

HILIC.neg_Cluster_1303..lithocholate

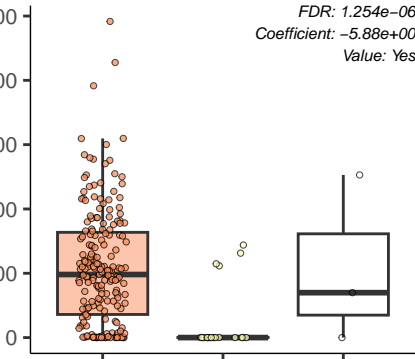
FDR: $1.254e-06$
Coefficient: $-5.88e+00$
Value: Yes

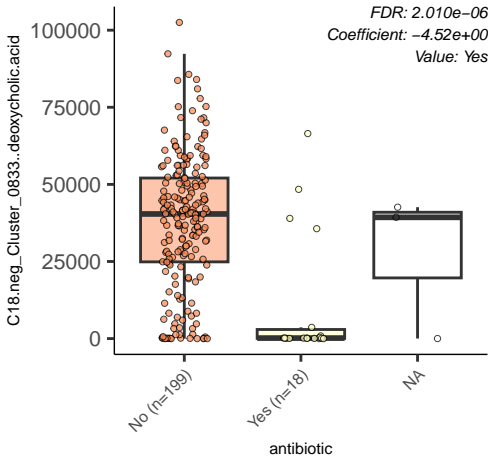
No (n=199)

Yes (n=18)

NA

antibiotic





C18.neg_Cluster_0731..lithocholic.acid

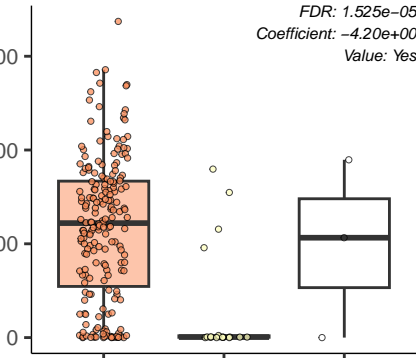
FDR: 1.525e-05
Coefficient: -4.20e+00
Value: Yes

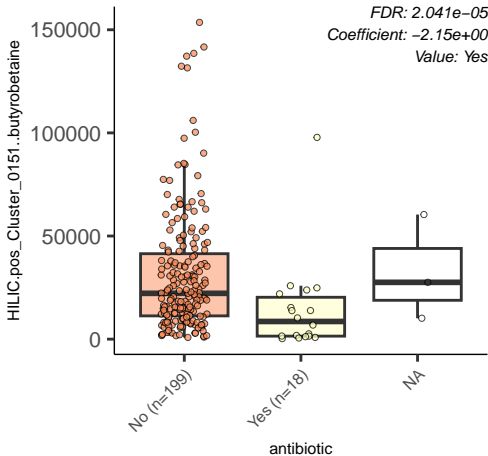
No (n=199)

Yes (n=18)

NA

antibiotic





C18.neg_Cluster_0031..phenyllactate

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

$1e+05$

$5e+04$

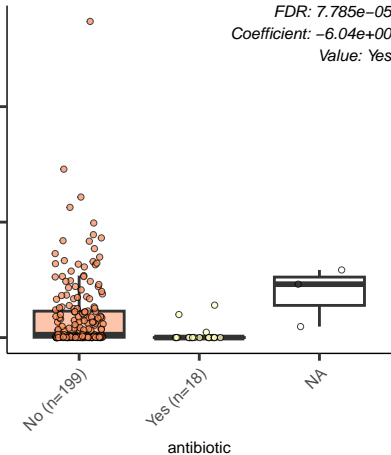
$0e+00$

No (n=199)

Yes (n=18)

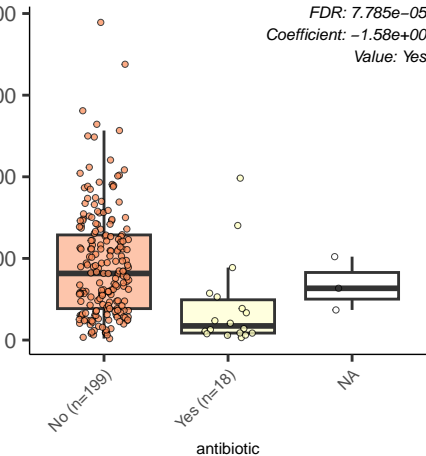
NA

antibiotic



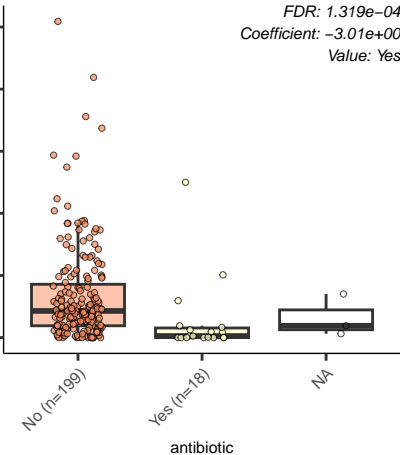
HILIC.neg_Cluster_0082..nicotinate

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



HILIC.neg_Cluster_0401..glucurorate

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



HILIC.neg_Cluster_0824..inosine

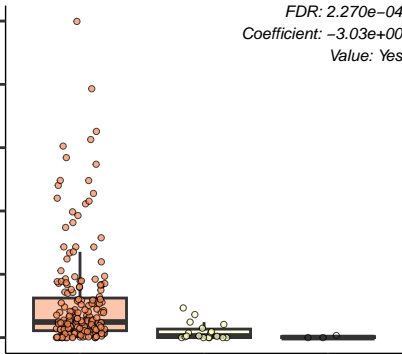
FDR: 2.270e-04
Coefficient: -3.03e+00
Value: Yes

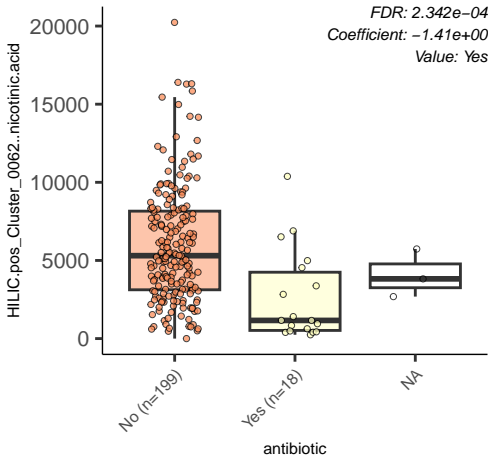
No (n=199)

Yes (n=18)

NA

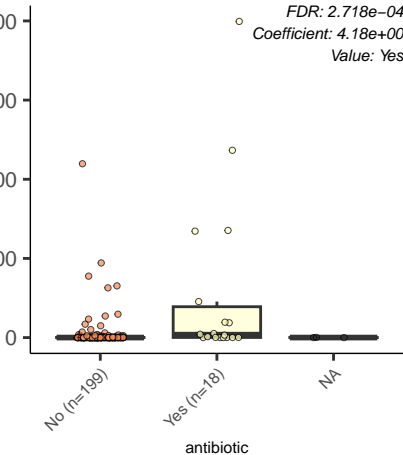
antibiotic

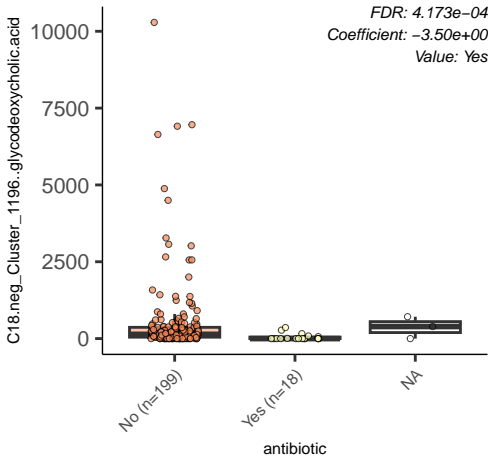




HILIC_pos_Cluster_0453..C2.carnitine

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





HILIC_pos_Cluster_0108..hypoxanthine

FDR: $4.173e-04$
Coefficient: $-1.39e+00$
Value: Yes

100000

75000

50000

25000

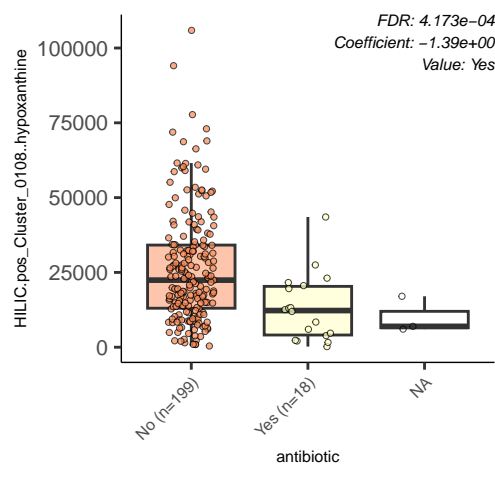
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.neg_Cluster_0187..xanthine

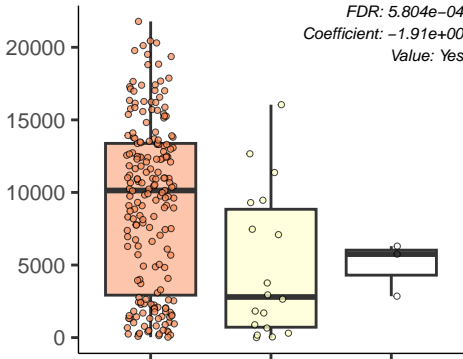
FDR: 5.804e-04
Coefficient: -1.91e+00
Value: Yes

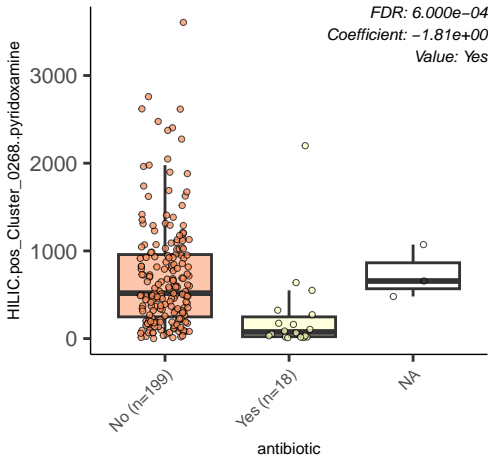
No (n=199)

Yes (n=18)

NA

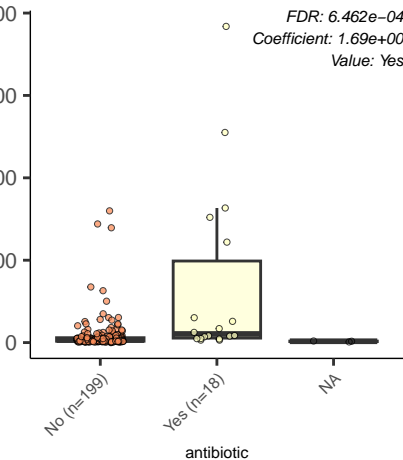
antibiotic





HILIC.pos_Cluster_0230..carnitine

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



HILIC_pos_Cluster_0184..pyridoxamine

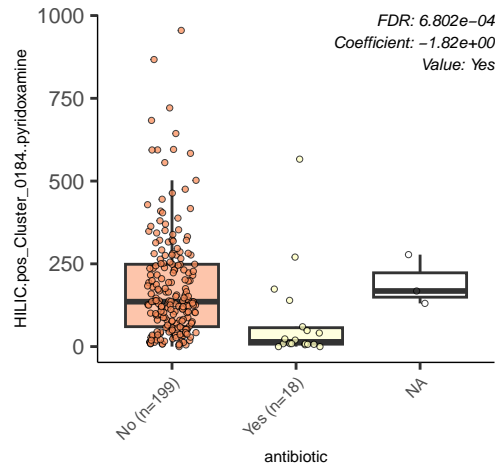
FDR: $6.802e-04$
Coefficient: $-1.82e+00$
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.neg_Cluster_0296..citrulline

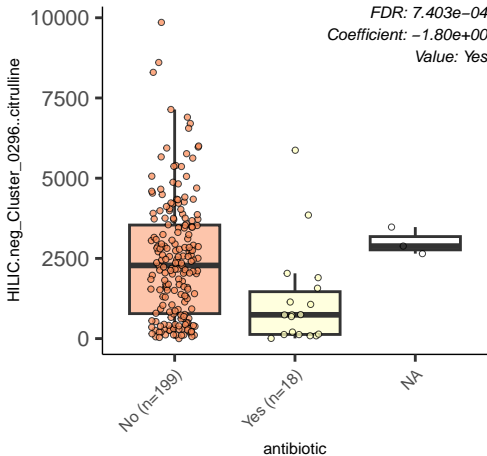
FDR: $7.403e-04$
Coefficient: $-1.80e+00$
Value: Yes

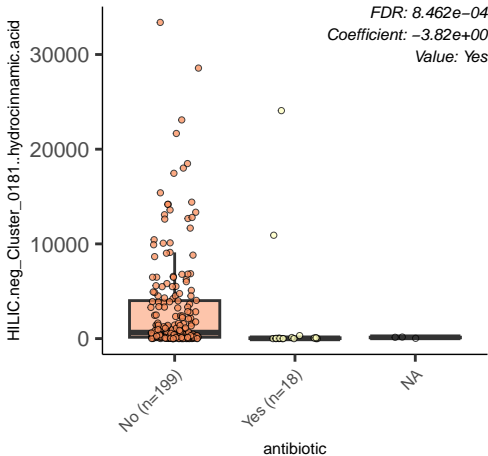
No (n=199)

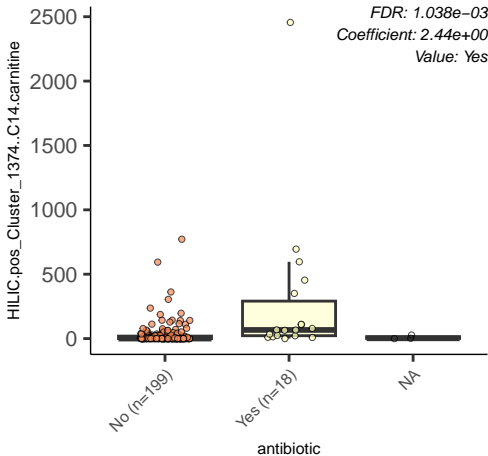
Yes (n=18)

NA

antibiotic







HILIC.neg_Cluster_0299..ascorbate

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

20000

10000

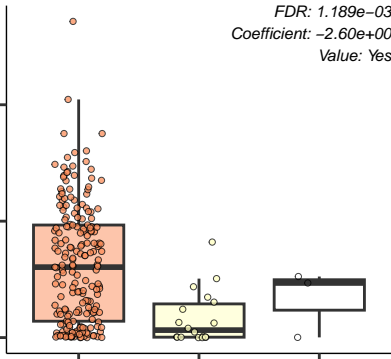
0

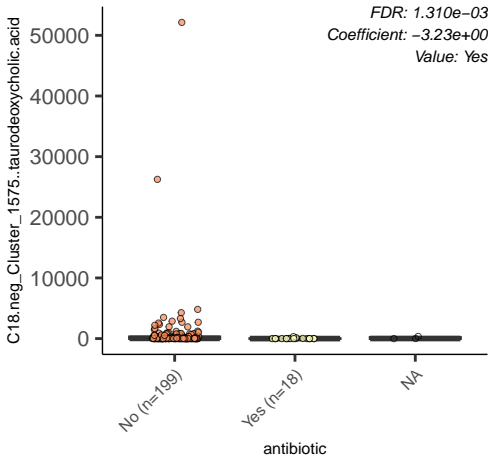
No (n=199)

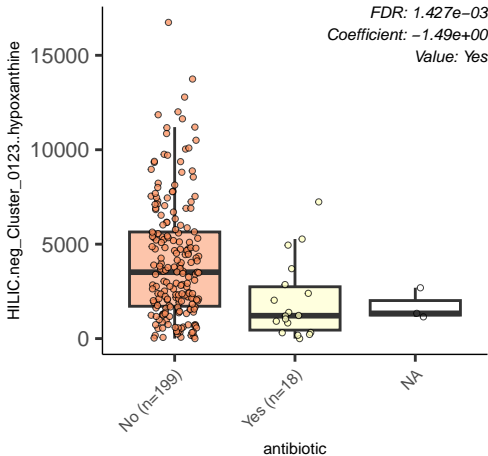
Yes (n=18)

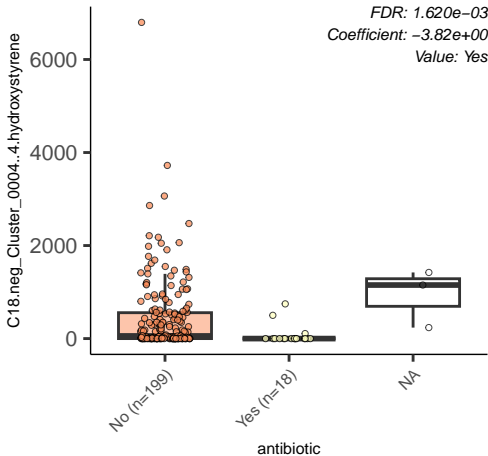
NA

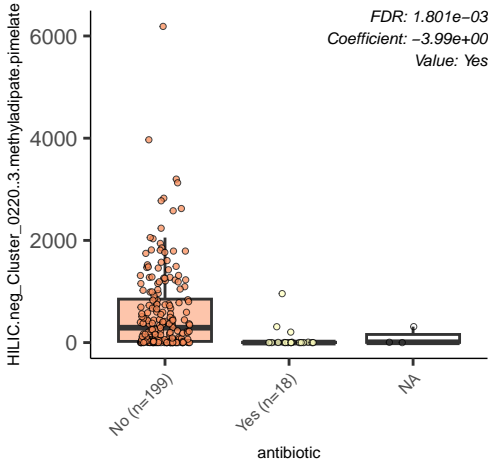
antibiotic

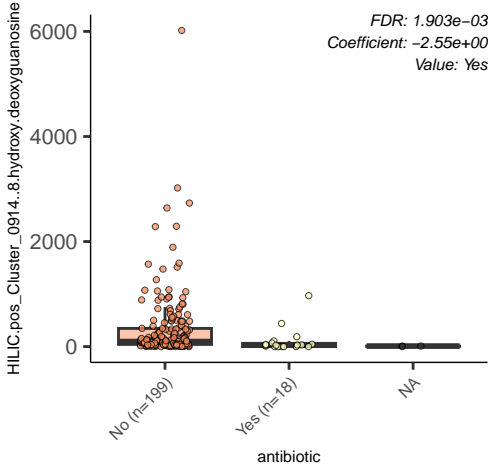












HILIC.neg_Cluster_1300...riboflavin

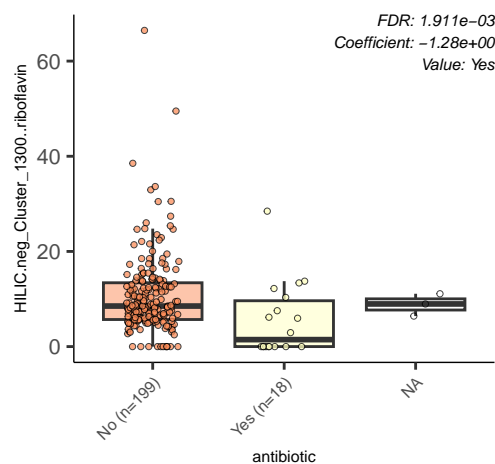
FDR: $1.911\text{e-}03$
Coefficient: $-1.28\text{e}+00$
Value: Yes

No (n=199)

Yes (n=18)

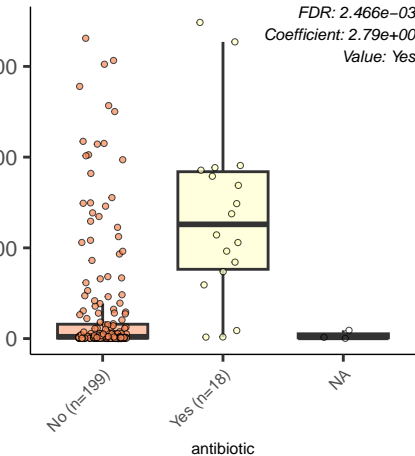
NA

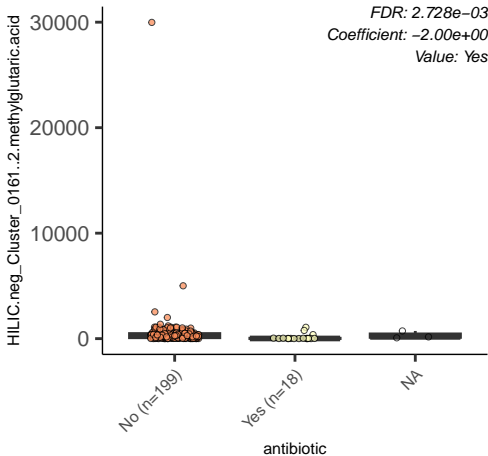
antibiotic



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

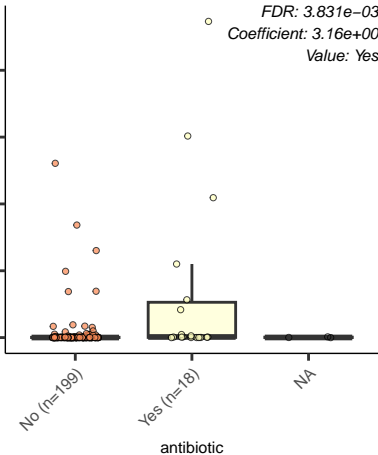
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos_Cluster_1017..sphinganine

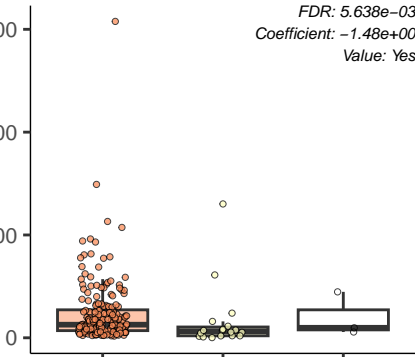
FDR: 5.638e-03
Coefficient: -1.48e+00
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos_Cluster_0540..pantothenate

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

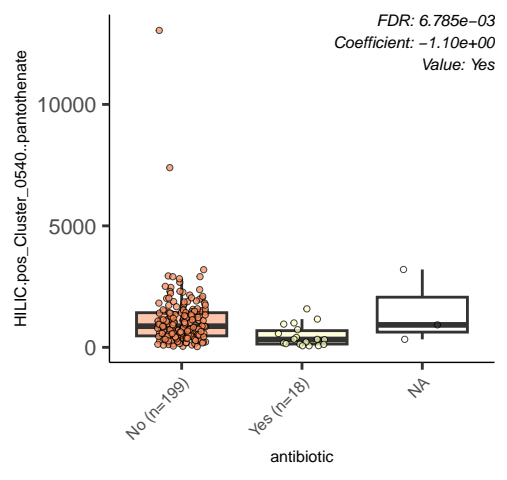
10000
5000
0

No (n=199)

Yes (n=18)

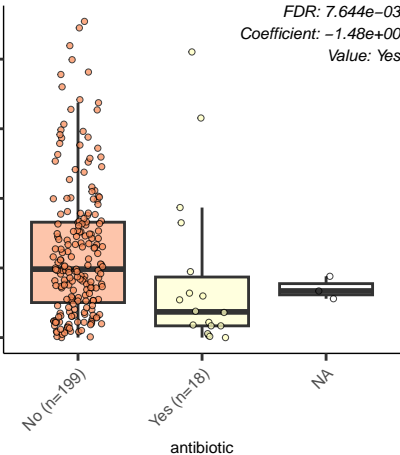
NA

antibiotic



HILIC.neg_Cluster_0003..propionate

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



HILIC_pos_Cluster_0822..inosine

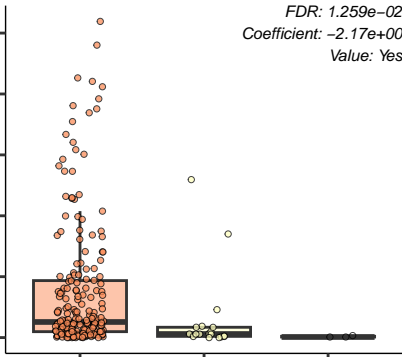
FDR: 1.259e-02
Coefficient: -2.17e+00
Value: Yes

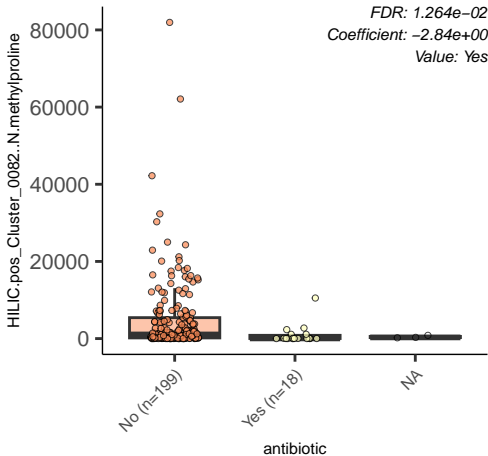
No (n=199)

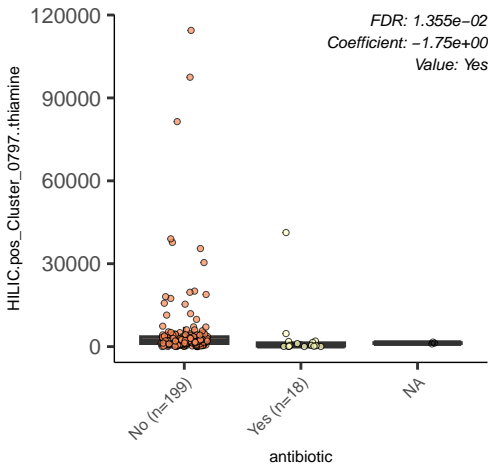
Yes (n=18)

NA

antibiotic







HILIC.neg_Cluster_0166..glutamate

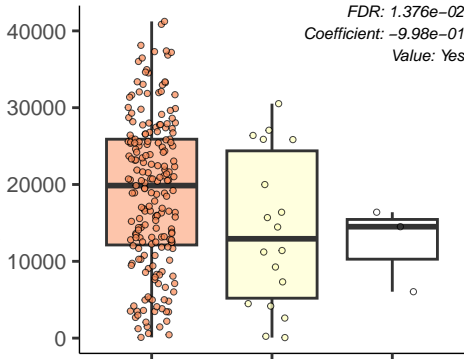
FDR: 1.376e-02
Coefficient: -9.98e-01
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.neg_Cluster_0049..uracil

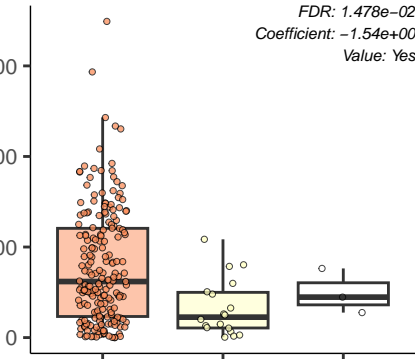
FDR: $1.478e-02$
Coefficient: $-1.54e+00$
Value: Yes

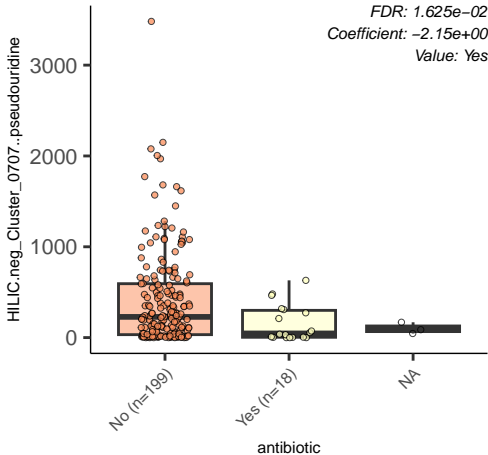
No (n=199)

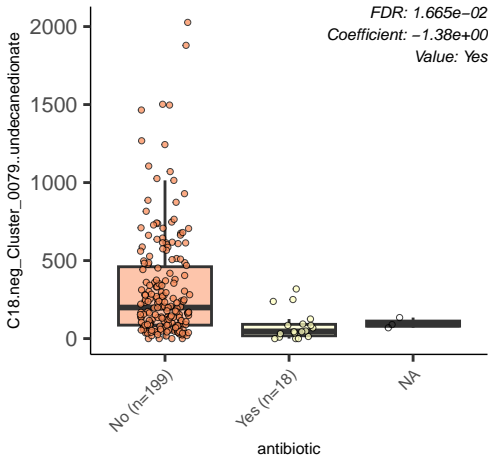
Yes (n=18)

NA

antibiotic







C8.pos_Cluster_0554..cholestenone

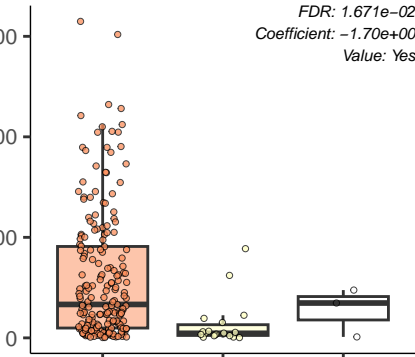
FDR: 1.671e-02
Coefficient: -1.70e+00
Value: Yes

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

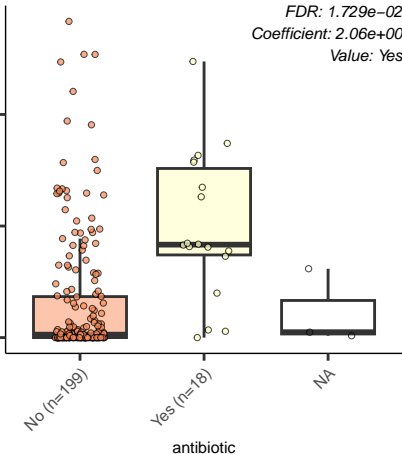
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos_Cluster_0048..betaine

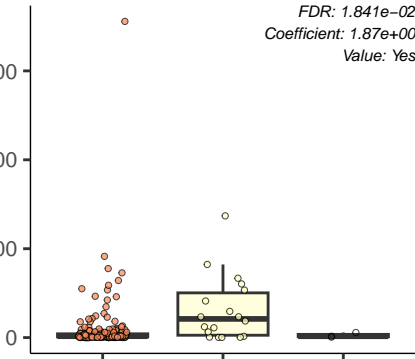
FDR: 1.841e-02
Coefficient: 1.87e+00
Value: Yes

No (n=199)

Yes (n=18)

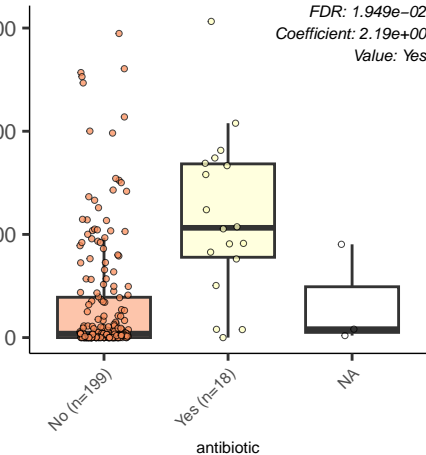
NA

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

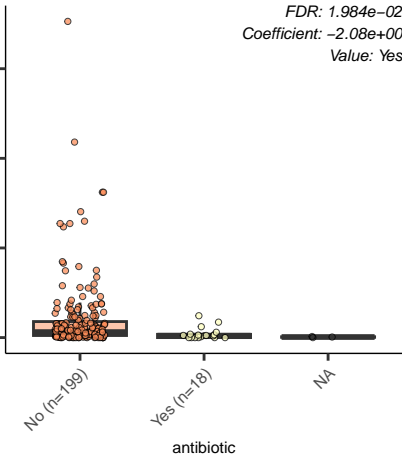
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.neg_Cluster_0176..xylose

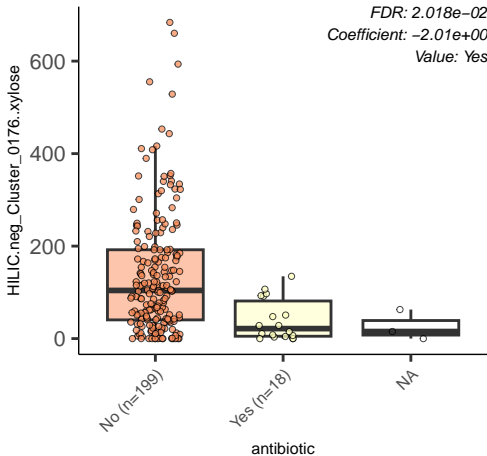
FDR: 2.018e-02
Coefficient: -2.01e+00
Value: Yes

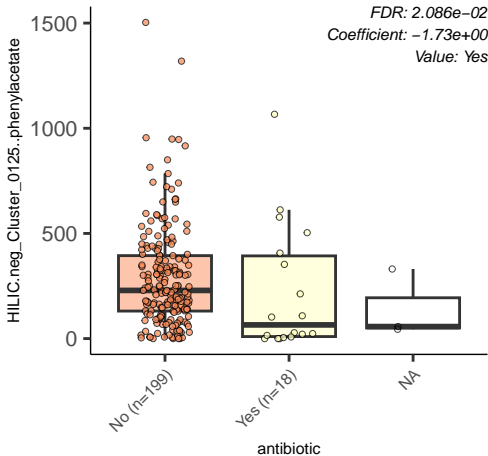
No (n=199)

Yes (n=18)

NA

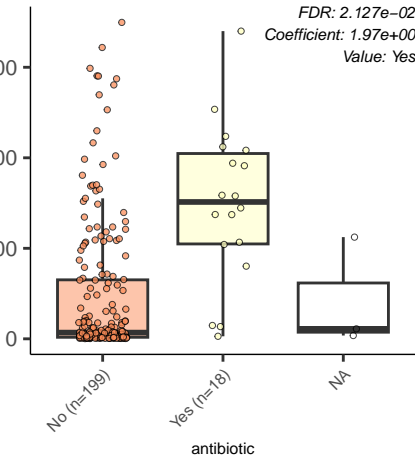
antibiotic

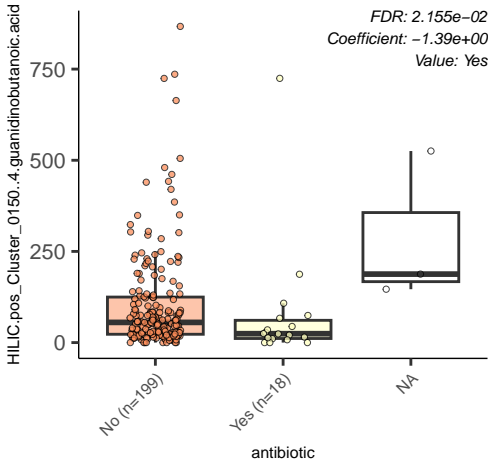




C18.neg_Cluster_0930..cholate

FDR: 2.127e-02
Coefficient: 1.97e+00
Value: Yes





C18.neg_Cluster_1621..cholate

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

2000

1000

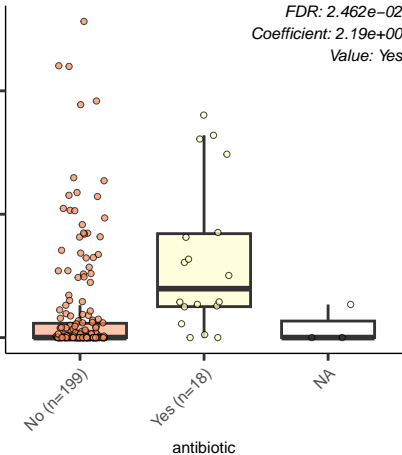
0

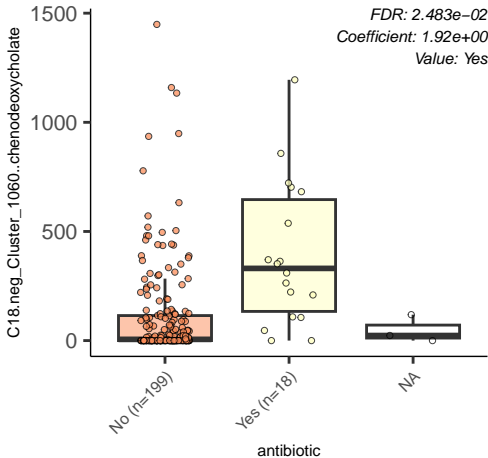
No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.pos_Cluster_0306..citrulline

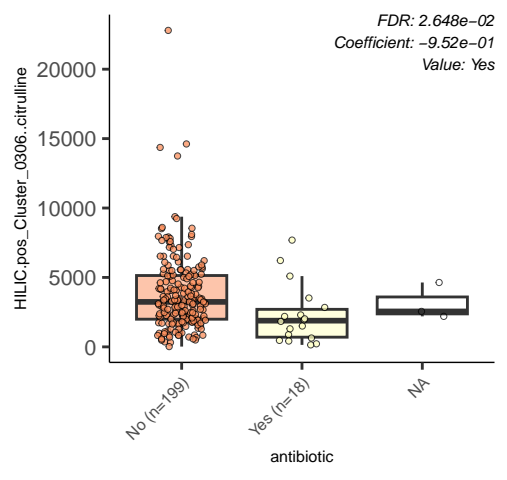
FDR: 2.648e-02
Coefficient: -9.52e-01
Value: Yes

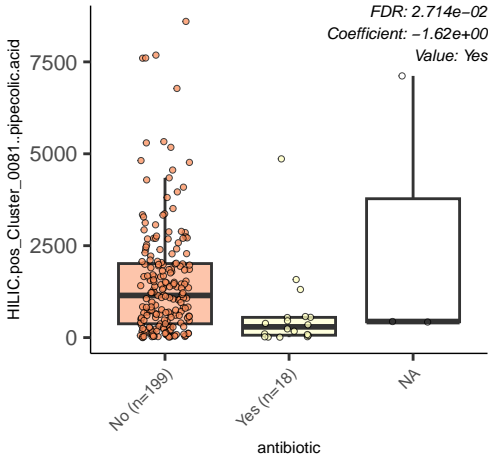
No (n=199)

Yes (n=18)

NA

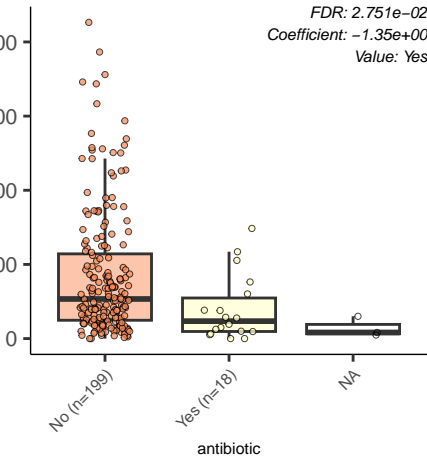
antibiotic





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)

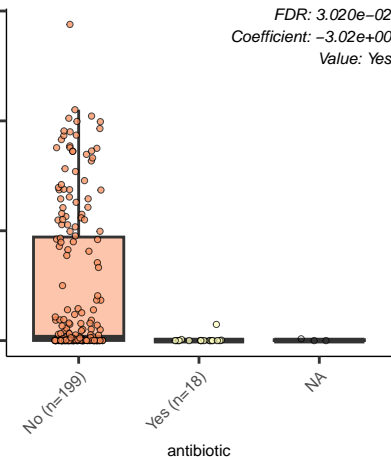
NA

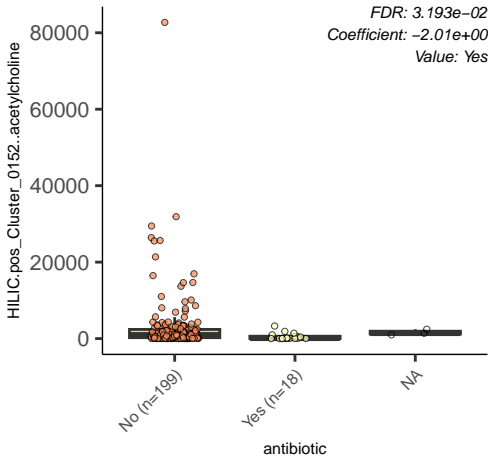
antibiotic

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

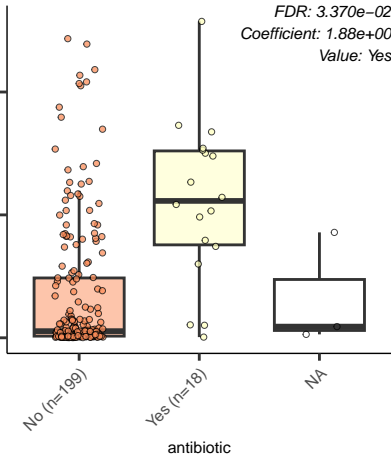
0e+00

No (n=199)

Yes (n=18)

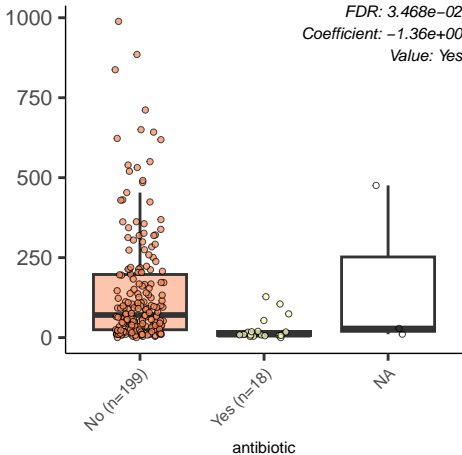
NA

antibiotic



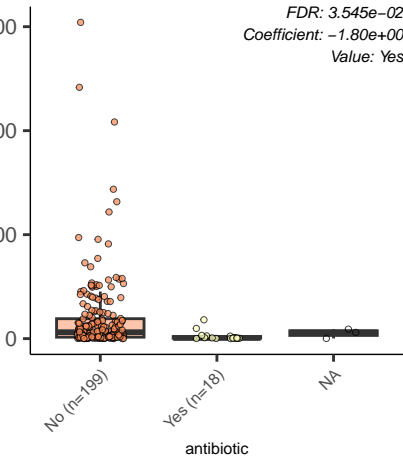
HILIC.neg_Cluster_0441..sebacate

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



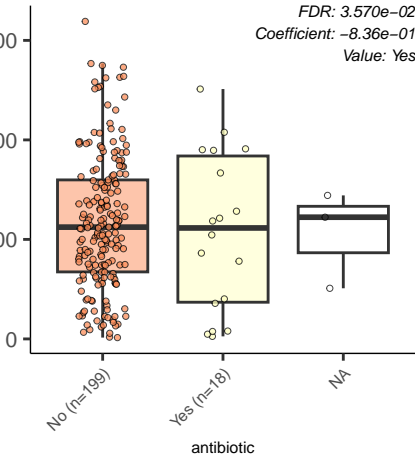
C8.pos_Cluster_0478..cholestenone

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



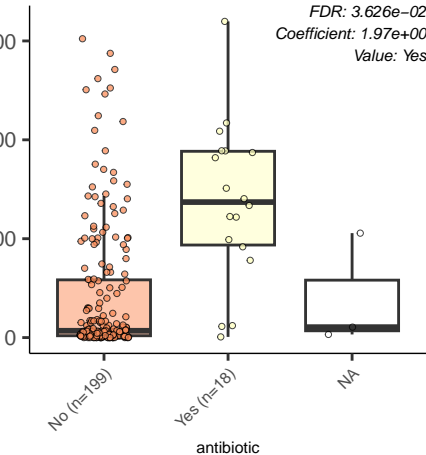
HILIC.neg_Cluster_0117.aspartate

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

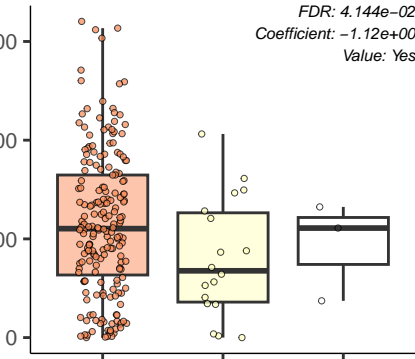
FDR: $4.144e-02$
Coefficient: $-1.12e+00$
Value: Yes

No (n=199)

Yes (n=18)

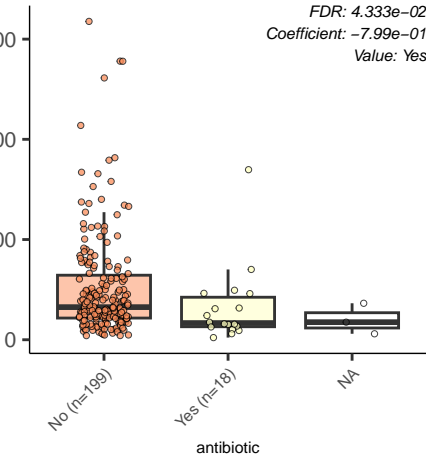
NA

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

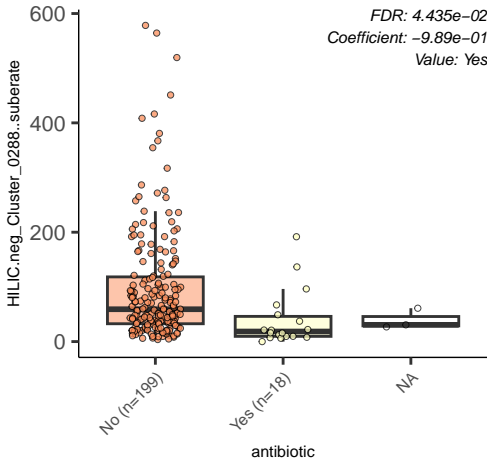
FDR: 4.435e-02
Coefficient: -9.89e-01
Value: Yes

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

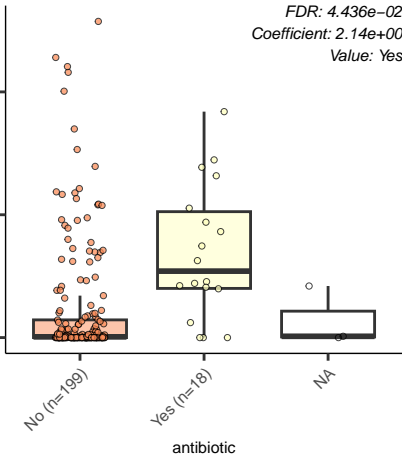
0

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos_Cluster_2093..urobilin.

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

30000

20000

10000

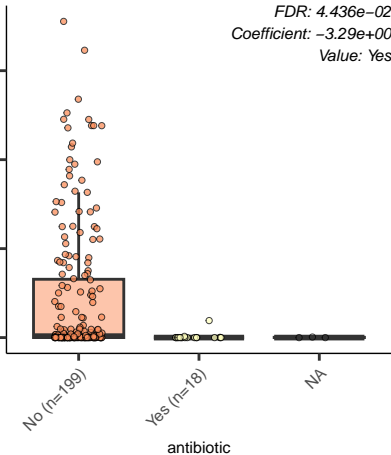
0

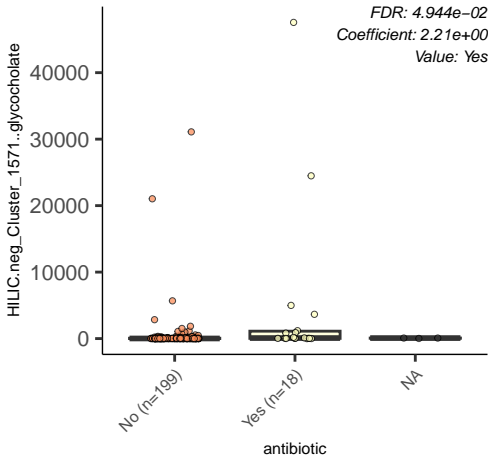
No (n=199)

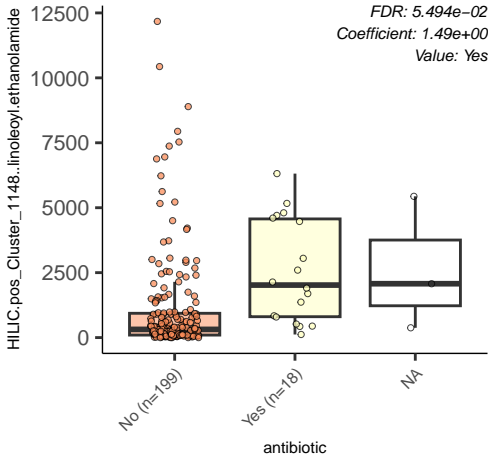
Yes (n=18)

NA

antibiotic







HILIC.neg_Cluster_0174..tartarate

FDR: 6.027e-02
Coefficient: 1.78e+00
Value: Yes

40000

20000

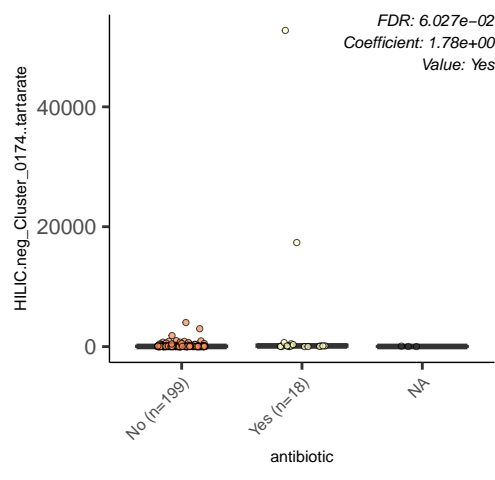
0

No (n=199)

Yes (n=18)

NA

antibiotic



C18.neg_Cluster_0045..azelate

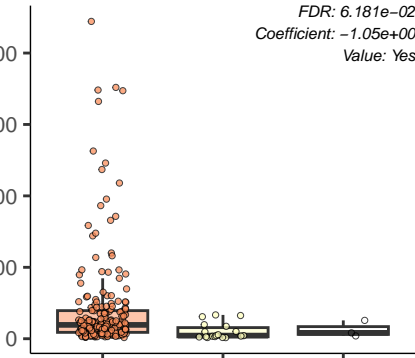
FDR: $6.181e-02$
Coefficient: $-1.05e+00$
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



HILIC.pos_Cluster_0295..arginine

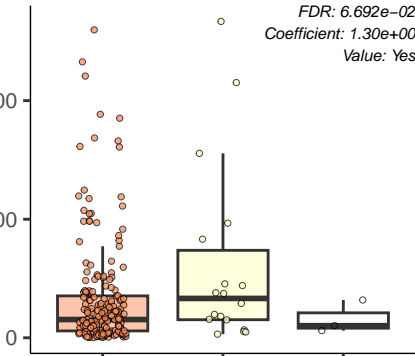
FDR: 6.692e-02
Coefficient: 1.30e+00
Value: Yes

No (n=199)

Yes (n=18)

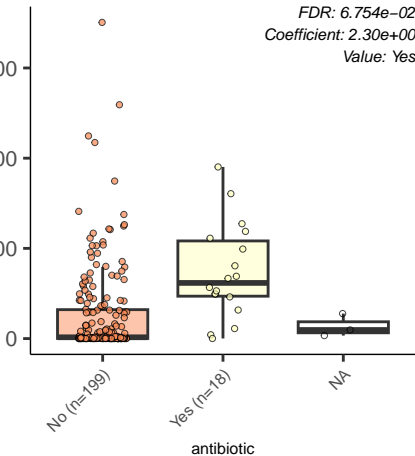
NA

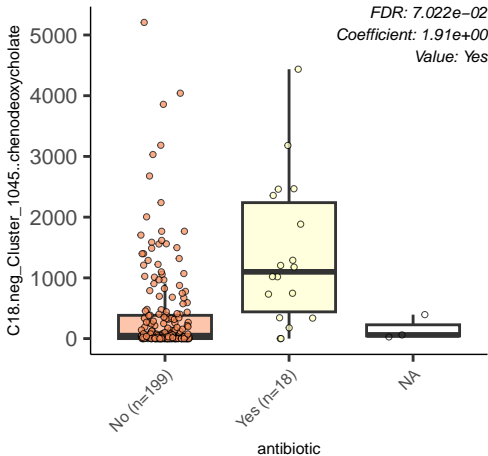
antibiotic



HILIC_pos_Cluster_0036..creatinine

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





HILIC_pos_Cluster_0167..methionine

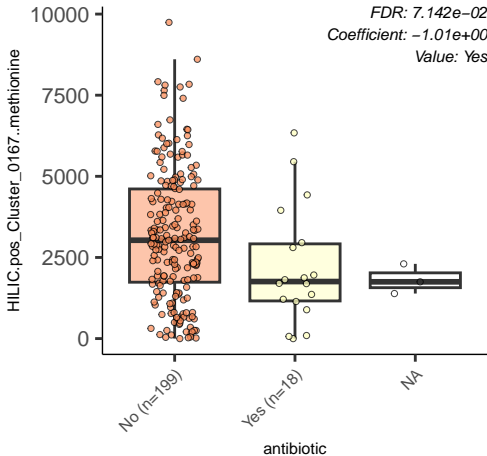
FDR: $7.142e-02$
Coefficient: $-1.01e+00$
Value: Yes

No (n=199)

Yes (n=18)

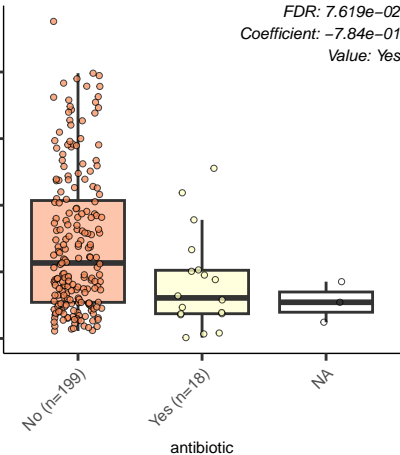
NA

antibiotic



HILIC.neg_Cluster_0372..N.acetylglutamate

FDR: $7.619e-02$
Coefficient: $-7.84e-01$
Value: Yes



HILIC.pos_Cluster_2052...bilirubin

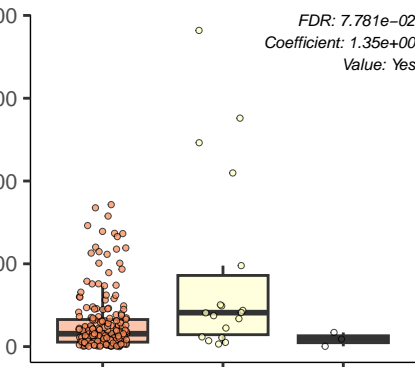
FDR: 7.781e-02
Coefficient: 1.35e+00
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



C8.pos_Cluster_1900..cholestenone

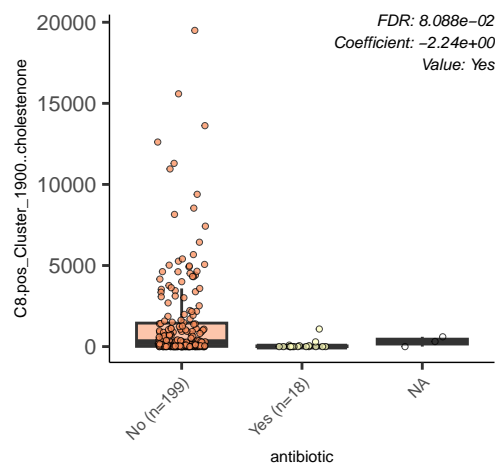
FDR: 8.088e-02
Coefficient: -2.24e+00
Value: Yes

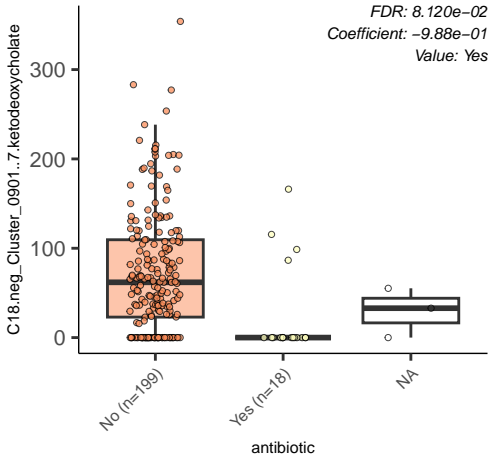
No (n=199)

Yes (n=18)

NA

antibiotic





HILIC.neg_Cluster_0365..azelaic.acid

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

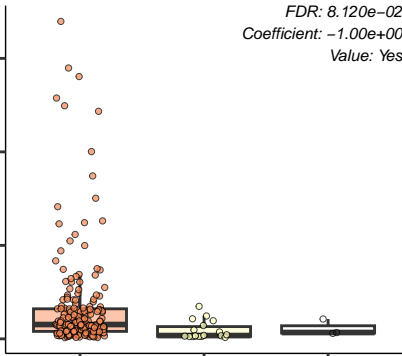
3000
2000
1000
0

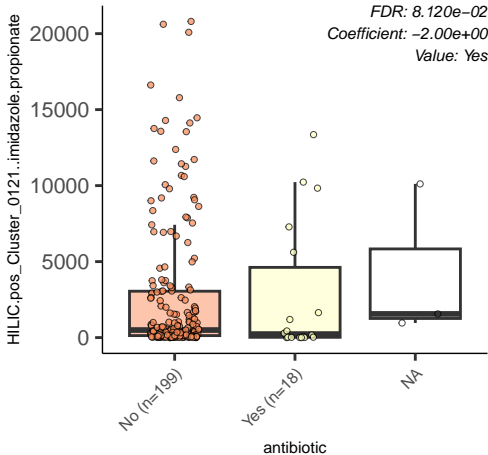
No (n=199)

Yes (n=18)

NA

antibiotic





C18.neg_Cluster_0064..sebacate

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

7500

5000

2500

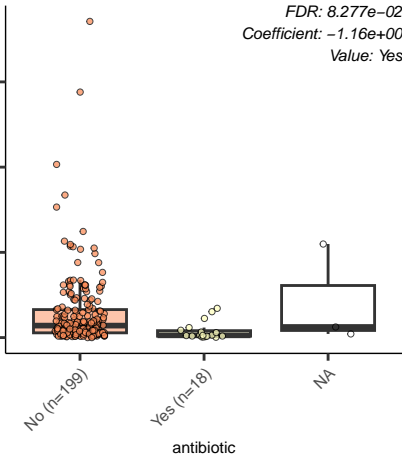
0

No (n=199)

Yes (n=18)

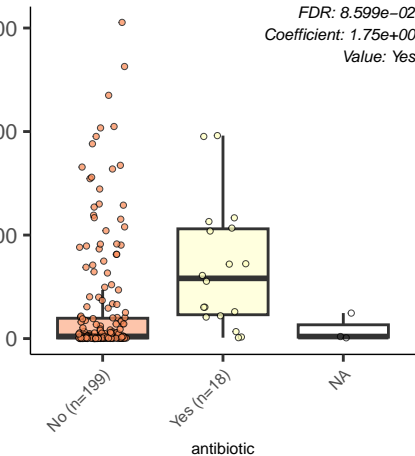
NA

antibiotic



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

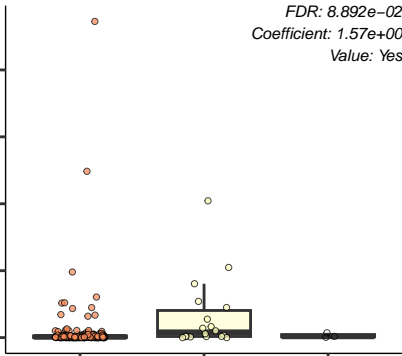
4000
3000
2000
1000
0

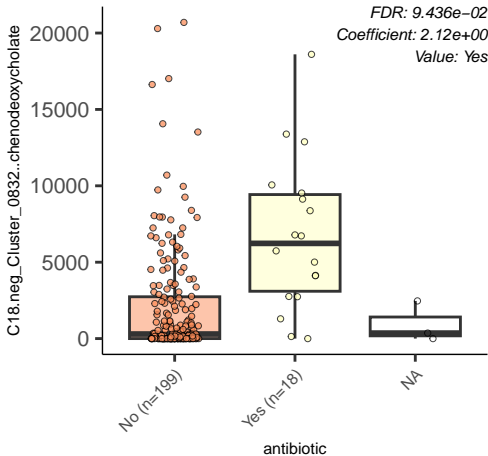
No (n=199)

Yes (n=18)

NA

antibiotic





C8.pos_Cluster_0705..cholestenone

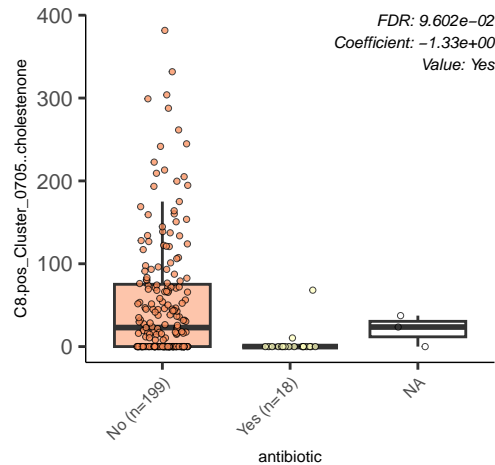
FDR: $9.602e-02$
Coefficient: $-1.33e+00$
Value: Yes

No (n=199)

Yes (n=18)

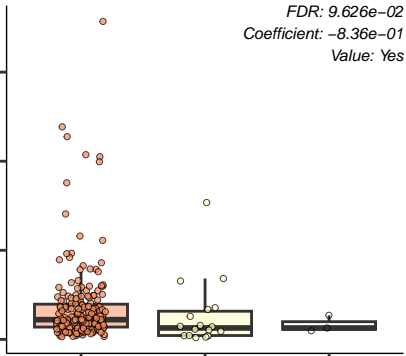
NA

antibiotic



HILIC.neg_Cluster_0079...4.hydroxybenzaldehyde

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



No (n=199)

Yes (n=18)

NA

antibiotic

C18.neg.Cluster_1465..tauroolithocholic.acid

FDR: $9.692e-02$
Coefficient: $-1.74e+00$
Value: Yes

10000

5000

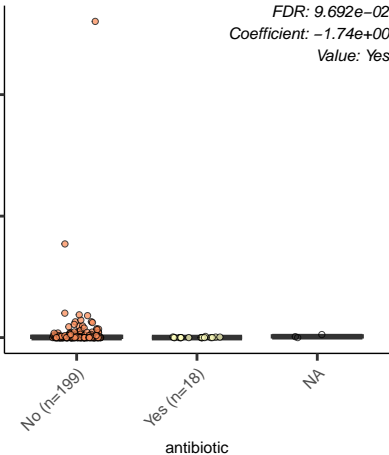
0

No (n=199)

Yes (n=18)

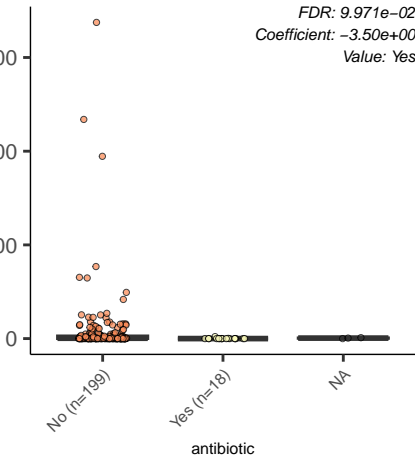
NA

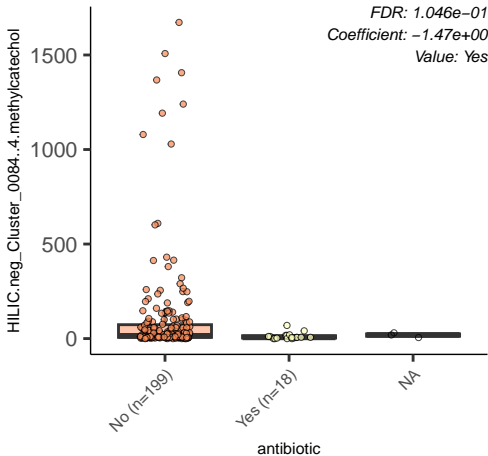
antibiotic



C8.pos_Cluster_1849..cholestenone

FDR: 9.971e-02
Coefficient: -3.50e+00
Value: Yes





HILIC.pos_Cluster_0113..trigonelline

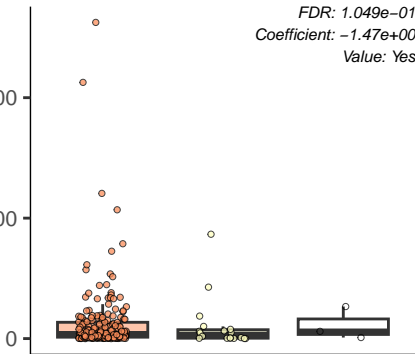
FDR: 1.049e-01
Coefficient: -1.47e+00
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



C18.neg_Cluster_1081..glycolithocholic.acid

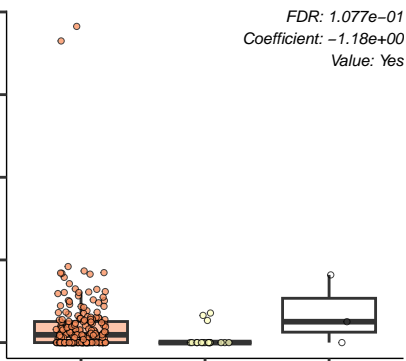
FDR: 1.077e-01
Coefficient: -1.18e+00
Value: Yes

No (n=199)

Yes (n=18)

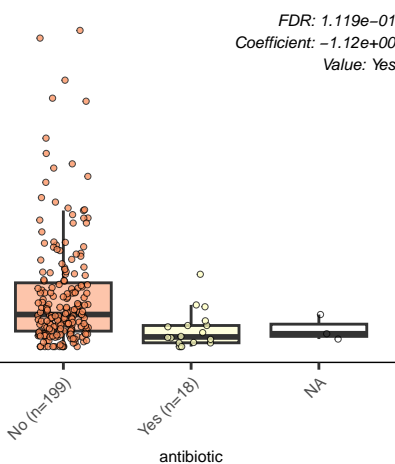
NA

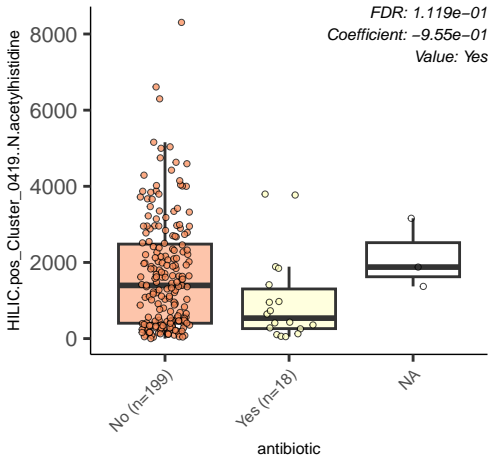
antibiotic



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

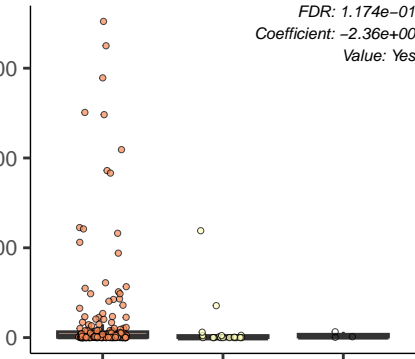
FDR: $1.174e-01$
Coefficient: $-2.36e+00$
Value: Yes

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

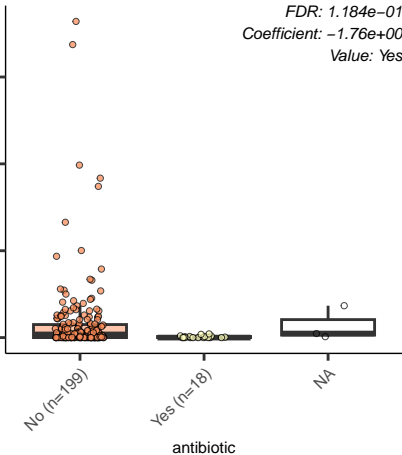
0

No (n=199)

Yes (n=18)

NA

antibiotic



C8.pos_Cluster_0629..cholestenone

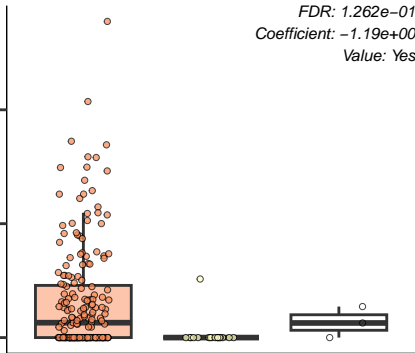
FDR: 1.262e-01
Coefficient: -1.19e+00
Value: Yes

No (n=199)

Yes (n=18)

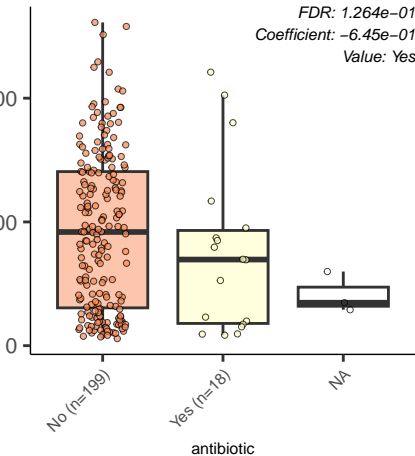
NA

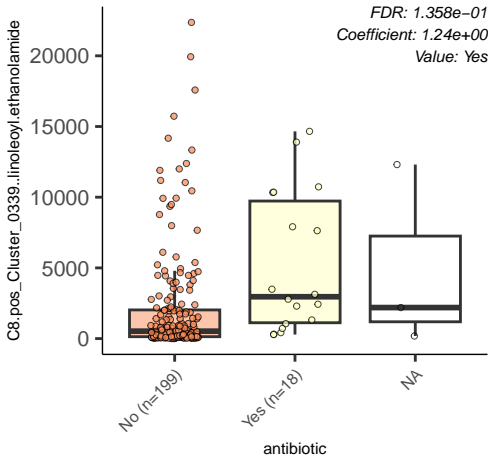
antibiotic

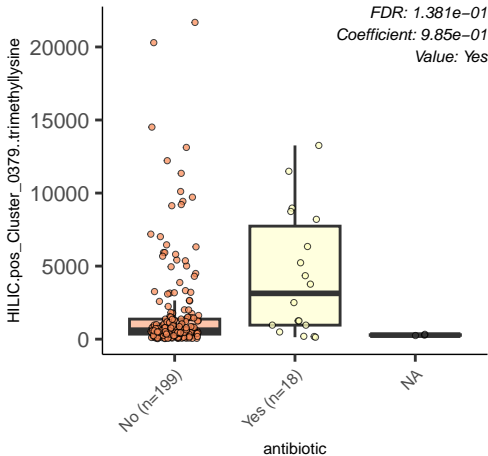


HILIC.neg_Cluster_0118..malate

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

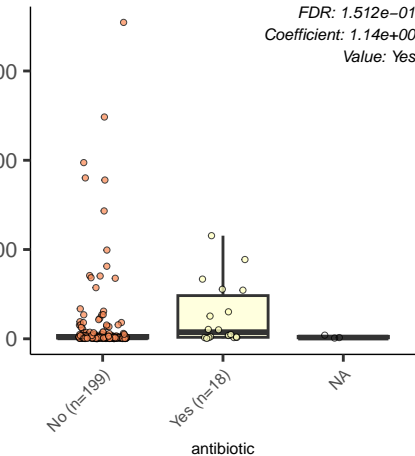






HILIC.neg_Cluster_0020..lactate

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

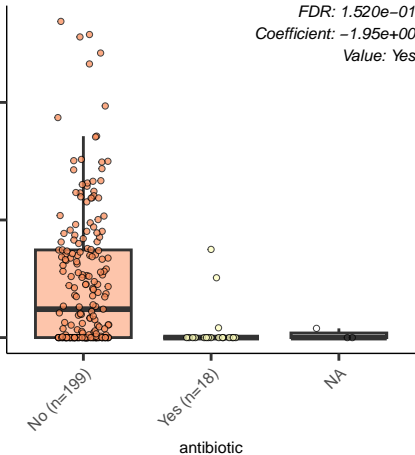
0

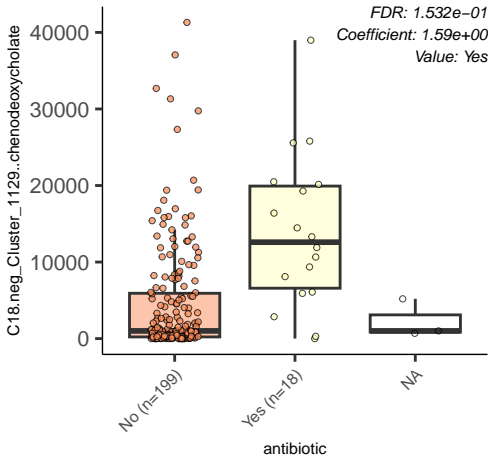
No (n=199)

Yes (n=18)

NA

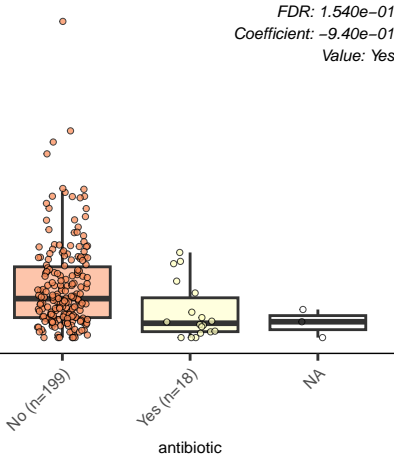
antibiotic





HILIC_pos_Cluster_0177_4.hydroxy.3.methylacetophenone

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



HILIC.neg_Cluster_0392...citrate

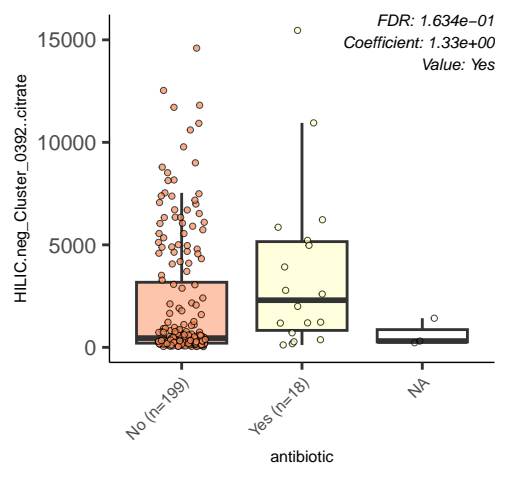
FDR: 1.634e-01
Coefficient: 1.33e+00
Value: Yes

No (n=199)

Yes (n=18)

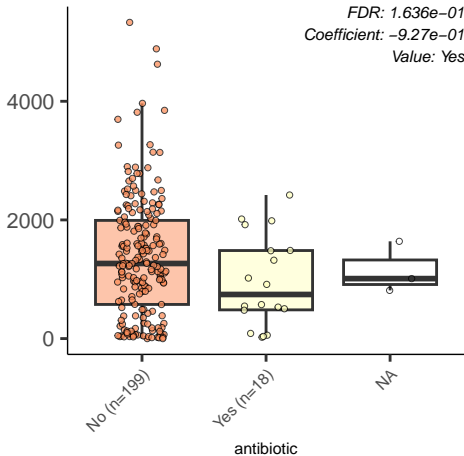
NA

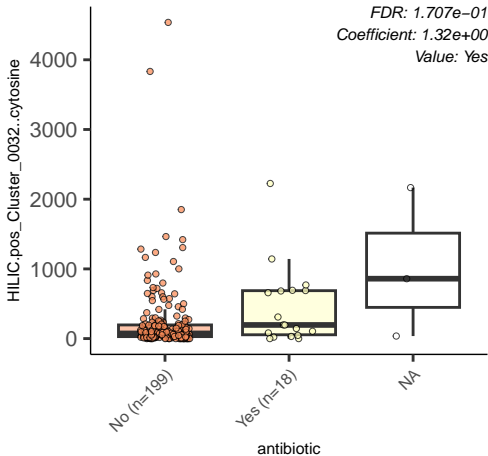
antibiotic

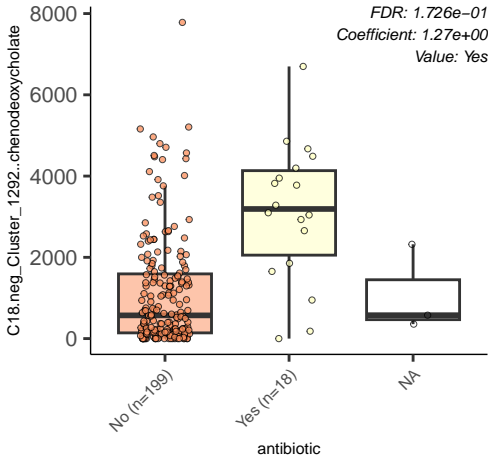


HILIC.neg_Cluster_0035..serine

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







HILIC.pos_Cluster_1580..C18.2.carnitine

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

2000

1000

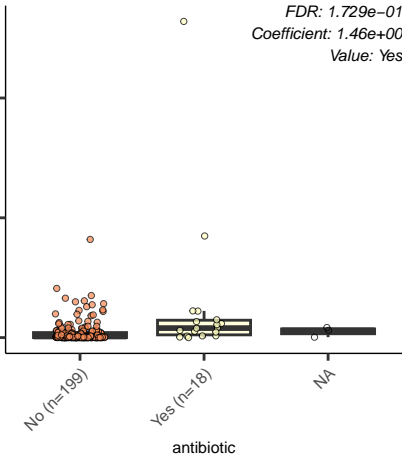
0

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

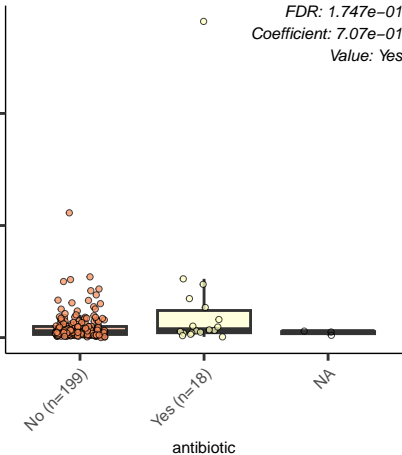
0

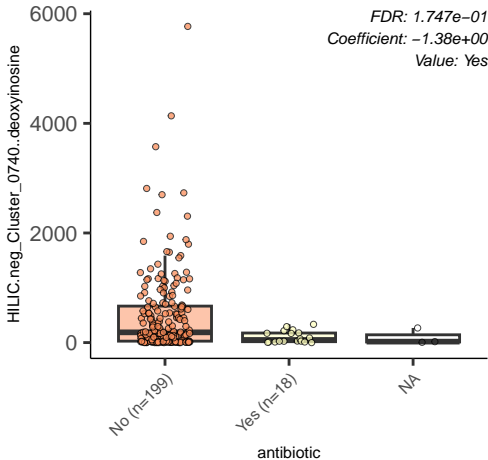
No (n=199)

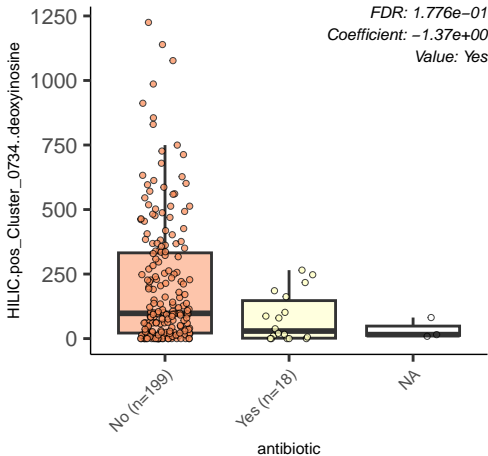
Yes (n=18)

NA

antibiotic







HILIC.neg.Cluster_0062...alpha.ketoisovalerate

FDR: 1.790×10^{-1}
Coefficient: -1.18×10^0
Value: Yes

2000

1000

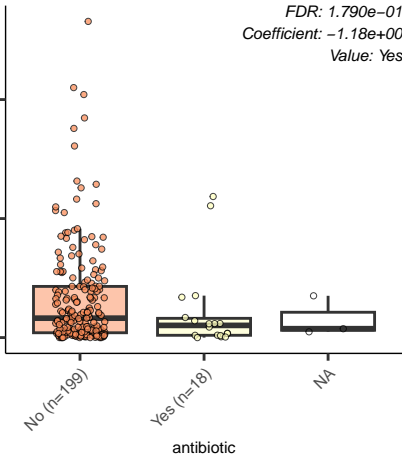
0

No (n=199)

Yes (n=18)

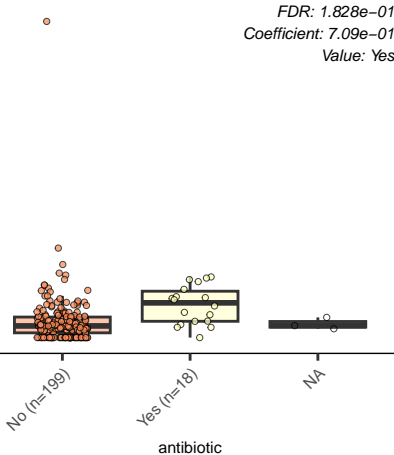
NA

antibiotic



C18.neg_Cluster_1941..arachidonic.acid

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



HILIC.pos_Cluster_0817..atenolol

FDR: 1.844e-01
Coefficient: -1.87e+00
Value: Yes

60000

40000

20000

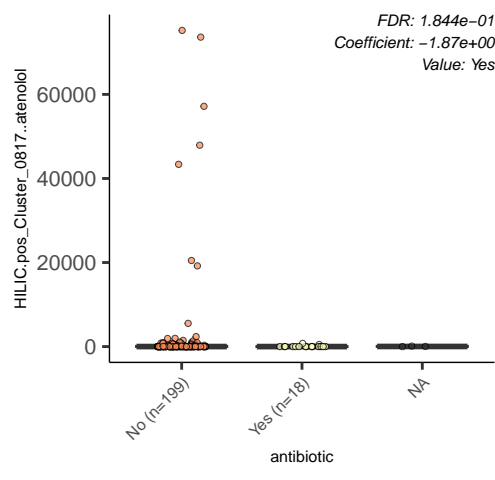
0

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

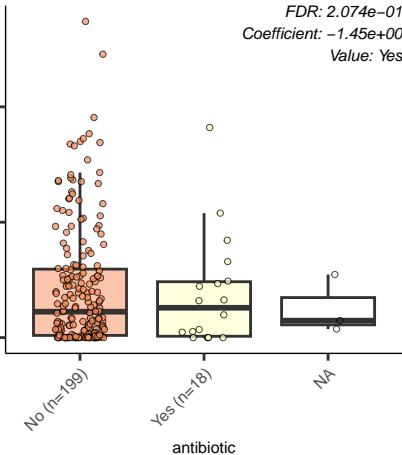
0

No (n=199)

Yes (n=18)

NA

antibiotic



C18.neg_Cluster_0394...9.10.diHOME

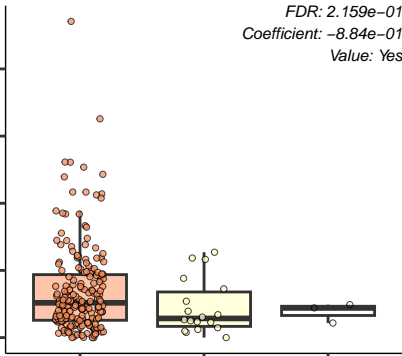
FDR: $2.159e-01$
Coefficient: $-8.84e-01$
Value: Yes

No (n=199)

Yes (n=18)

NA

antibiotic



C18.neg_Cluster_1596..oleanolic.acid

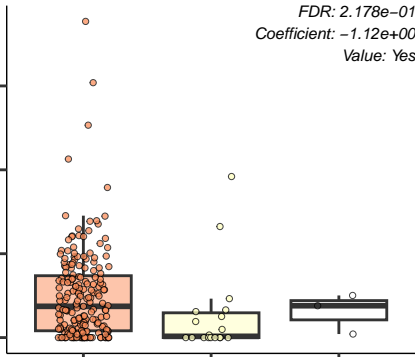
FDR: 2.178e-01
Coefficient: -1.12e+00
Value: Yes

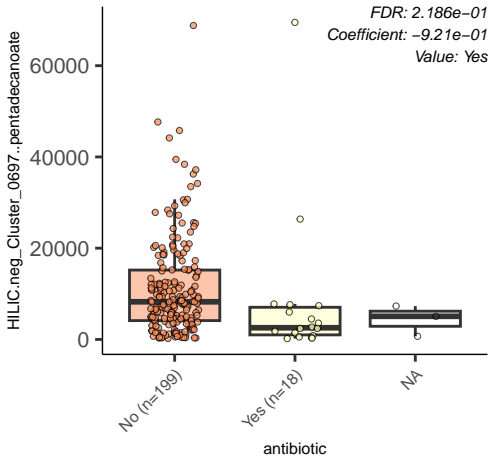
No (n=199)

Yes (n=18)

NA

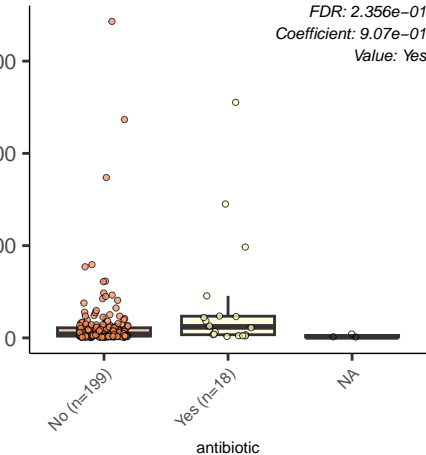
antibiotic





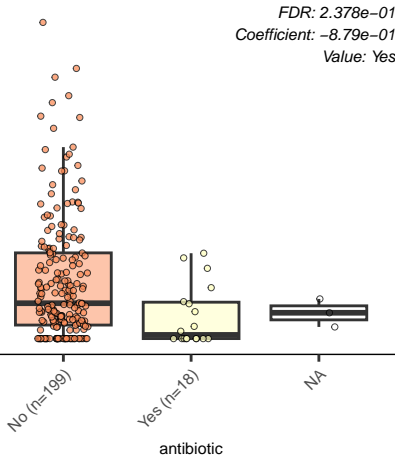
HILIC.pos_Cluster_0089...hydroxyproline

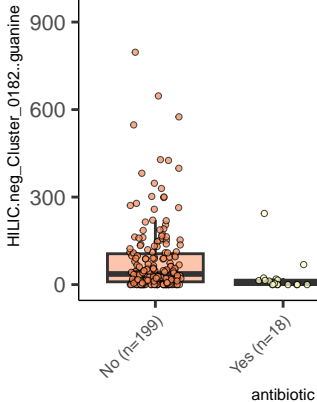
FDR: 2.356e-01
Coefficient: 9.07e-01
Value: Yes



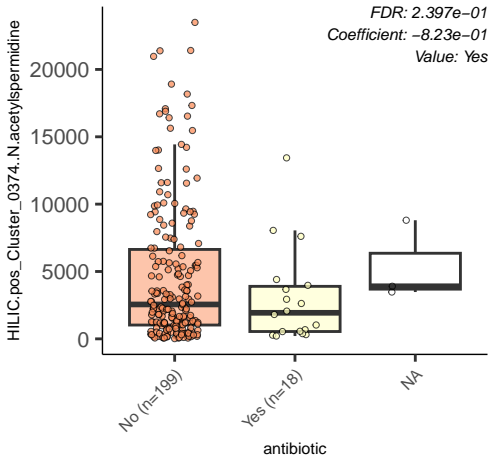
C18.neg.Cluster_0183...1.2.3.4.tetrahydro.b.carboline.1.3.dicarb

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



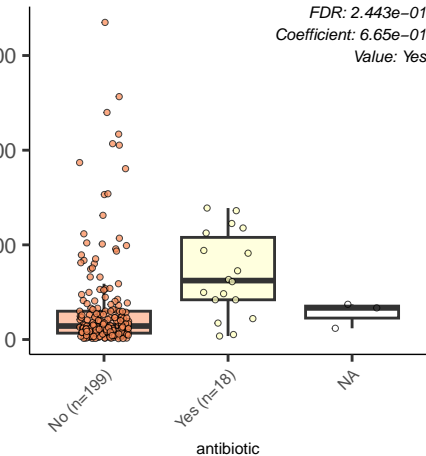


FDR: 2.378e-01
Coefficient: -1.28e+00
Value: Yes



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

