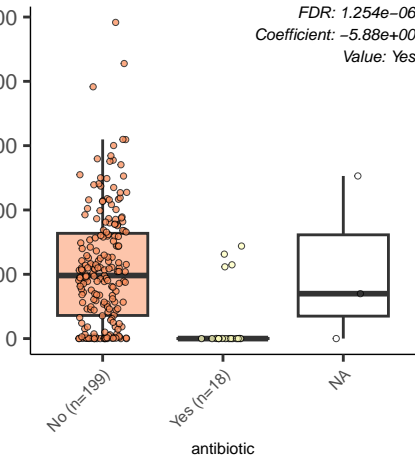
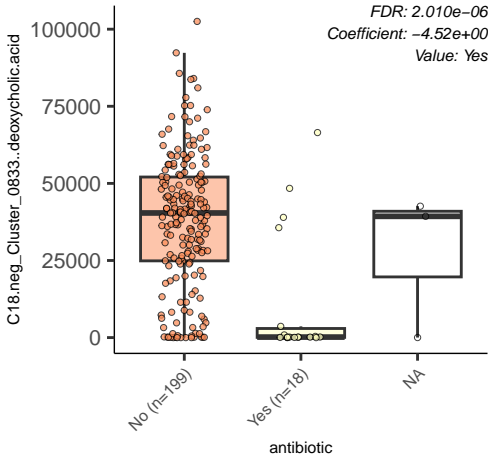


HILIC.neg\_Cluster\_1303..lithocholate

FDR:  $1.254e-06$   
Coefficient:  $-5.88e+00$   
Value: Yes





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

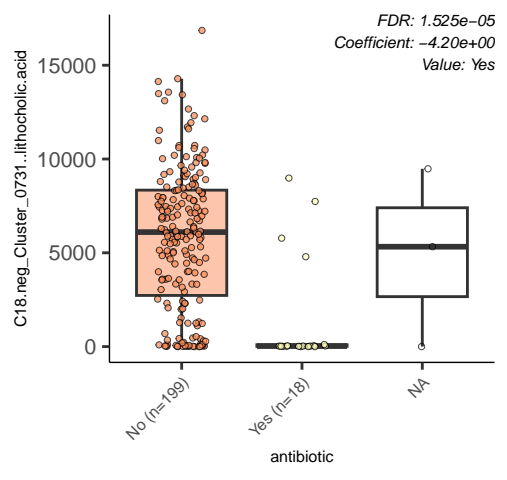
FDR: 1.525e-05  
Coefficient: -4.20e+00  
Value: Yes

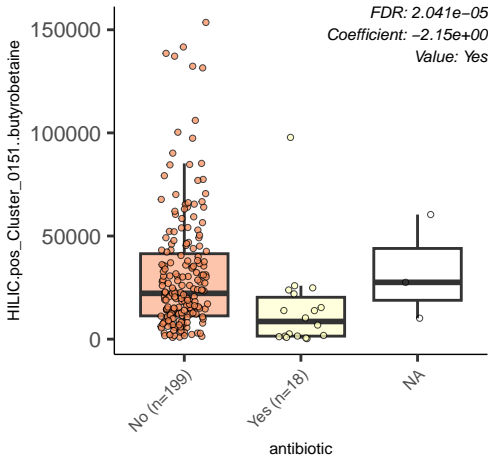
No (n=199)

Yes (n=18)

NA

antibiotic





C18.neg\_Cluster\_0031..phenyllactate

FDR:  $7.785e-05$   
Coefficient:  $-6.04e+00$   
Value: Yes

1e+05

5e+04

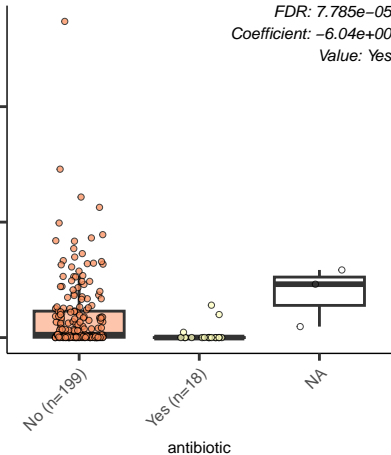
0e+00

No (n=199)

Yes (n=18)

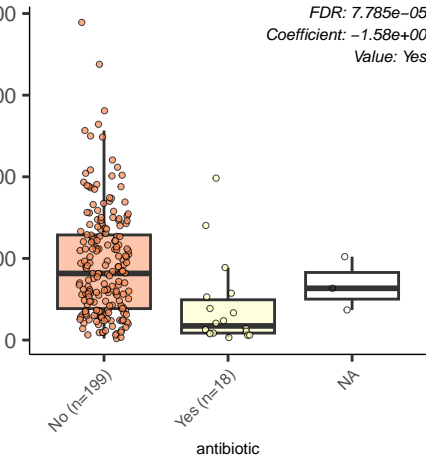
NA

antibiotic



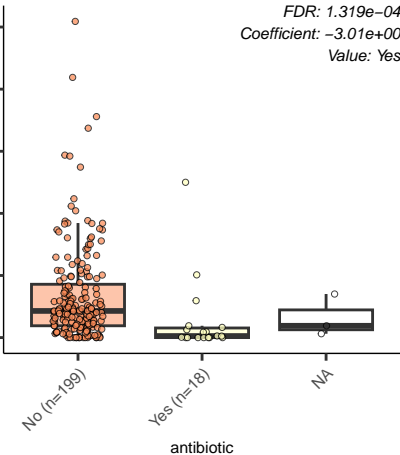
HILIC.neg\_Cluster\_0082..nicotinate

FDR:  $7.785e-05$   
Coefficient:  $-1.58e+00$   
Value: Yes



HILIC.neg\_Cluster\_0401..glucurotate

FDR:  $1.319\text{e-}04$   
Coefficient:  $-3.01\text{e}+00$   
Value: Yes



HILIC.neg\_Cluster\_0824..inosine

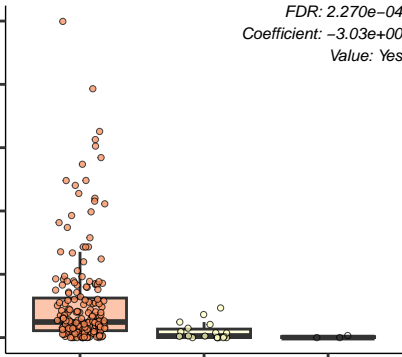
FDR: 2.270e-04  
Coefficient: -3.03e+00  
Value: Yes

No (n=199)

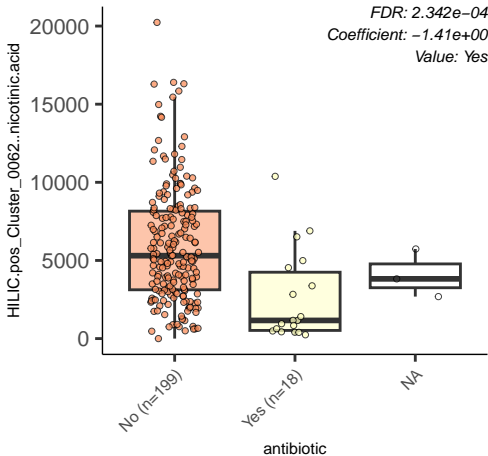
Yes (n=18)

NA

antibiotic

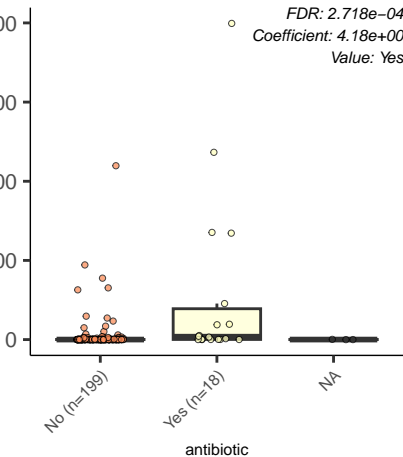


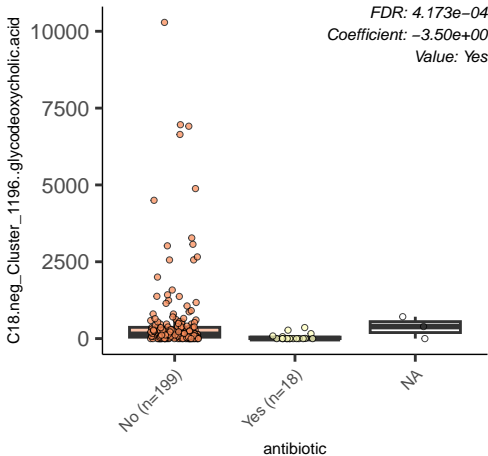


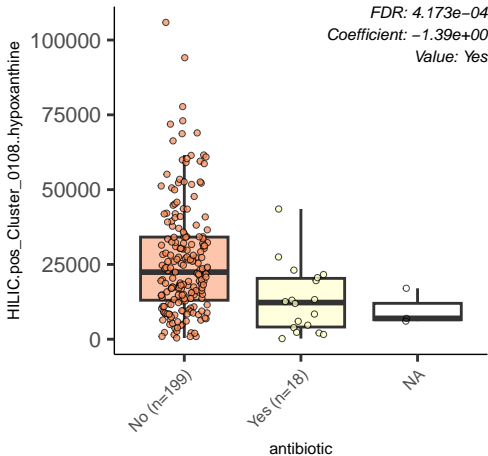


HILIC\_pos\_Cluster\_0453..C2.carnitine

FDR: 2.718e-04  
Coefficient: 4.18e+00  
Value: Yes







HILIC.neg\_Cluster\_0187..xanthine

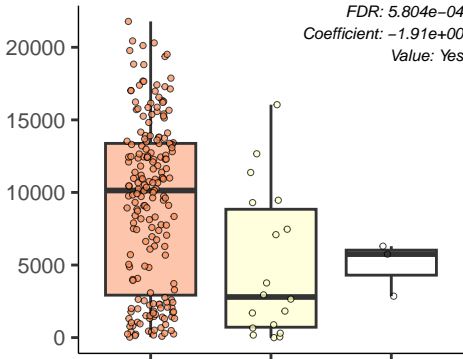
*FDR: 5.804e-04*  
*Coefficient: -1.91e+00*  
*Value: Yes*

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC\_pos\_Cluster\_0268..pyridoxamine

FDR:  $6.000\text{e-}04$   
Coefficient:  $-1.81\text{e}+00$   
Value: Yes

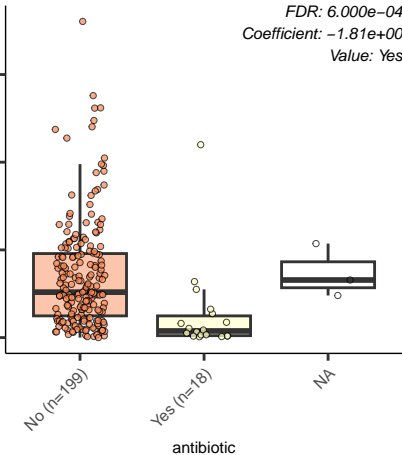
3000  
2000  
1000  
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos\_Cluster\_0230..carnitine

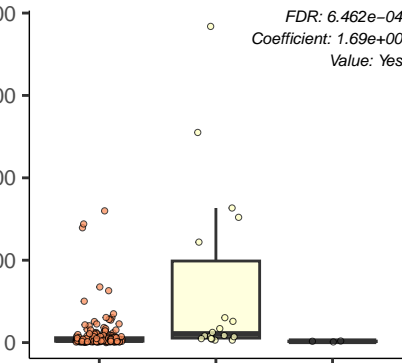
*FDR: 6.462e-04*  
*Coefficient: 1.69e+00*  
*Value: Yes*

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC\_pos\_Cluster\_0184..pyridoxamine

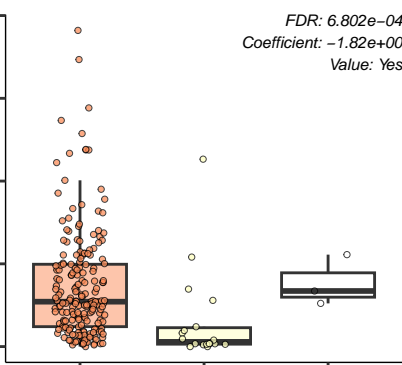
*FDR: 6.802e-04*  
*Coefficient: -1.82e+00*  
*Value: Yes*

No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.neg\_Cluster\_0296..citrulline

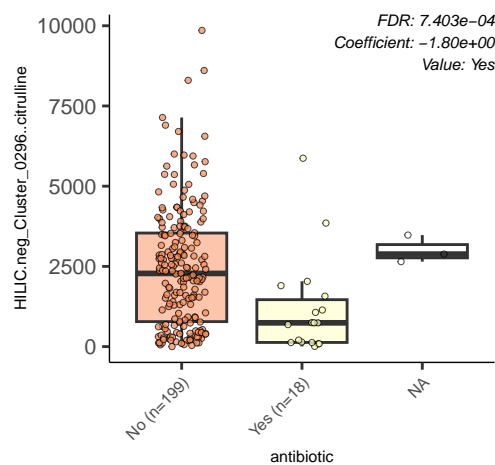
FDR:  $7.403e-04$   
Coefficient:  $-1.80e+00$   
Value: Yes

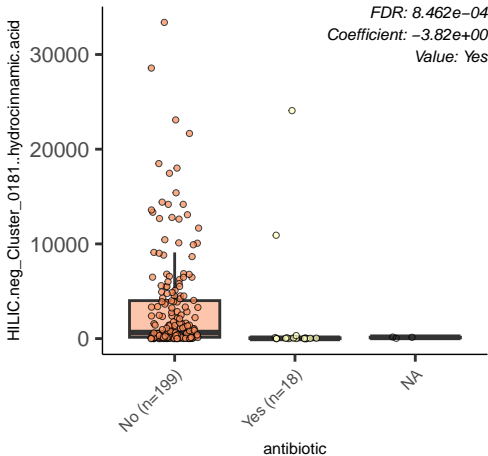
No (n=199)

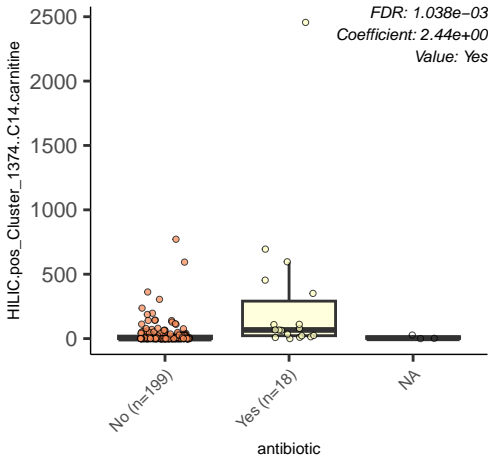
Yes (n=18)

NA

antibiotic







HILIC.neg\_Cluster\_0299..ascorbate

FDR:  $1.189\text{e-}03$   
Coefficient:  $-2.60\text{e}+00$   
Value: Yes

20000

10000

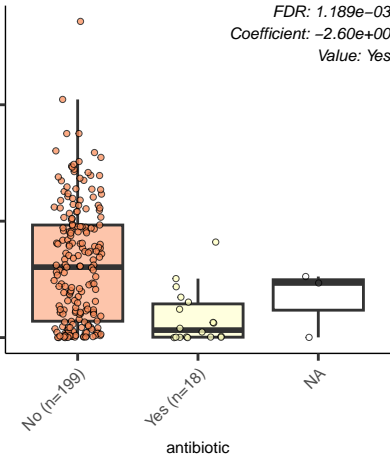
0

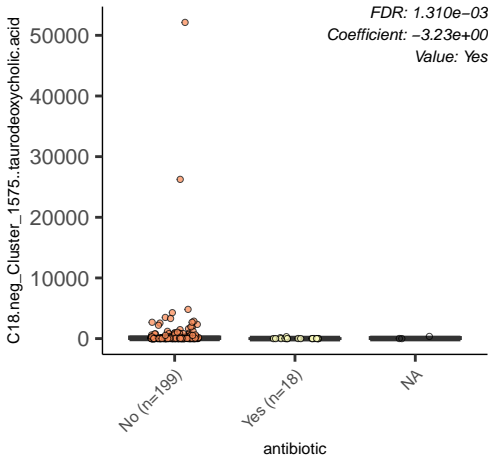
No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.neg\_Cluster\_0123...hypoxanthine

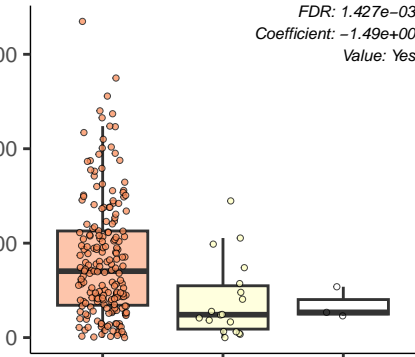
FDR:  $1.427e-03$   
Coefficient:  $-1.49e+00$   
Value: Yes

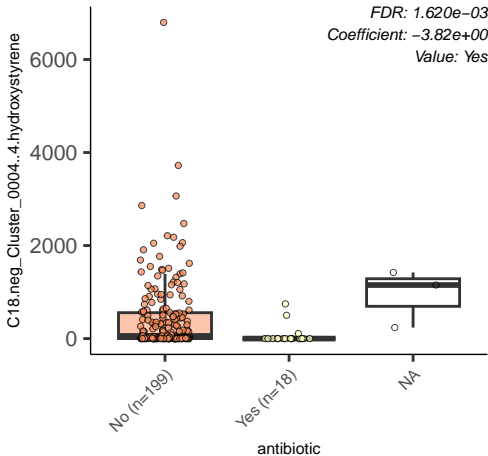
No (n=199)

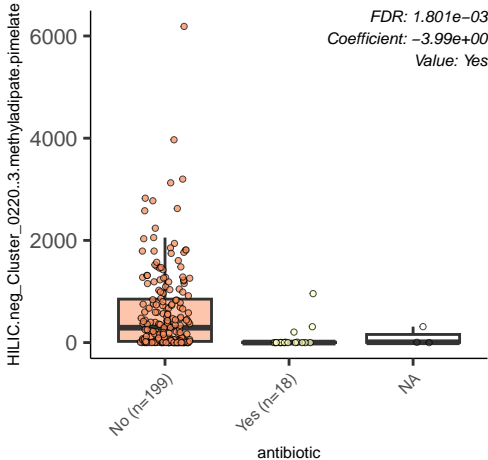
Yes (n=18)

NA

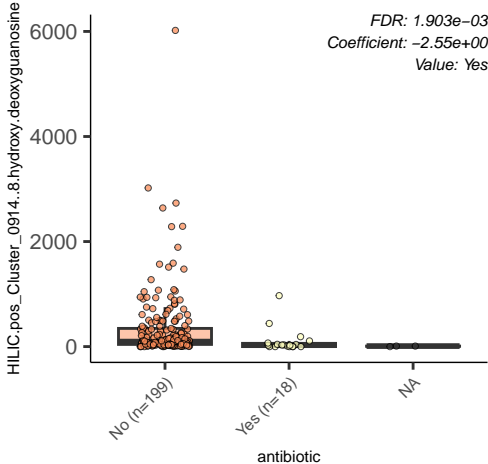
antibiotic











HILIC.neg\_Cluster\_1300...riboflavin

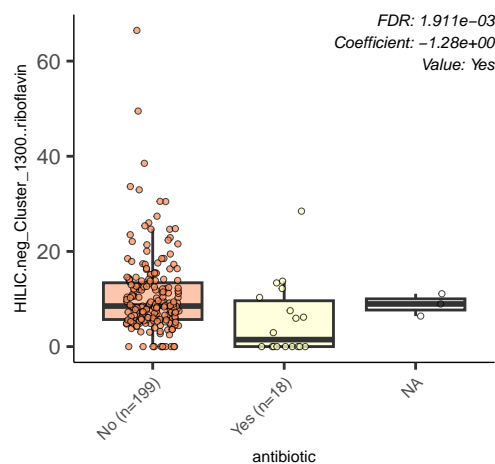
FDR:  $1.911e-03$   
Coefficient:  $-1.28e+00$   
Value: Yes

No (n=199)

Yes (n=18)

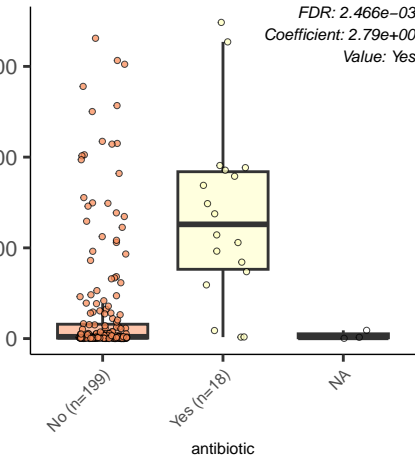
NA

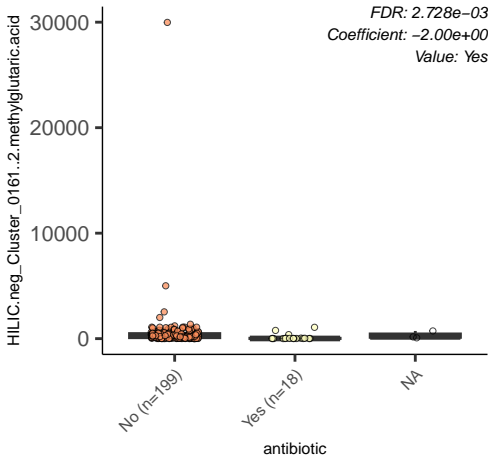
antibiotic



HILIC\_pos\_Cluster\_0090..creatine

FDR:  $2.466e-03$   
Coefficient:  $2.79e+00$   
Value: Yes





C18.neg\_Cluster\_1574..taurochenodesoxycholic.acid

FDR: 3.831e-03  
Coefficient: 3.16e+00  
Value: Yes

200000

150000

100000

50000

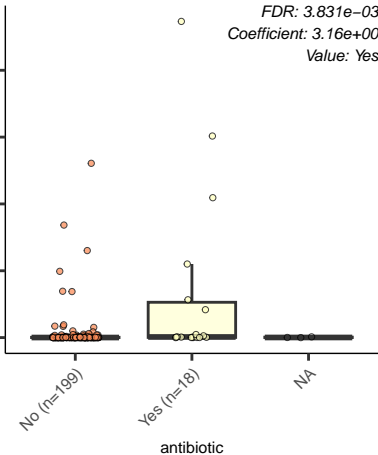
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos\_Cluster\_1017..sphinganine

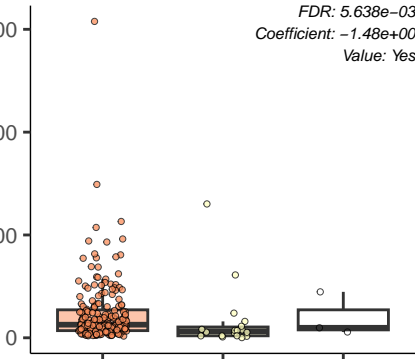
*FDR: 5.638e-03*  
*Coefficient: -1.48e+00*  
*Value: Yes*

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos\_Cluster\_0540..pantothenate

FDR: 6.785e-03  
Coefficient: -1.10e+00  
Value: Yes

10000

5000

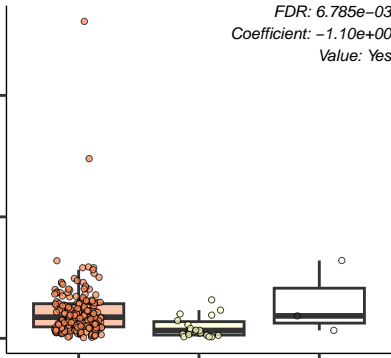
0

No (n=199)

Yes (n=18)

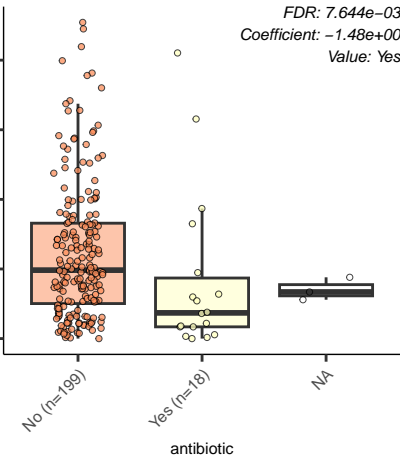
NA

antibiotic



HILIC.neg\_Cluster\_0003..propionate

FDR:  $7.644e-03$   
Coefficient:  $-1.48e+00$   
Value: Yes





HILIC\_pos\_Cluster\_0822..inosine

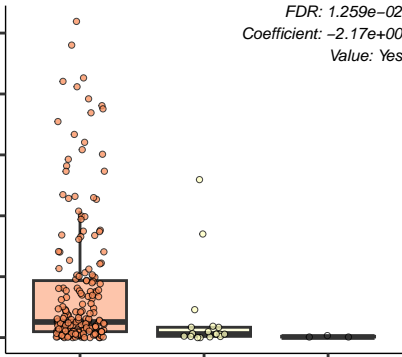
FDR: 1.259e-02  
Coefficient: -2.17e+00  
Value: Yes

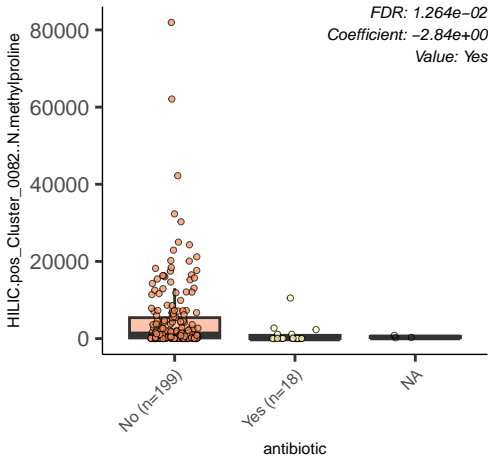
No (n=199)

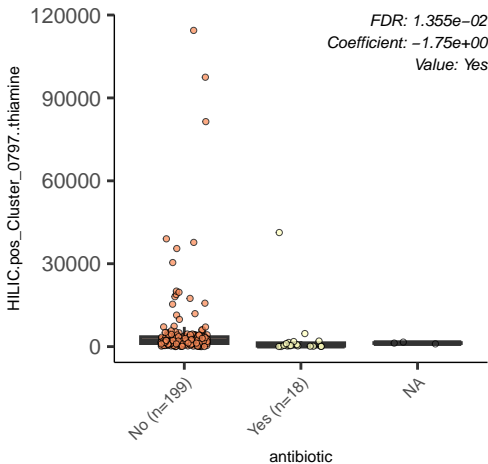
Yes (n=18)

NA

antibiotic

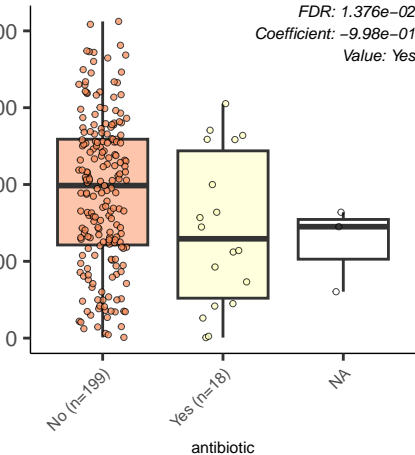






HILIC.neg\_Cluster\_0166..glutamate

*FDR: 1.376e-02*  
*Coefficient: -9.98e-01*  
*Value: Yes*



HILIC.neg\_Cluster\_0049..uracil

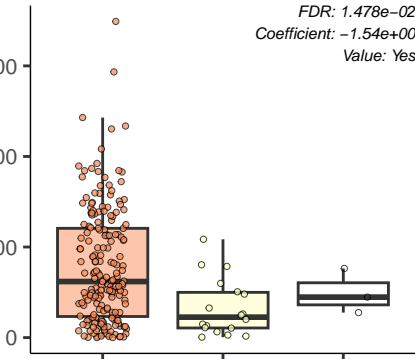
FDR:  $1.478e-02$   
Coefficient:  $-1.54e+00$   
Value: Yes

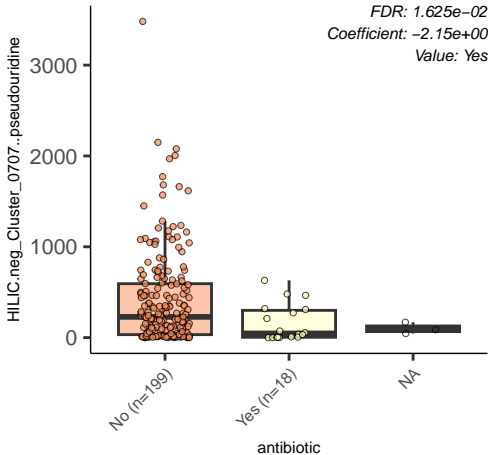
No (n=199)

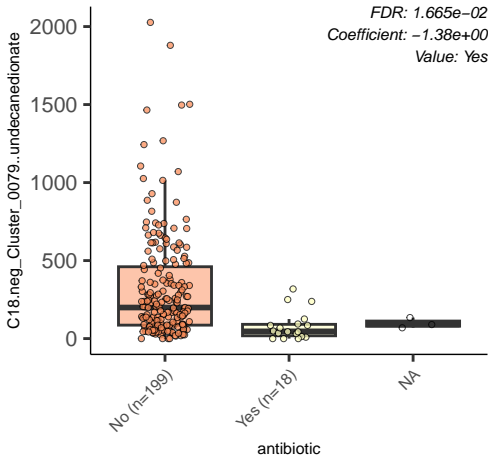
Yes (n=18)

NA

antibiotic







C8.pos\_Cluster\_0554..cholestenone

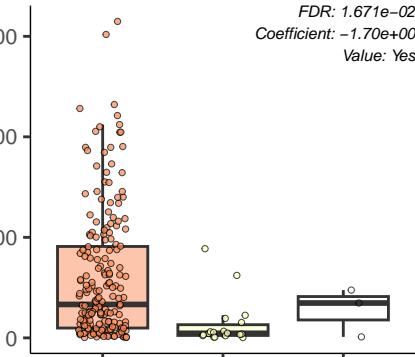
FDR: 1.671e-02  
Coefficient: -1.70e+00  
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic





C18.neg\_Cluster\_1722..cholate

FDR: 1.729e-02  
Coefficient: 2.06e+00  
Value: Yes

1000

500

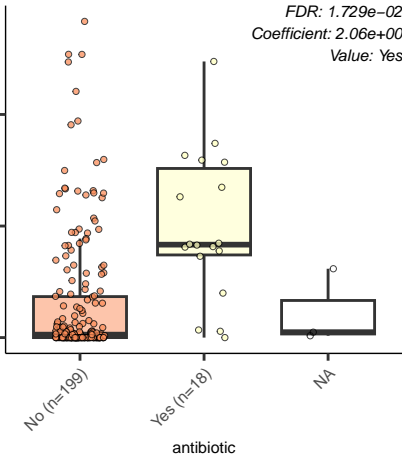
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos\_Cluster\_0048..betaine

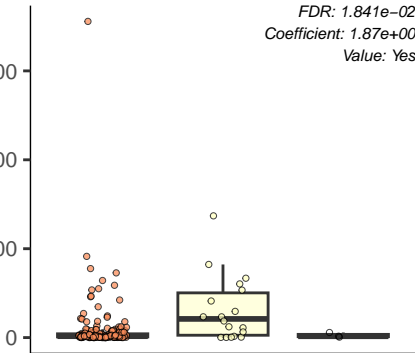
FDR: 1.841e-02  
Coefficient: 1.87e+00  
Value: Yes

No (n=199)

Yes (n=18)

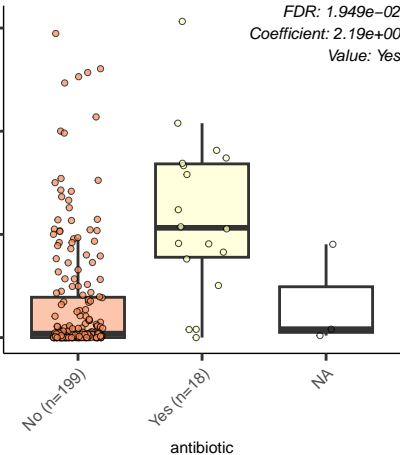
NA

antibiotic



C18.neg\_Cluster\_1178..cholate

*FDR: 1.949e-02*  
*Coefficient: 2.19e+00*  
*Value: Yes*



HILIC.neg\_Cluster\_0909..guanosine

*FDR: 1.984e-02*  
*Coefficient: -2.08e+00*  
*Value: Yes*

1500

1000

500

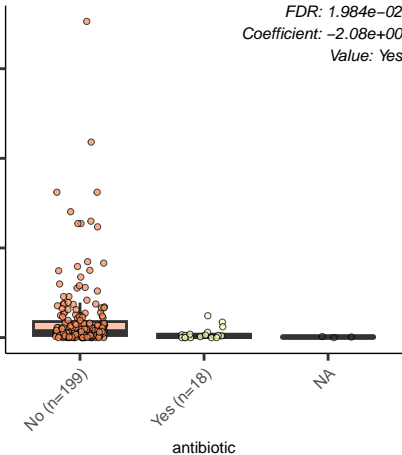
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.neg\_Cluster\_0176..xylose

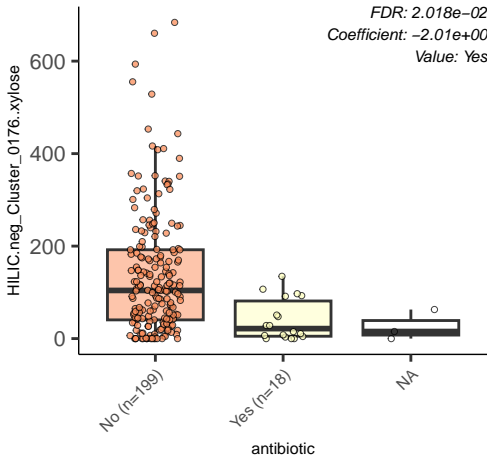
FDR: 2.018e-02  
Coefficient: -2.01e+00  
Value: Yes

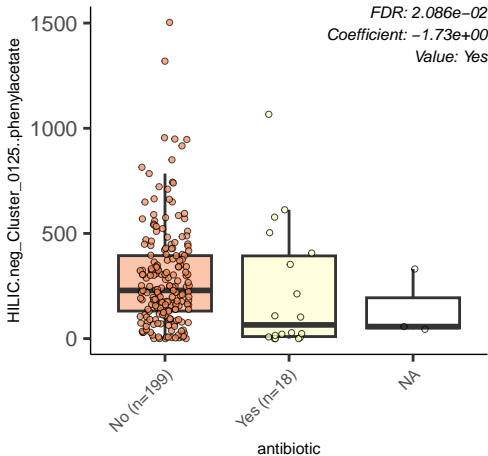
No (n=199)

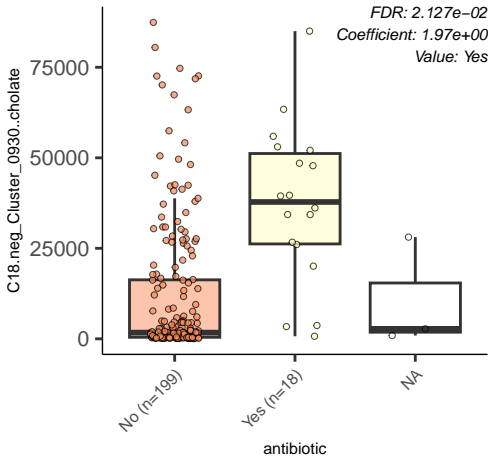
Yes (n=18)

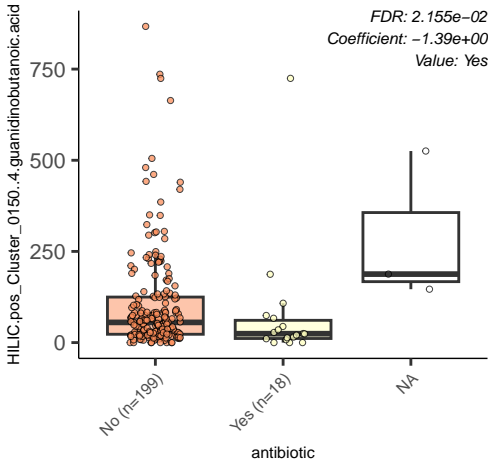
NA

antibiotic











C18.neg\_Cluster\_1621..cholate

FDR: 2.462e-02  
Coefficient: 2.19e+00  
Value: Yes

2000

1000

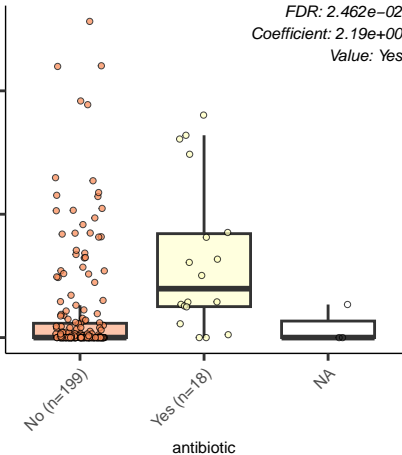
0

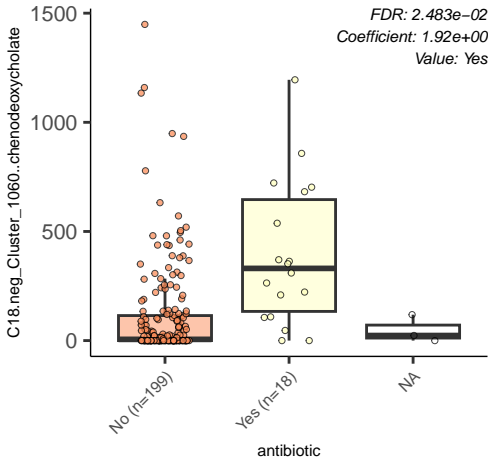
No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.pos\_Cluster\_0306..citruiline

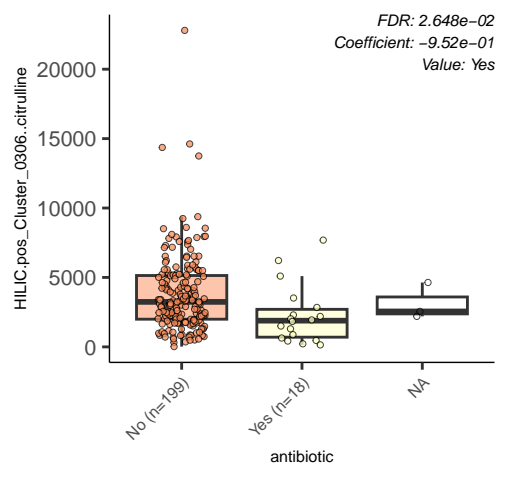
FDR: 2.648e-02  
Coefficient: -9.52e-01  
Value: Yes

No (n=199)

Yes (n=18)

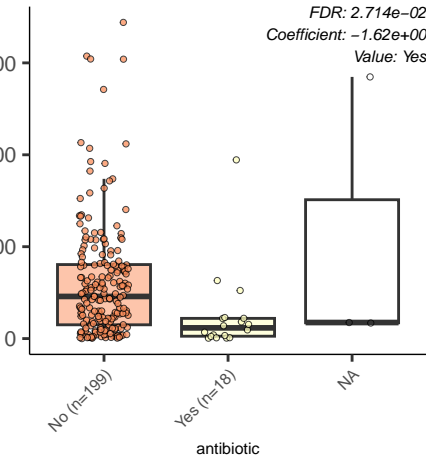
NA

antibiotic



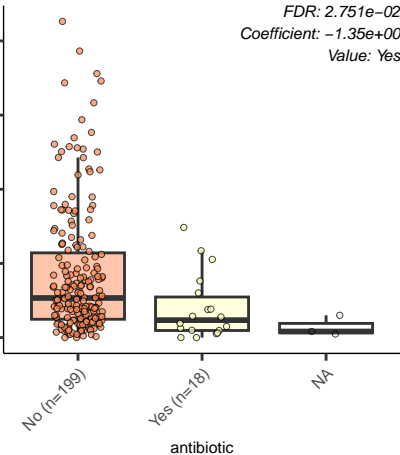
HILIC.pos\_Cluster\_0081..pipecolic.acid

FDR:  $2.714e-02$   
Coefficient:  $-1.62e+00$   
Value: Yes



HILIC.neg\_Cluster\_0706...uridine

FDR:  $2.751e-02$   
Coefficient:  $-1.35e+00$   
Value: Yes



C18.neg\_Cluster\_2021..urobilin

60000

40000

20000

0

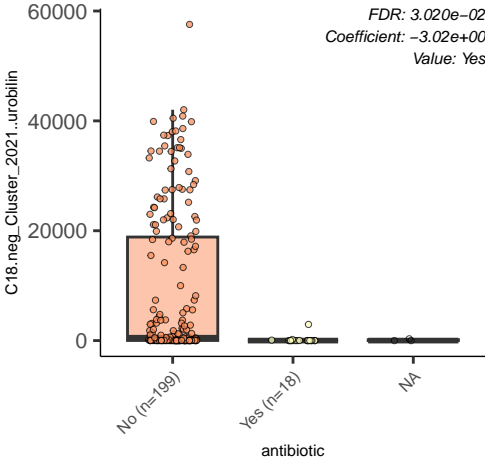
No (n=199)

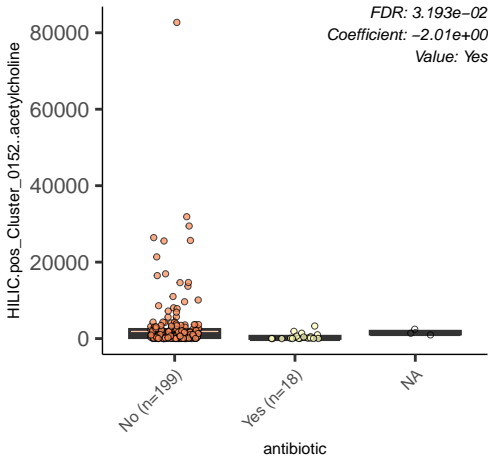
Yes (n=18)

NA

antibiotic

FDR:  $3.020e-02$   
Coefficient:  $-3.02e+00$   
Value: Yes





C18.neg\_Cluster\_1258..cholate

*FDR: 3.370e-02*  
*Coefficient: 1.88e+00*  
*Value: Yes*

1e+05

5e+04

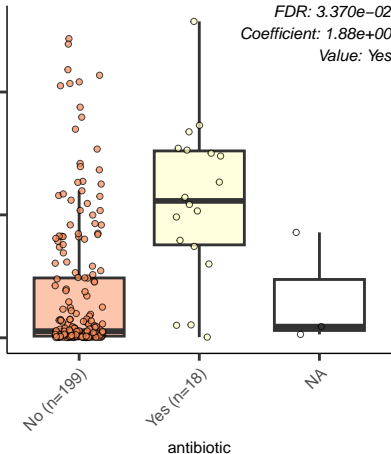
0e+00

No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.neg\_Cluster\_0441..sebacate

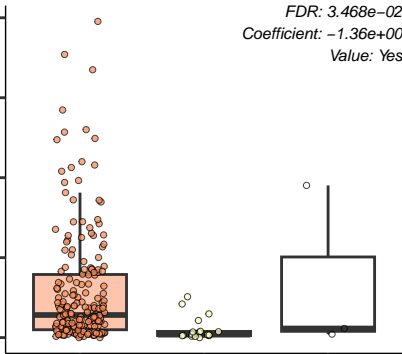
FDR: 3.468e-02  
Coefficient: -1.36e+00  
Value: Yes

No (n=199)

Yes (n=18)

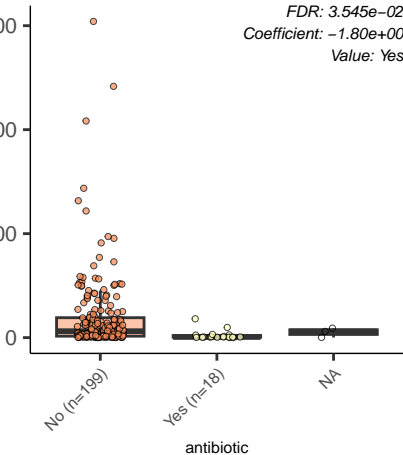
NA

antibiotic



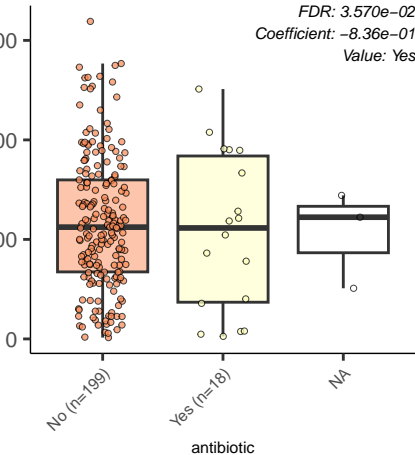
C8.pos\_Cluster\_0478..cholestenone

*FDR: 3.545e-02*  
*Coefficient: -1.80e+00*  
*Value: Yes*



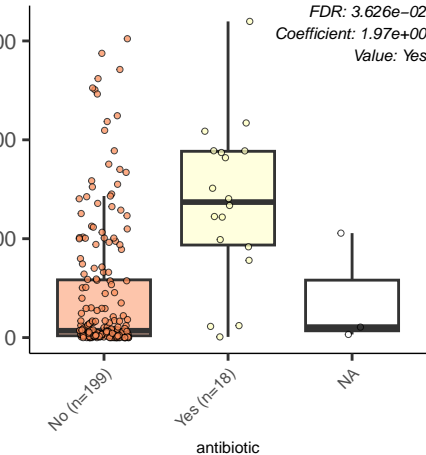
HILIC.neg\_Cluster\_0117.aspartate

FDR:  $3.570e-02$   
Coefficient:  $-8.36e-01$   
Value: Yes



C18.neg\_Cluster\_1273..cholate

*FDR: 3.626e-02*  
*Coefficient: 1.97e+00*  
*Value: Yes*



HILIC.neg\_Cluster\_0173..methionine

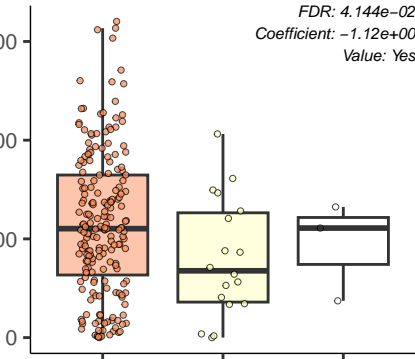
FDR:  $4.144e-02$   
Coefficient:  $-1.12e+00$   
Value: Yes

No (n=199)

Yes (n=18)

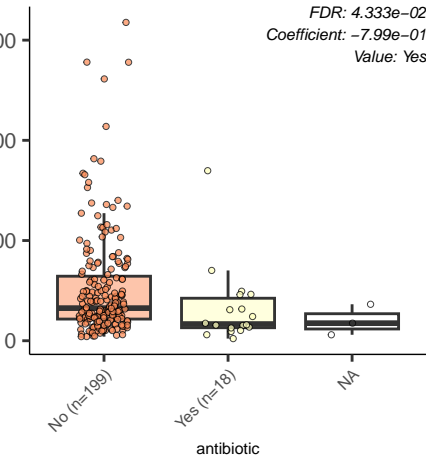
NA

antibiotic



HILIC.neg\_Cluster\_0036..glycerate

FDR:  $4.333\text{e-}02$   
Coefficient:  $-7.99\text{e-}01$   
Value: Yes



HILIC.neg\_Cluster\_0288..suberate

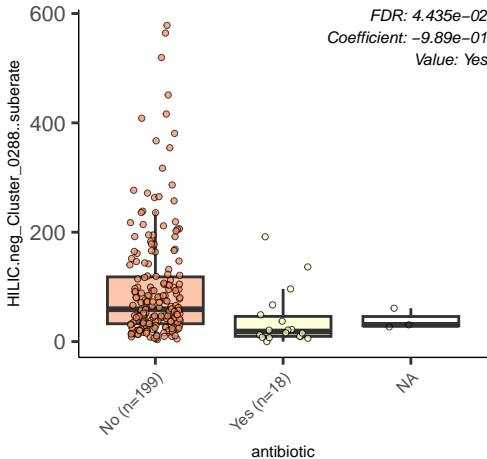
*FDR: 4.435e-02*  
*Coefficient: -9.89e-01*  
*Value: Yes*

No (n=199)

Yes (n=18)

NA

antibiotic



C18.neg\_Cluster\_1372..cholate

FDR: 4.436e-02  
Coefficient: 2.14e+00  
Value: Yes

2000

1000

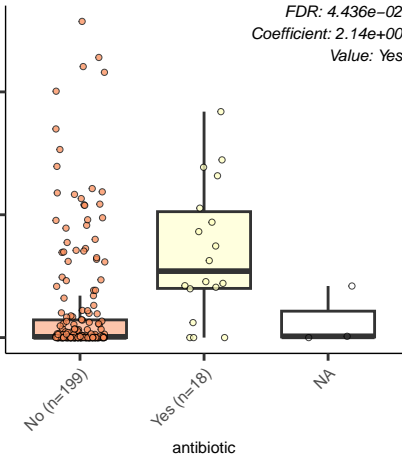
0

No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.pos\_Cluster\_2093..urobilin.

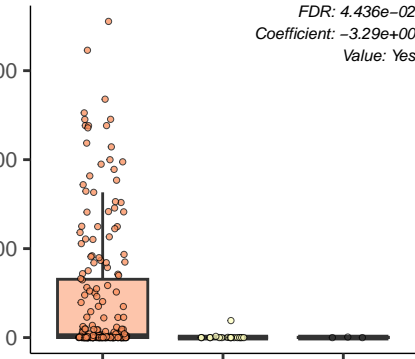
FDR:  $4.436e-02$   
Coefficient:  $-3.29e+00$   
Value: Yes

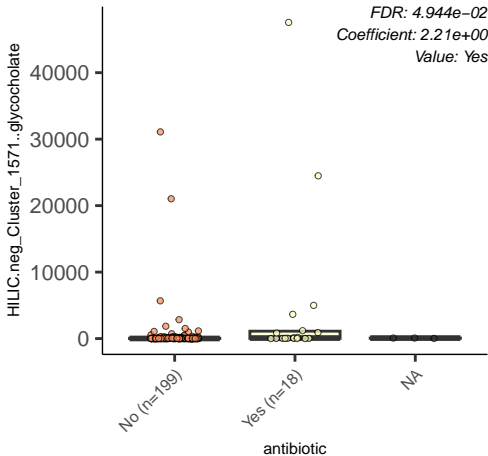
No (n=199)

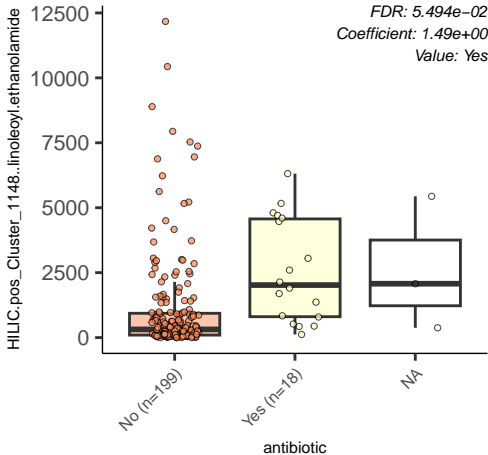
Yes (n=18)

NA

antibiotic









C18.neg\_Cluster\_0045..azelate

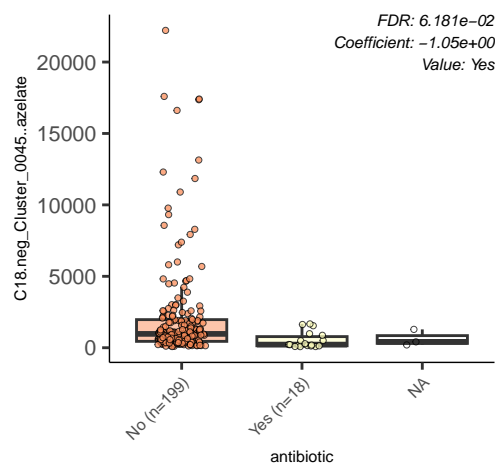
FDR: 6.181e-02  
Coefficient: -1.05e+00  
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos\_Cluster\_0295..arginine

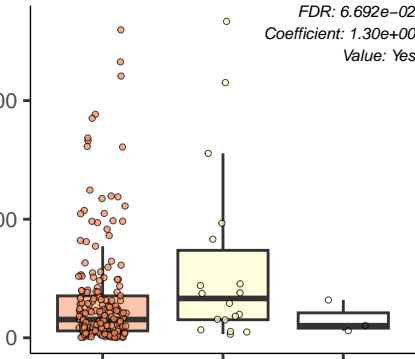
FDR: 6.692e-02  
Coefficient: 1.30e+00  
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos\_Cluster\_0036..creatinine

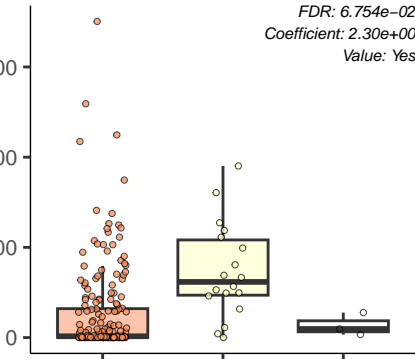
FDR:  $6.754e-02$   
Coefficient:  $2.30e+00$   
Value: Yes

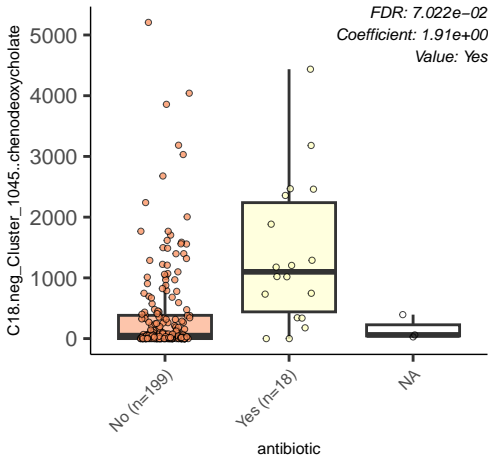
No (n=199)

Yes (n=18)

NA

antibiotic







HILIC\_pos\_Cluster\_0167..methionine

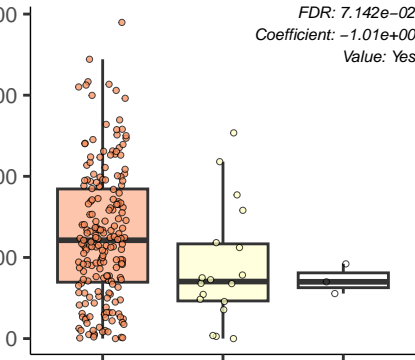
FDR:  $7.142e-02$   
Coefficient:  $-1.01e+00$   
Value: Yes

No (n=199)

Yes (n=18)

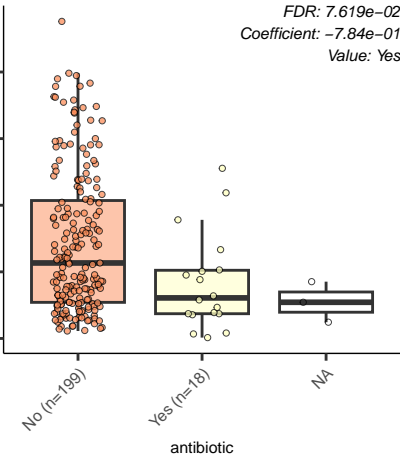
NA

antibiotic



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

FDR:  $7.619\text{e-}02$   
Coefficient:  $-7.84\text{e-}01$   
Value: Yes



HILIC.pos\_Cluster\_2052...bilirubin

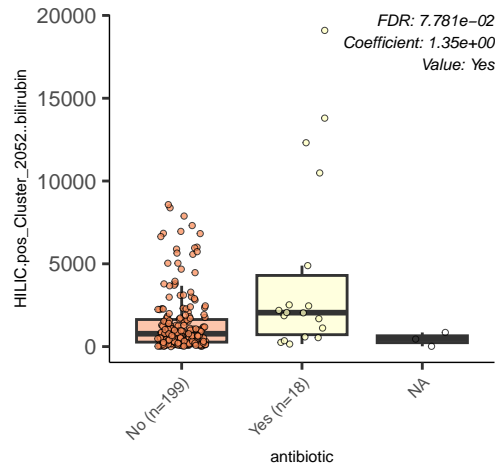
*FDR: 7.781e-02*  
*Coefficient: 1.35e+00*  
*Value: Yes*

No (n=199)

Yes (n=18)

NA

antibiotic



C8.pos\_Cluster\_1900..cholestenone

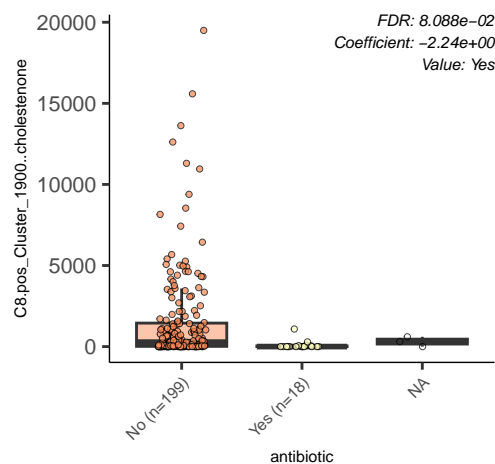
FDR: 8.088e-02  
Coefficient: -2.24e+00  
Value: Yes

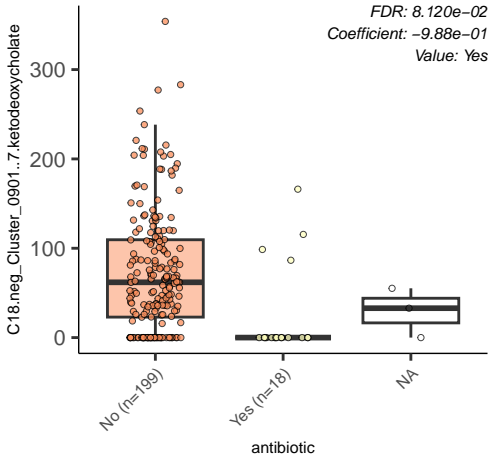
No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.neg\_Cluster\_0365..azelaic.acid

FDR:  $8.120e-02$   
Coefficient:  $-1.00e+00$   
Value: Yes

3000

2000

1000

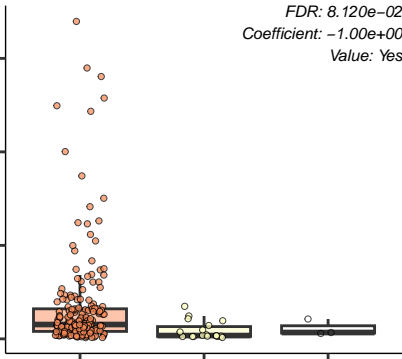
0

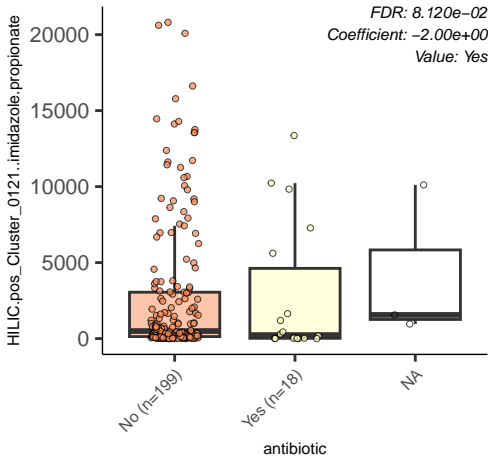
No (n=199)

Yes (n=18)

NA

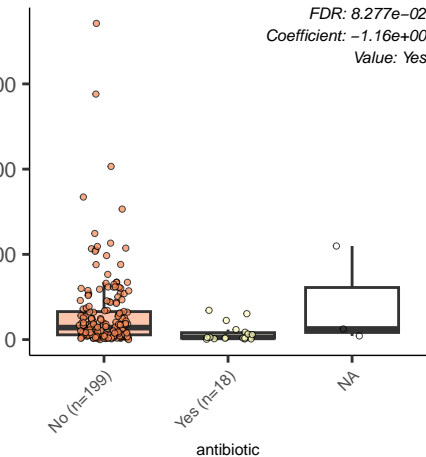
antibiotic





C18.neg\_Cluster\_0064..sebacate

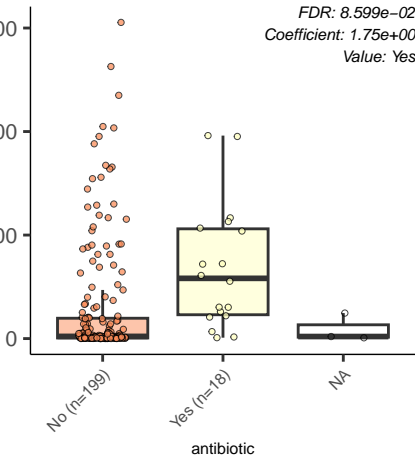
FDR:  $8.277e-02$   
Coefficient:  $-1.16e+00$   
Value: Yes





HILIC.neg\_Cluster\_1403..cholate

FDR:  $8.599e-02$   
Coefficient:  $1.75e+00$   
Value: Yes



HILIC.neg\_Cluster\_0677..cystine

FDR: 8.892e-02  
Coefficient: 1.57e+00  
Value: Yes

4000

3000

2000

1000

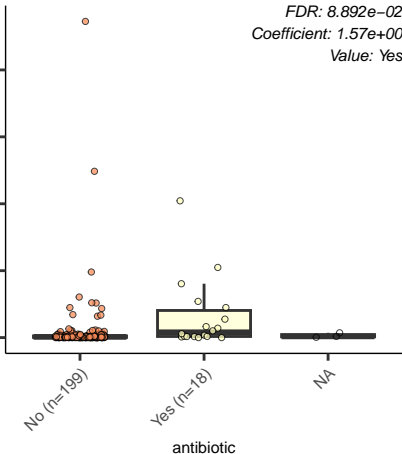
0

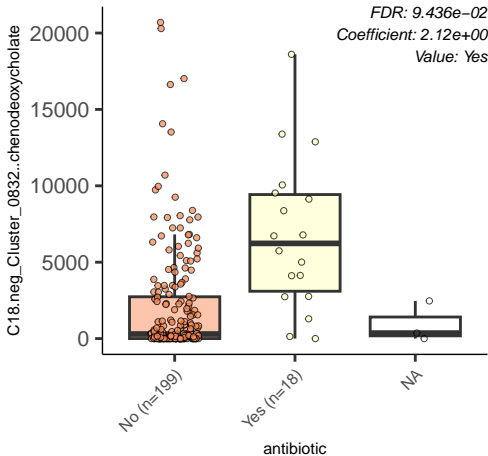
No (n=199)

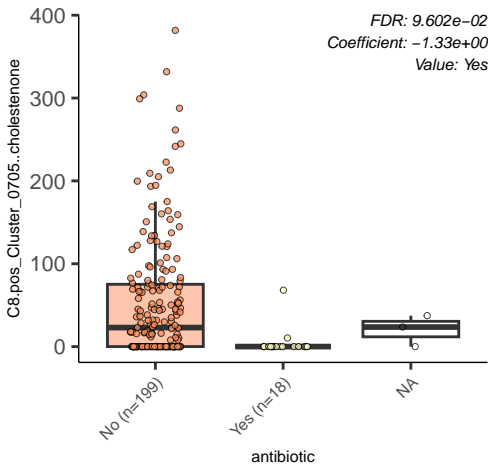
Yes (n=18)

NA

antibiotic

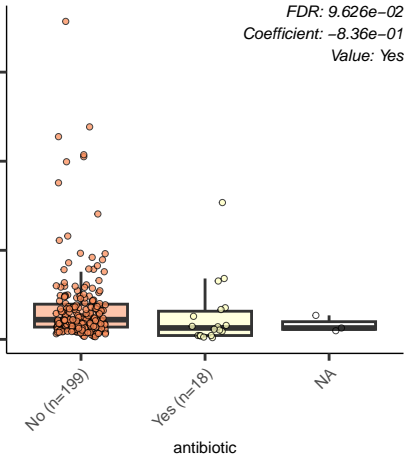




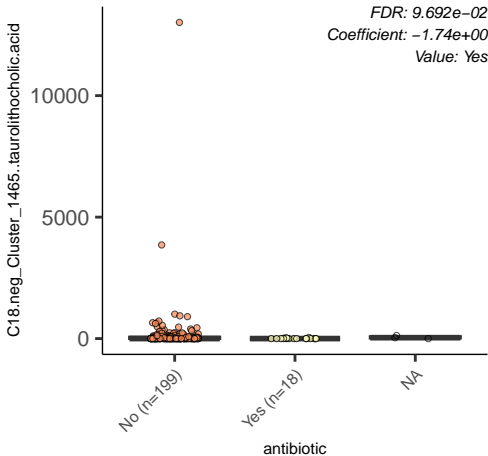


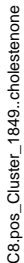
HILIC.neg\_Cluster\_0079...4.hydroxybenzaldehyde

FDR:  $9.626e-02$   
Coefficient:  $-8.36e-01$   
Value: Yes



antibiotic

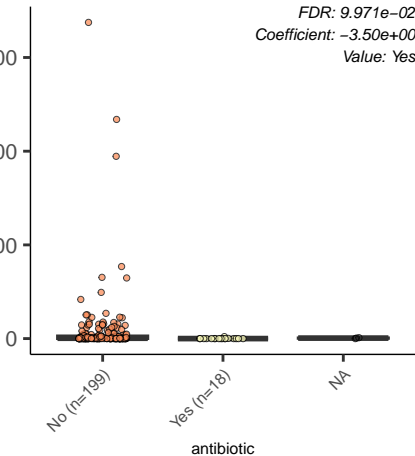


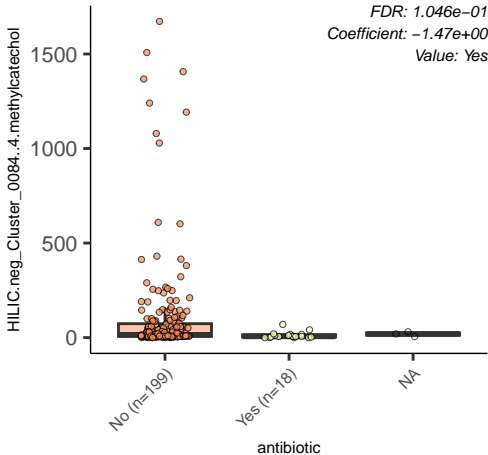


*FDR: 9.971e-02*

Coefficient:  $-3.50e+00$

Value: Yes







HILIC.pos\_Cluster\_0113..trigonelline

FDR: 1.049e-01  
Coefficient: -1.47e+00  
Value: Yes

20000

10000

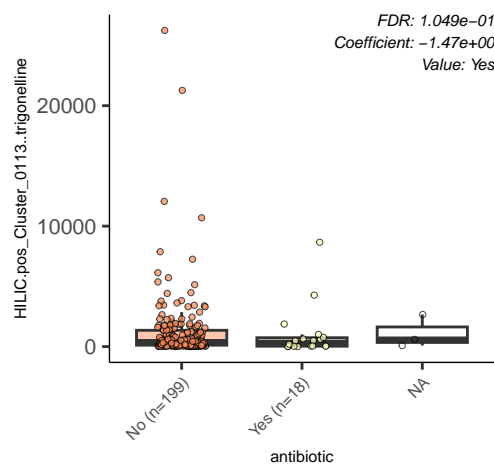
0

No (n=199)

Yes (n=18)

NA

antibiotic



C18.neg\_Cluster\_1081..glycolithocholic.acid

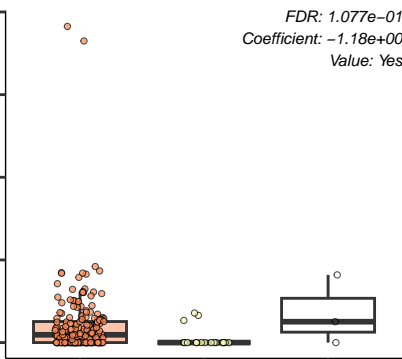
*FDR: 1.077e-01*  
*Coefficient: -1.18e+00*  
*Value: Yes*

No (n=199)

Yes (n=18)

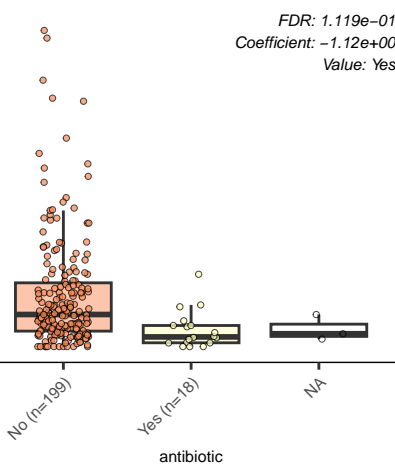
NA

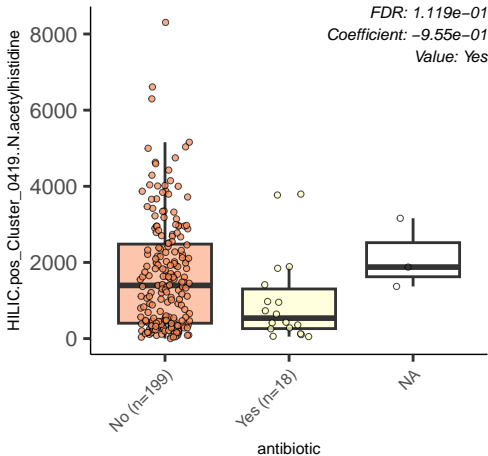
antibiotic



ILIC.neg.Cluster\_0622...1.2.3.4.tetrahydro.1.methyl.beta.carboline.3

FDR: 1.119e-01  
Coefficient: -1.12e+00  
Value: Yes





HILIC.neg\_Cluster\_0332...saccharin

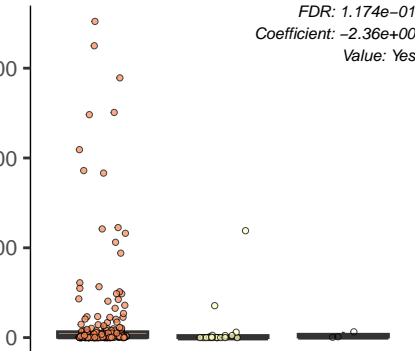
FDR: 1.174e-01  
Coefficient: -2.36e+00  
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



C18.neg\_Cluster\_0486..carnosol

FDR:  $1.184e-01$   
Coefficient:  $-1.76e+00$   
Value: Yes

7500

5000

2500

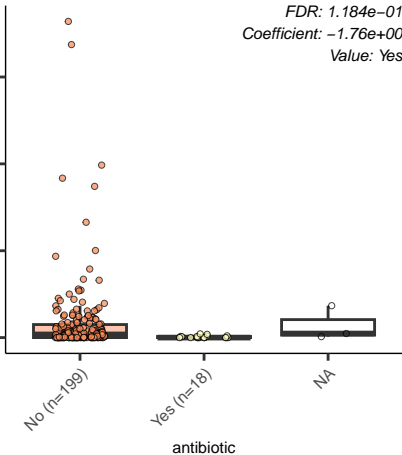
0

No (n=199)

Yes (n=18)

NA

antibiotic



C8.pos\_Cluster\_0629..cholestenone

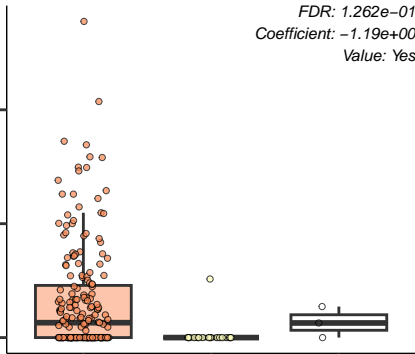
FDR: 1.262e-01  
Coefficient: -1.19e+00  
Value: Yes

No (n=199)

Yes (n=18)

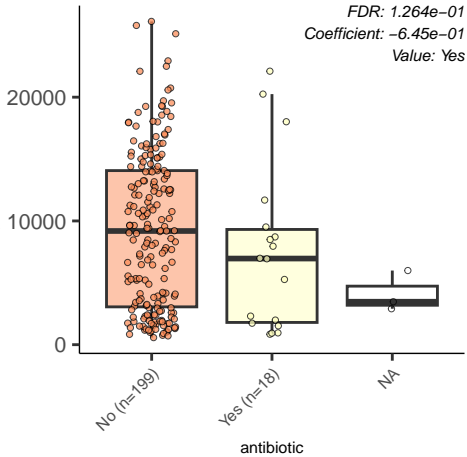
NA

antibiotic

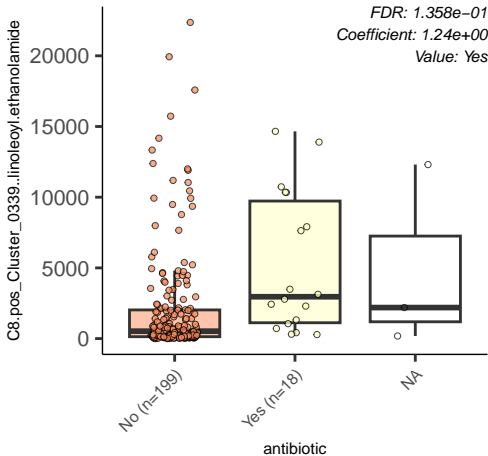


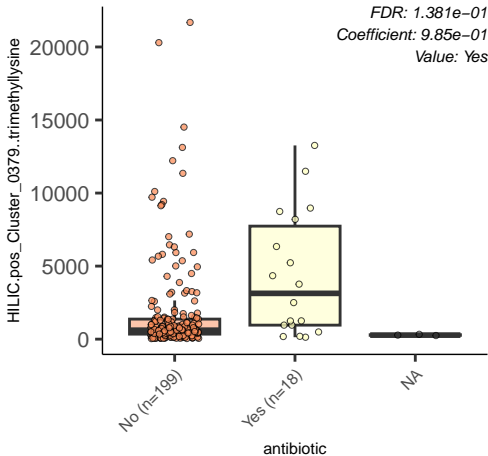
HILIC.neg\_Cluster\_0118..malate

FDR: 1.264e-01  
Coefficient: -6.45e-01  
Value: Yes



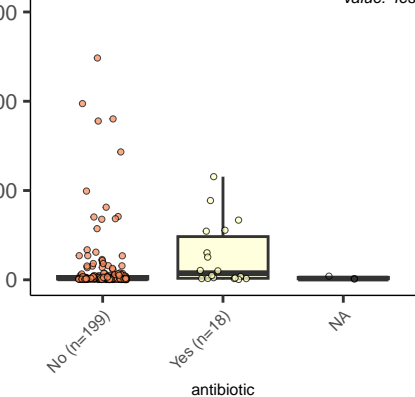






HILIC.neg\_Cluster\_0020..lactate

FDR: 1.512e-01  
Coefficient: 1.14e+00  
Value: Yes



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

FDR: 1.520e-01  
Coefficient: -1.95e+00  
Value: Yes

400

200

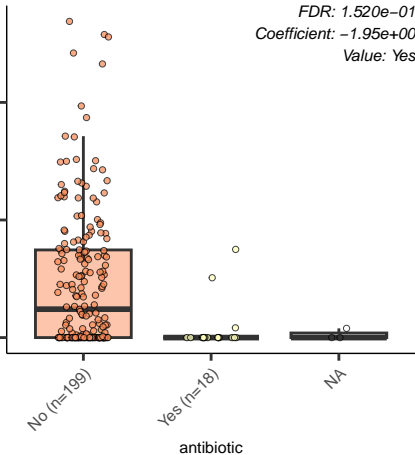
0

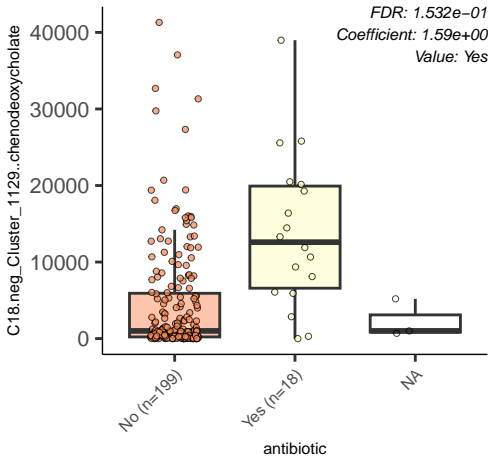
No (n=199)

Yes (n=18)

NA

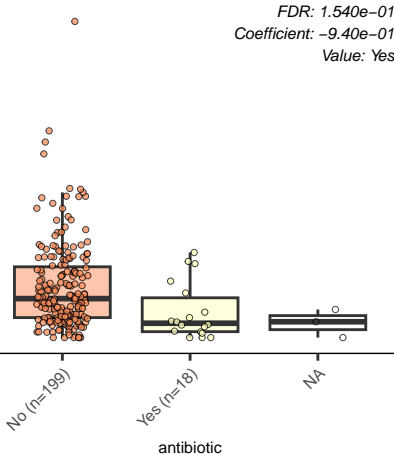
antibiotic





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

FDR: 1.540e-01  
Coefficient: -9.40e-01  
Value: Yes



HILIC.neg\_Cluster\_0392...citrate

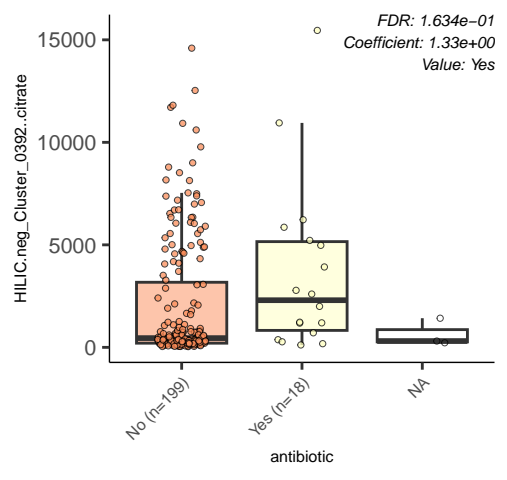
FDR: 1.634e-01  
Coefficient: 1.33e+00  
Value: Yes

No (n=199)

Yes (n=18)

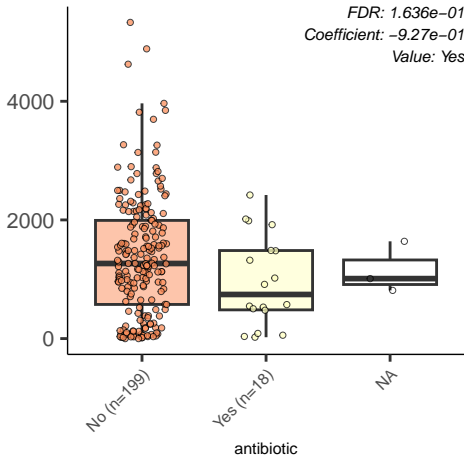
NA

antibiotic



HILIC.neg\_Cluster\_0035..serine

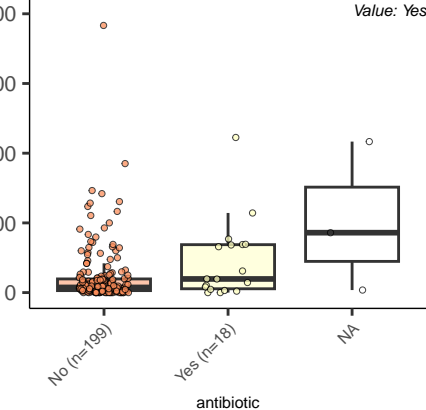
FDR:  $1.636e-01$   
Coefficient:  $-9.27e-01$   
Value: Yes

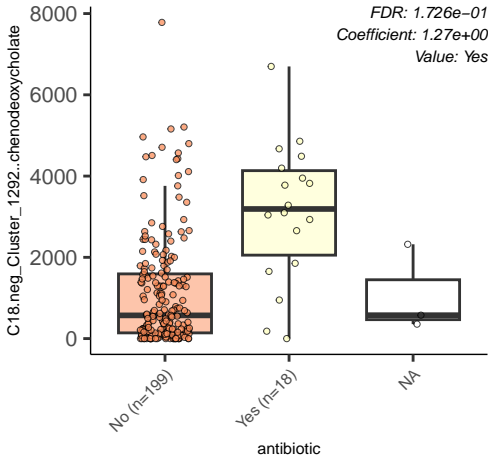




HILIC.pos\_Cluster\_0032...cytosine

FDR: 1.707e-01  
Coefficient: 1.32e+00  
Value: Yes





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

FDR: 1.729e-01  
Coefficient: 1.46e+00  
Value: Yes

2000

1000

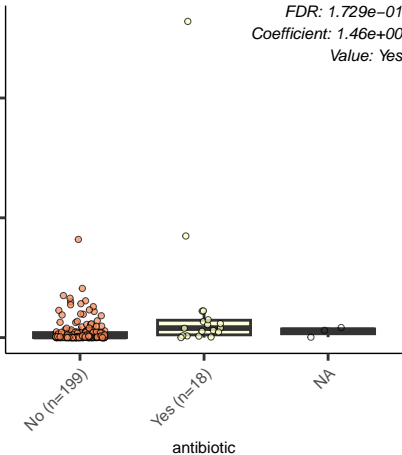
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.neg\_Cluster\_0192..ribitol

*FDR: 1.747e-01*  
*Coefficient: 7.07e-01*  
*Value: Yes*

1000

500

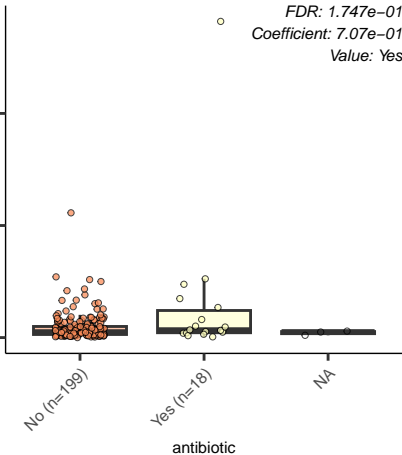
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.neg\_Cluster\_0740...deoxyinosine

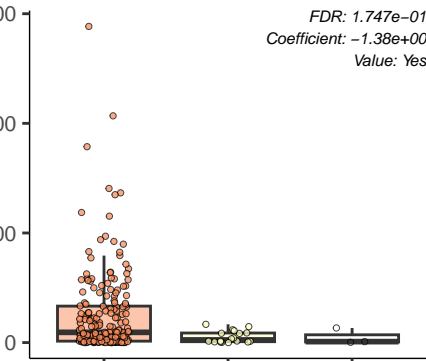
FDR: 1.747e-01  
Coefficient: -1.38e+00  
Value: Yes

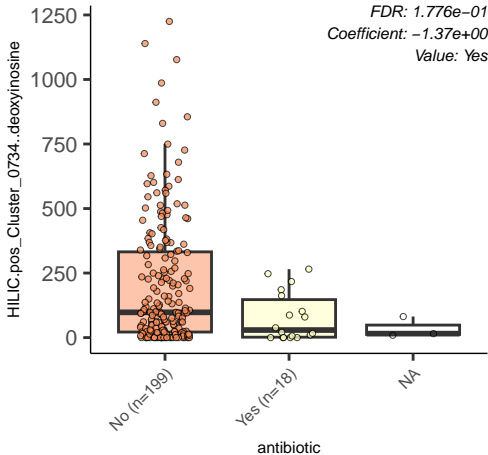
No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.neg\_Cluster\_0062...alpha.ketoisovalerate

FDR: 1.790e-01  
Coefficient: -1.18e+00  
Value: Yes

2000

1000

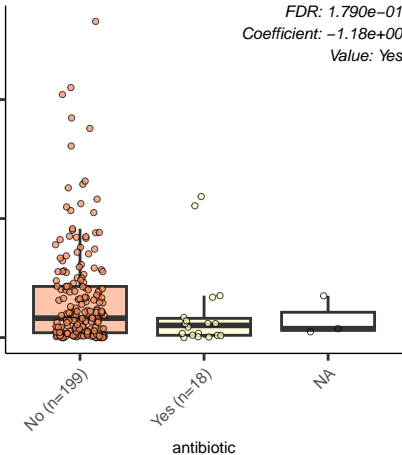
0

No (n=199)

Yes (n=18)

NA

antibiotic



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

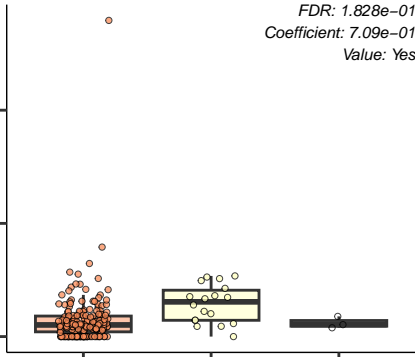
FDR: 1.828e-01  
Coefficient: 7.09e-01  
Value: Yes

No (n=199)

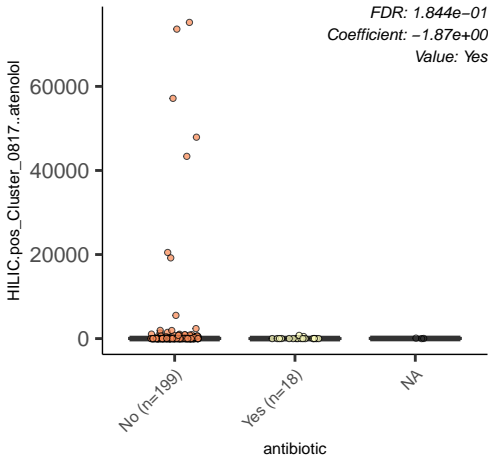
Yes (n=18)

NA

antibiotic







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

FDR:  $2.074e-01$   
Coefficient:  $-1.45e+00$   
Value: Yes

1000

500

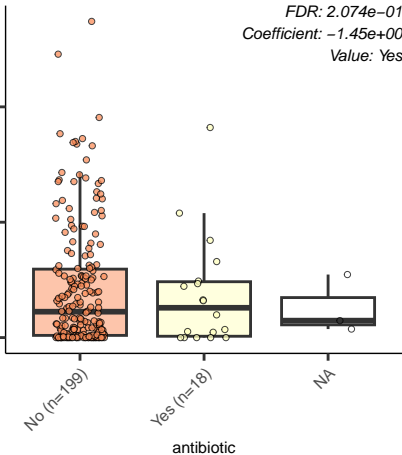
0

No (n=199)

Yes (n=18)

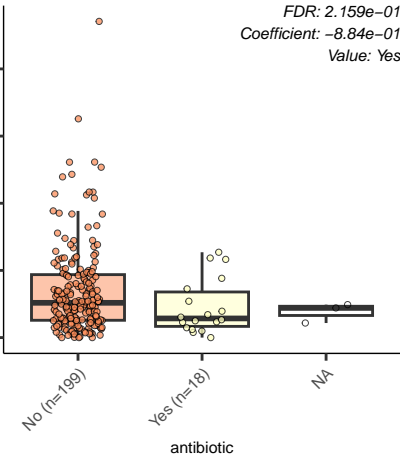
NA

antibiotic



C18.neg\_Cluster\_0394...9.10.diHOME

FDR:  $2.159e-01$   
Coefficient:  $-8.84e-01$   
Value: Yes



C18.neg\_Cluster\_1596..oleanolic.acid

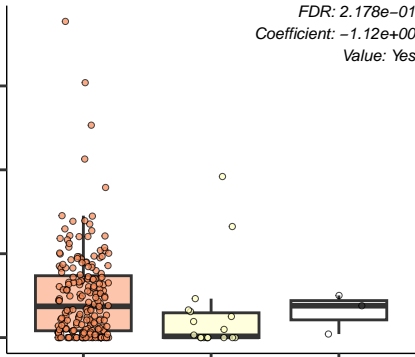
FDR: 2.178e-01  
Coefficient: -1.12e+00  
Value: Yes

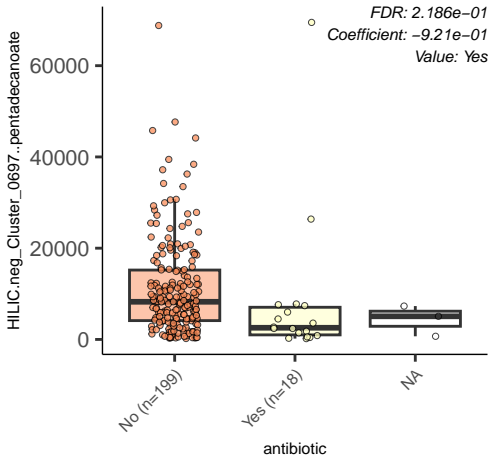
No (n=199)

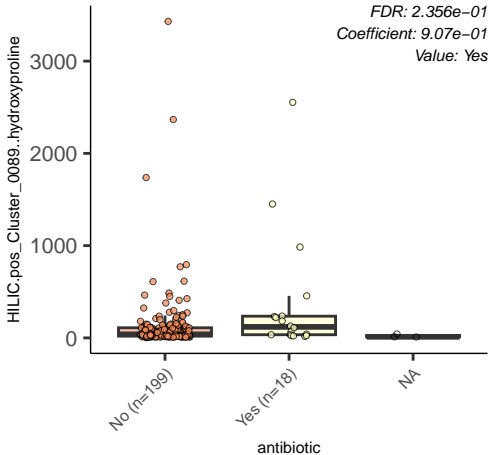
Yes (n=18)

NA

antibiotic

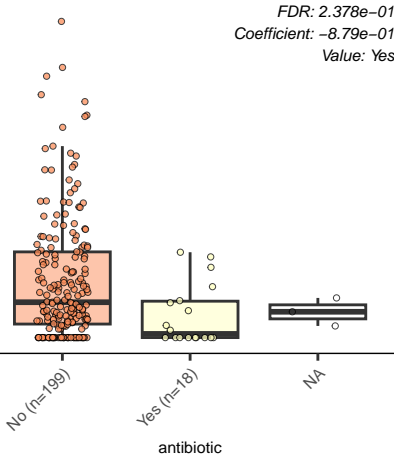






C18.neg.Cluster\_0183...1.2.3.4.tetrahydro.b.carboline.1.3.dicarb

FDR:  $2.378e-01$   
Coefficient:  $-8.79e-01$   
Value: Yes



HILIC.neg\_Cluster\_0182..guanine

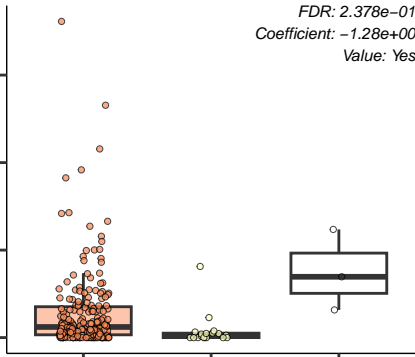
FDR: 2.378e-01  
Coefficient: -1.28e+00  
Value: Yes

No (n=199)

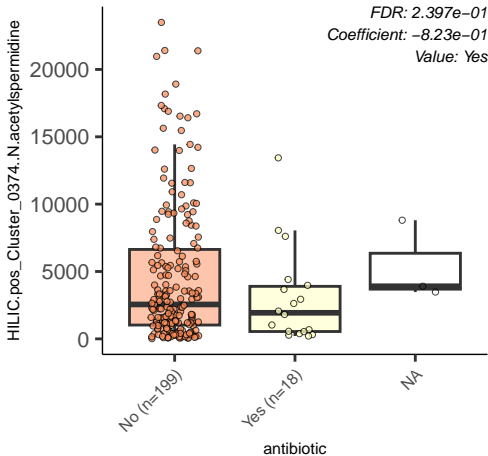
Yes (n=18)

NA

antibiotic

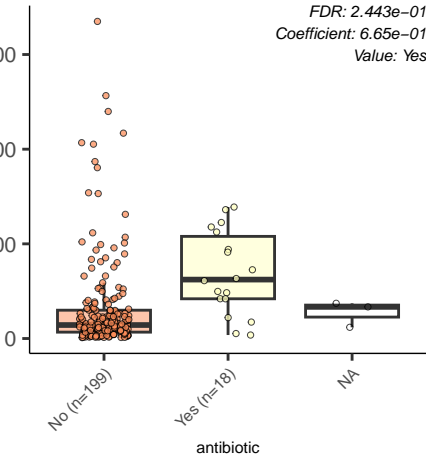






HILIC.pos\_Cluster\_0447..ADMA

FDR: 2.443e-01  
Coefficient: 6.65e-01  
Value: Yes



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

FDR: 2.493e-01  
Coefficient: -7.31e-01  
Value: Yes

