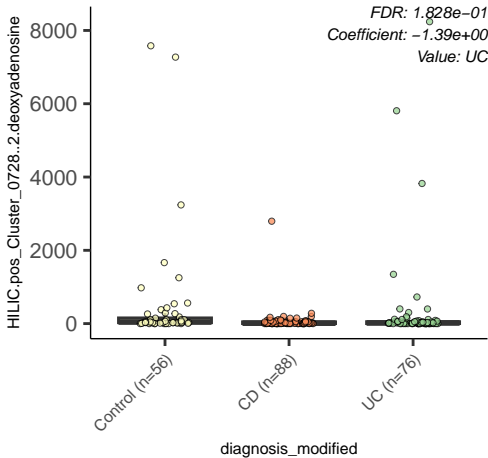












HILIC.pos\_Cluster\_0079..pyroglutamic.acid

FDR: 1.884e-01  
Coefficient: 6.30e-01  
Value: CD

10000

5000

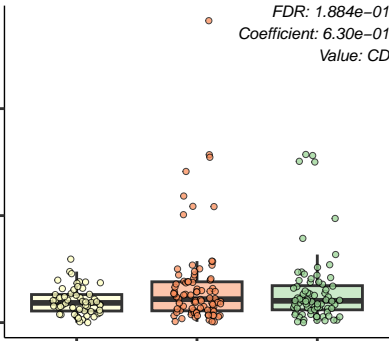
0

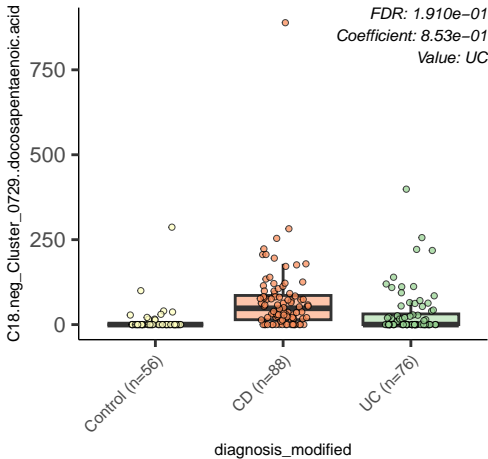
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.neg\_Cluster\_0059..proline

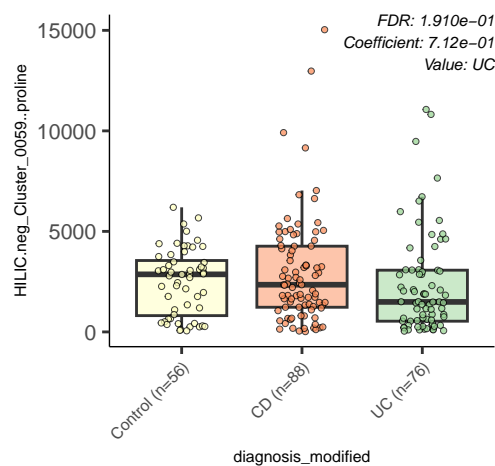
*FDR: 1.910e-01*  
*Coefficient: 7.12e-01*  
*Value: UC*

Control (n=56)

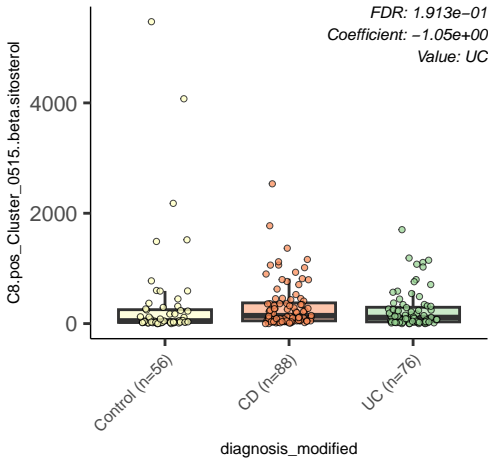
CD (n=88)

UC (n=76)

diagnosis\_modified

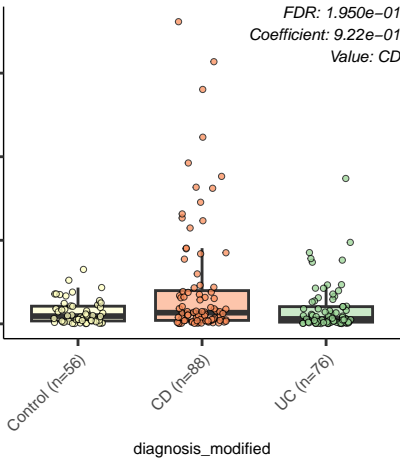


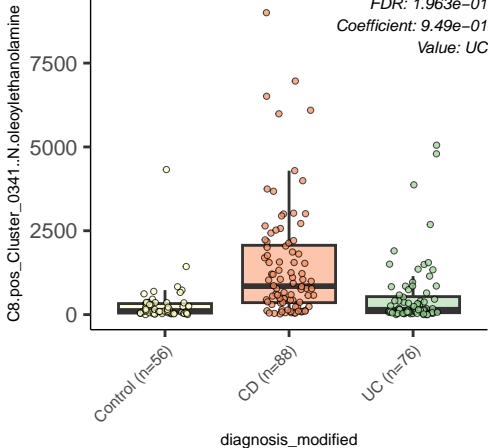




HILIC.neg\_Cluster\_0032...2.aminobutyric.acid

FDR: 1.950e-01  
Coefficient: 9.22e-01  
Value: CD





HILIC.neg\_Cluster\_0015..alanine

15000  
10000  
5000  
0

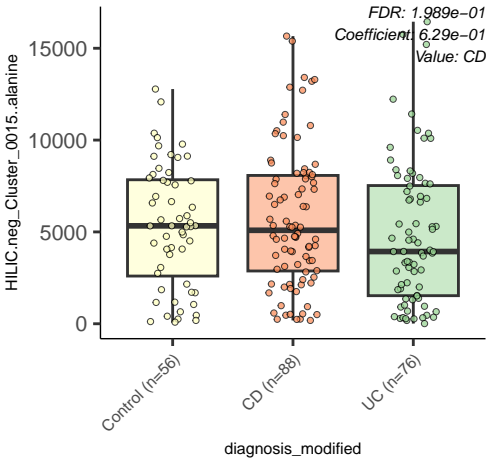
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified

FDR:  $1.989 \times 10^{-1}$   
Coefficient:  $6.29 \times 10^{-1}$   
Value: CD



C18.neg\_Cluster\_0591..eicosatrienoic.acid

FDR: 2.002e-01  
Coefficient: 9.04e-01  
Value: UC

400

200

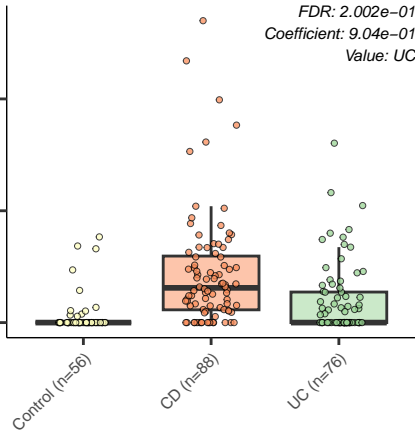
0

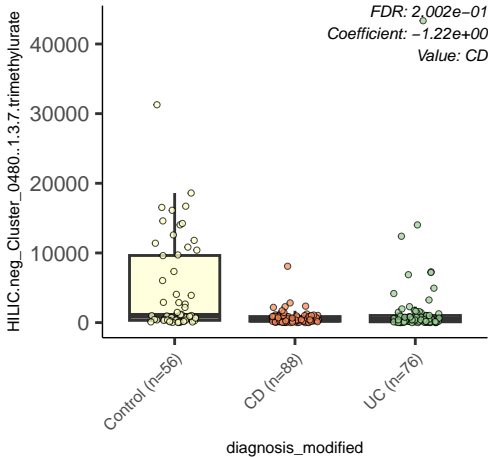
Control (n=56)

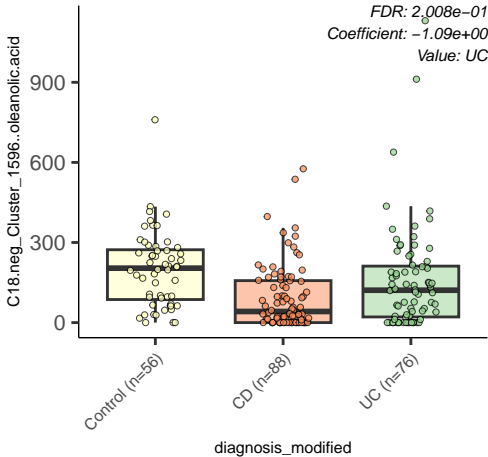
CD (n=88)

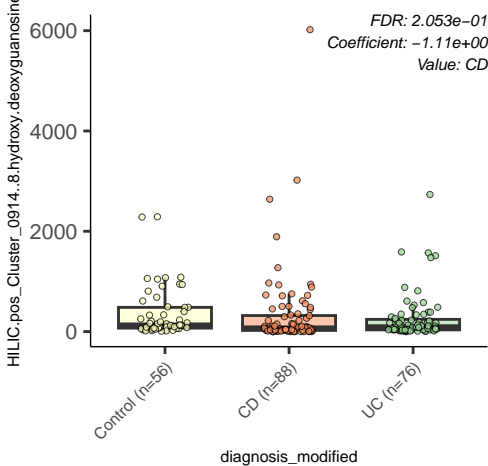
UC (n=76)

diagnosis\_modified

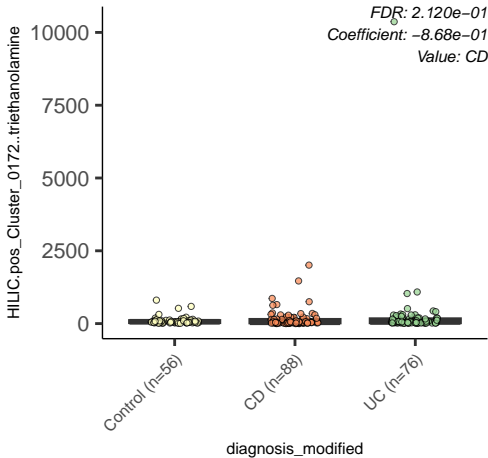






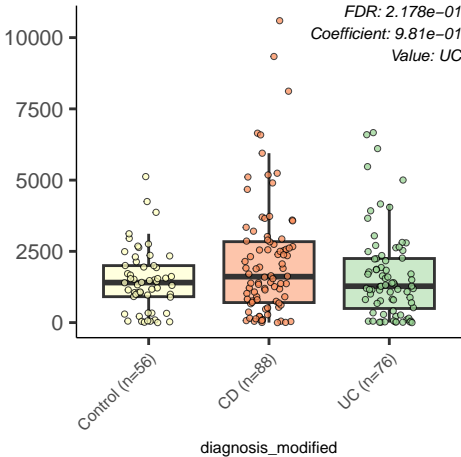






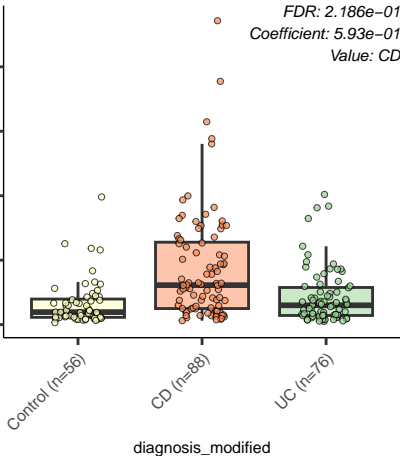
HILIC.neg\_Cluster\_0162..glutamine

*FDR: 2.178e-01*  
*Coefficient: 9.81e-01*  
*Value: UC*



HILIC\_pos\_Cluster\_1113..phytosphingosine

*FDR: 2.186e-01*  
*Coefficient: 5.93e-01*  
*Value: CD*



HILIC.neg\_Cluster\_0066..valine

*FDR: 2.199e-01*  
*Coefficient: 6.79e-01*  
*Value: UC*

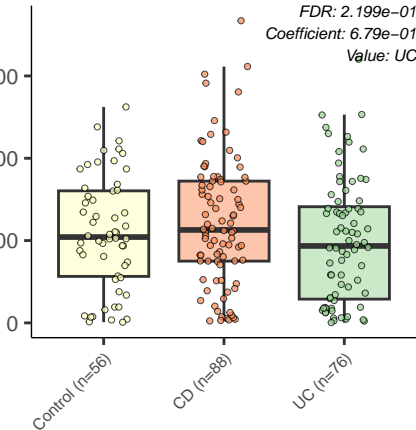
60000  
40000  
20000  
0

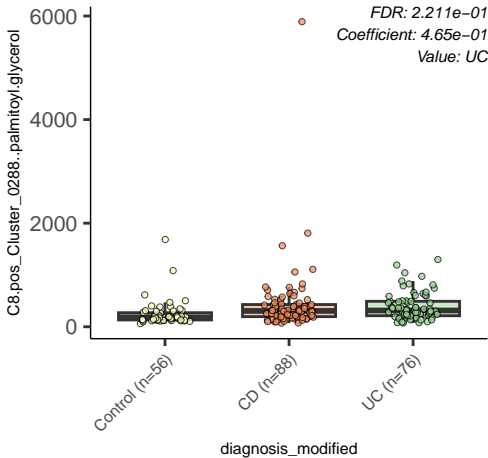
Control (n=56)

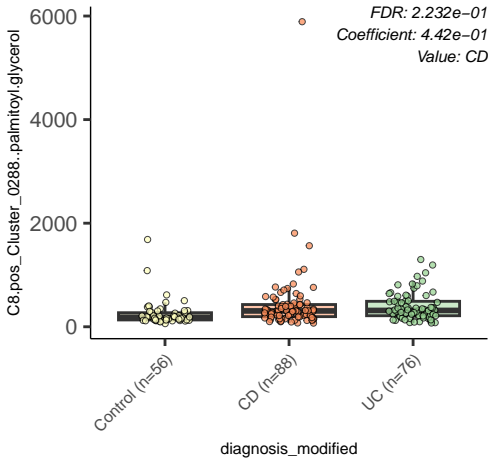
CD (n=88)

UC (n=76)

diagnosis\_modified

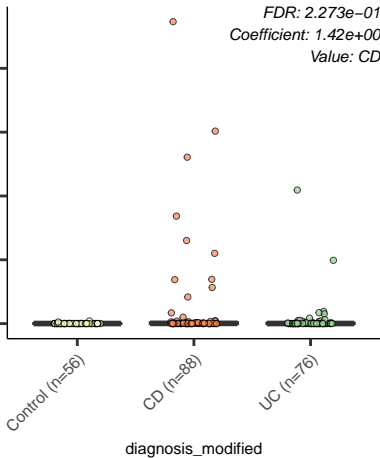






C18.neg\_Cluster\_1574..taurochenodesoxycholic.ac

FDR: 2.273e-01  
Coefficient: 1.42e+00  
Value: CD



C18.neg\_Cluster\_0250..oleic.acid

100000  
75000  
50000  
25000  
0

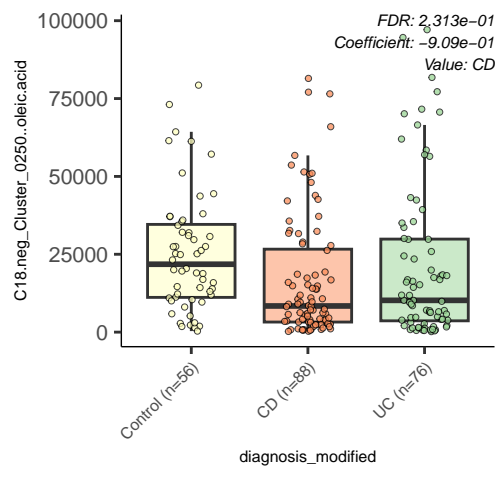
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified

FDR: 2.313e-01  
Coefficient: -9.09e-01  
Value: CD





HILIC.pos\_Cluster\_0046..valine

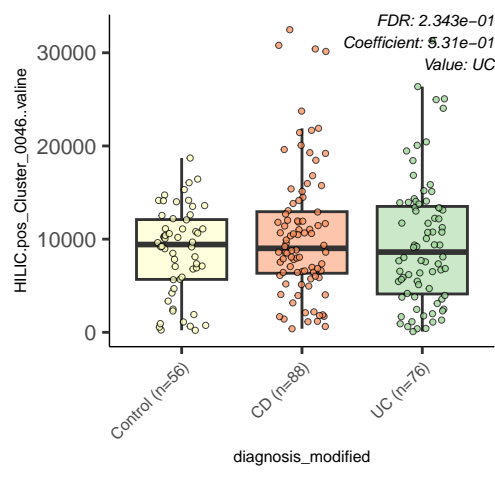
FDR: 2.343e-01  
Coefficient: 5.31e-01  
Value: UC

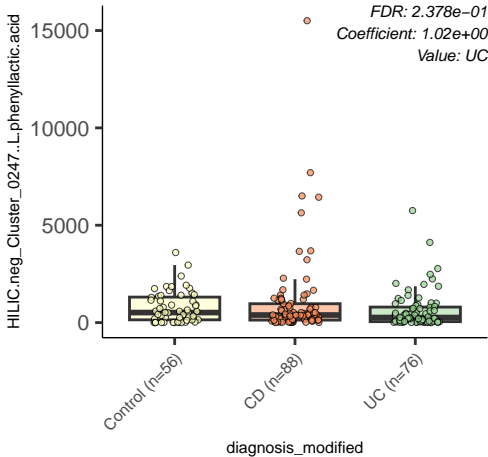
Control (n=56)

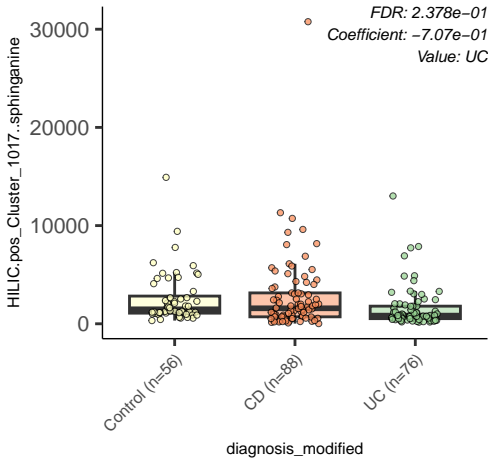
CD (n=88)

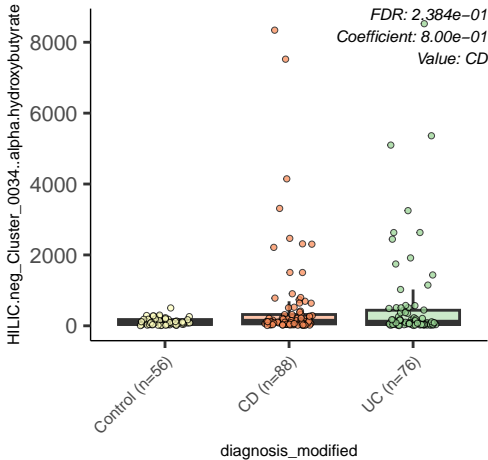
UC (n=76)

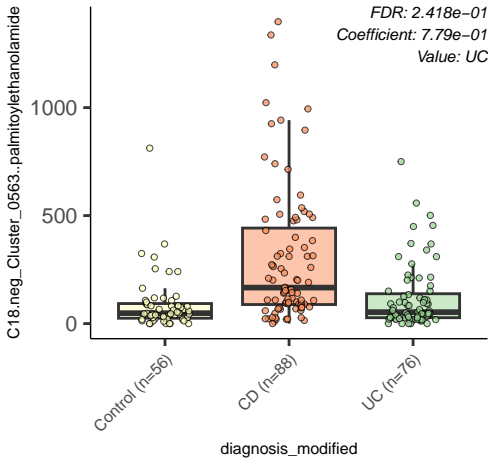
diagnosis\_modified











HILIC\_pos\_Cluster\_0022...choline

FDR: 2.418e-01  
Coefficient: 4.95e-01  
Value: CD

75000

50000

25000

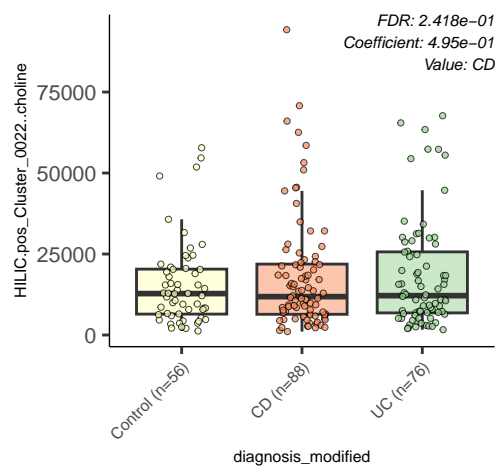
0

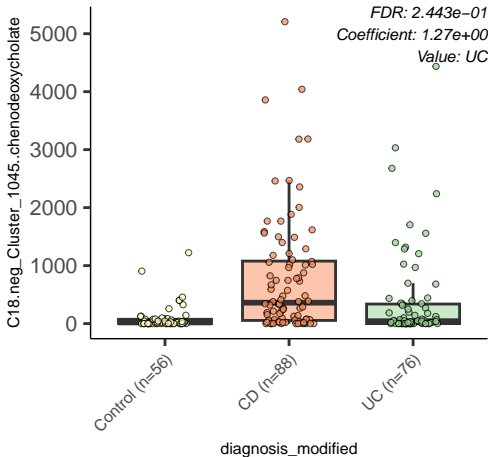
Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC\_pos\_Cluster\_0048..betaine

FDR: 2.443e-01  
Coefficient: 1.00e+00  
Value: UC

60000

40000

20000

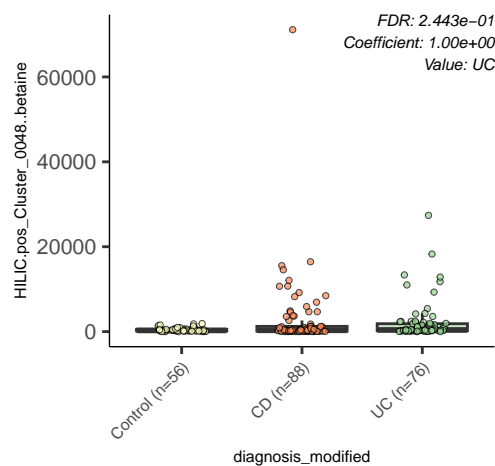
0

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified





HILIC.pos\_Cluster\_0046..valine

FDR: 2.496e-01  
Coefficient: 4.92e-01  
Value: CD

Control (n=56)

CD (n=88)

UC (n=76)

diagnosis\_modified

