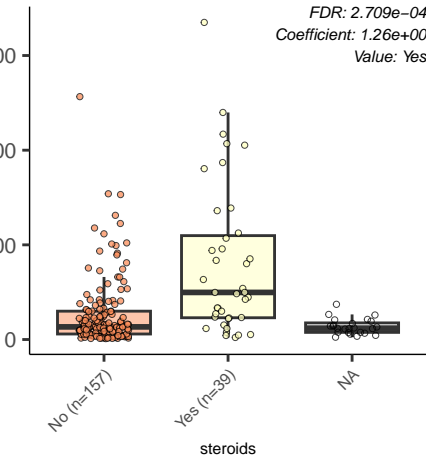


HILIC.pos_Cluster_0447..ADMA

FDR: 2.709e-04
Coefficient: 1.26e+00
Value: Yes



HILIC.pos_Cluster_0036..creatinine

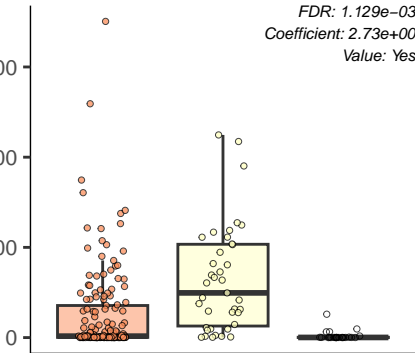
FDR: 1.129e-03
Coefficient: 2.73e+00
Value: Yes

No (n=157)

Yes (n=39)

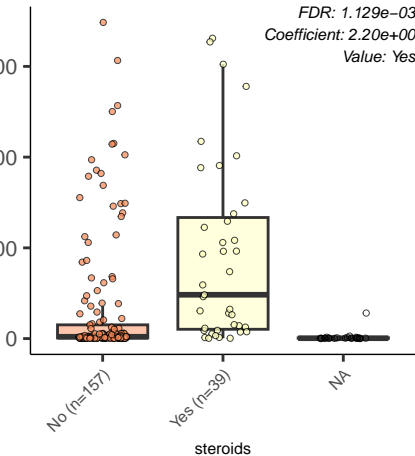
NA

steroids



HILIC_pos_Cluster_0090..creatine

FDR: 1.129e-03
Coefficient: 2.20e+00
Value: Yes

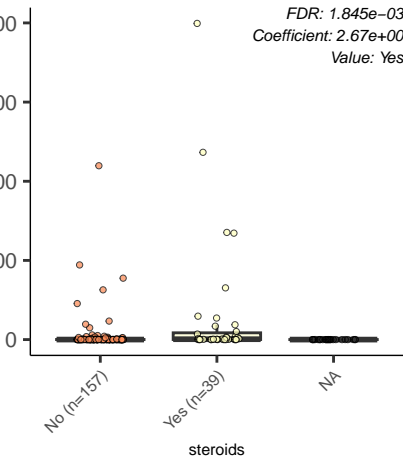


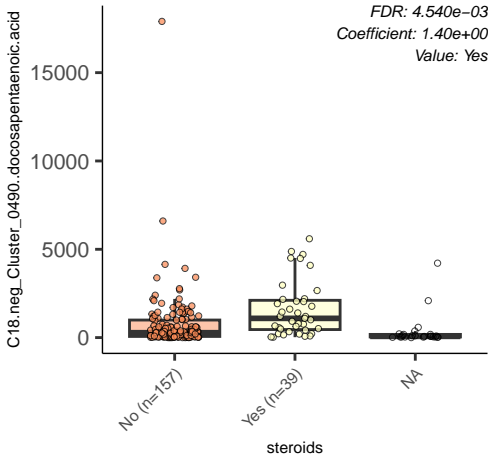


FDR: 1.845e-03

Coefficient: 2.67e+00

Value: Yes





C18.neg_Cluster_0729..docosapentaenoic.acid

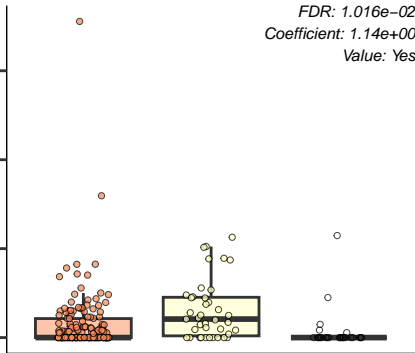
FDR: 1.016e-02
Coefficient: 1.14e+00
Value: Yes

No (n=157)

Yes (n=39)

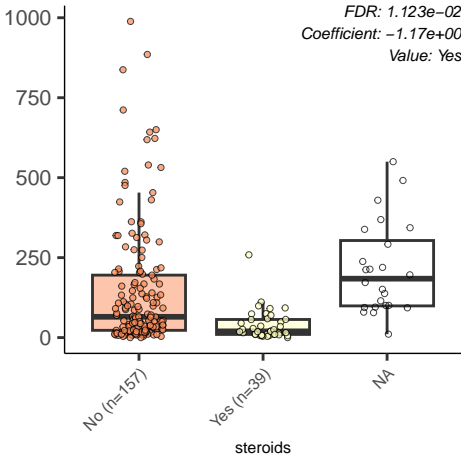
NA

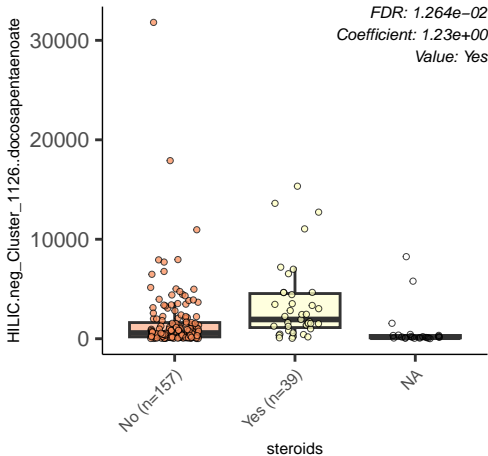
steroids



HILIC.neg_Cluster_0441..sebacate

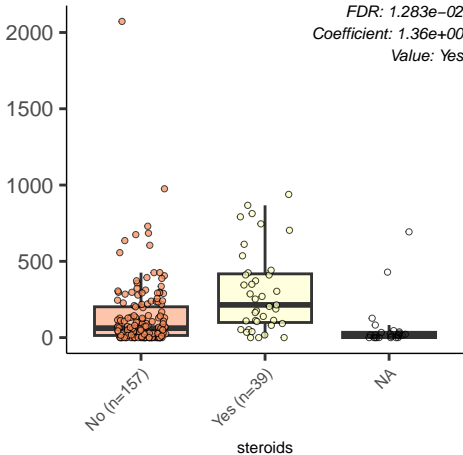
FDR: $1.123e-02$
Coefficient: $-1.17e+00$
Value: Yes





C18.neg_Cluster_0863..docosapentaenoic.acid

FDR: 1.283e-02
Coefficient: 1.36e+00
Value: Yes



HILIC_neg_Cluster_1303..lithocholate

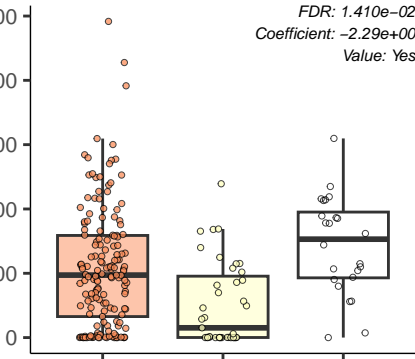
FDR: $1.410e-02$
Coefficient: $-2.29e+00$
Value: Yes

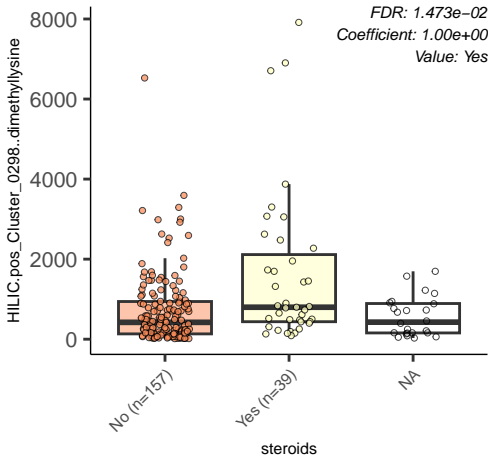
No (n=157)

Yes (n=39)

NA

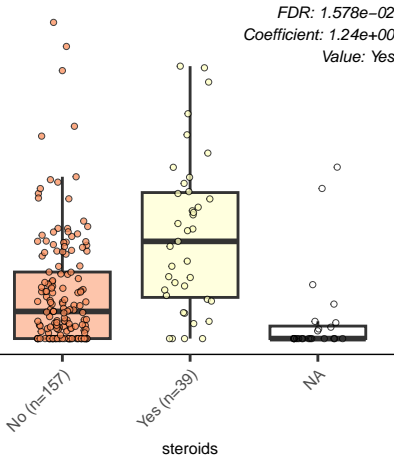
steroids





C18.neg_Cluster_1324..docosapentaenoic.acid

FDR: 1.578e-02
Coefficient: 1.24e+00
Value: Yes



C18.neg_Cluster_0111..dodecanedioic.acid

FDR: $2.125e-02$
Coefficient: $-9.05e-01$
Value: Yes

4000

2000

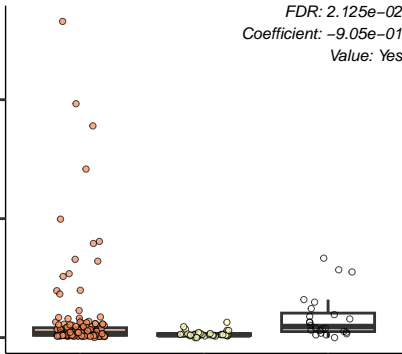
0

No (n=157)

Yes (n=39)

NA

steroids



C18.neg_Cluster_0064..sebacate

FDR: 2.165e-02
Coefficient: -1.07e+00
Value: Yes

7500

5000

2500

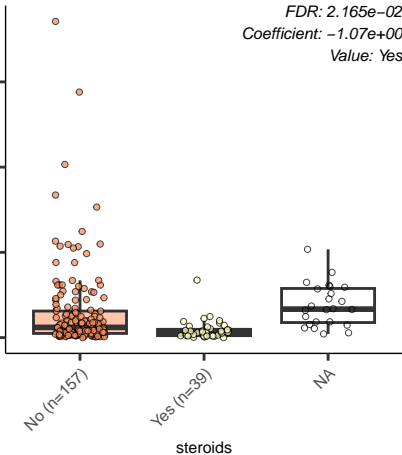
0

No (n=157)

Yes (n=39)

NA

steroids



C18.neg_Cluster_0731..lithocholic.acid

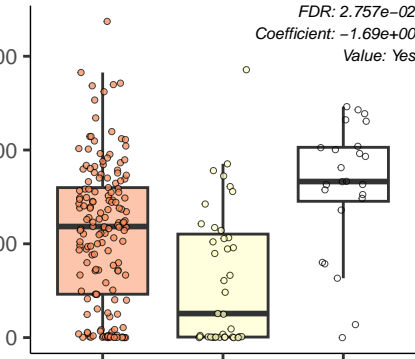
FDR: 2.757e-02
Coefficient: -1.69e+00
Value: Yes

No (n=157)

Yes (n=39)

NA

steroids



C18.neg_Cluster_0506..adrenic.acid

FDR: 2.837e-02

Coefficient: 1.53e+00

Value: Yes

3000

2000

1000

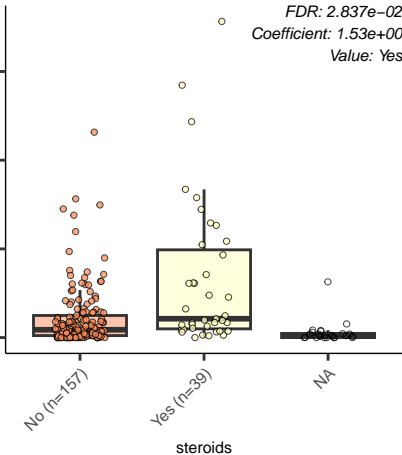
0

No (n=157)

Yes (n=39)

NA

steroids



HILIC.neg_Cluster_0288..suberate

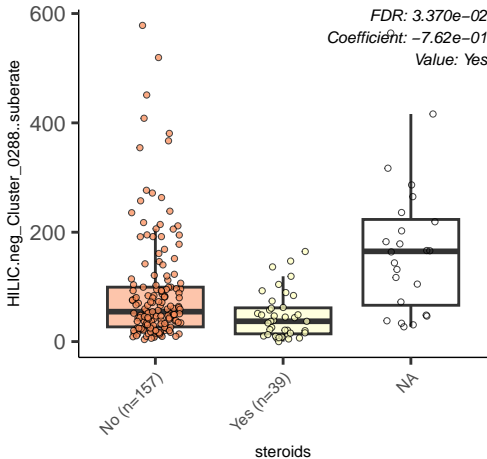
FDR: 3.370e-02
Coefficient: -7.62e-01
Value: Yes

No (n=157)

Yes (n=39)

NA

steroids



HILIC.neg_Cluster_0365..azelaic.acid

FDR: $3.528e-02$
Coefficient: $-8.54e-01$
Value: Yes

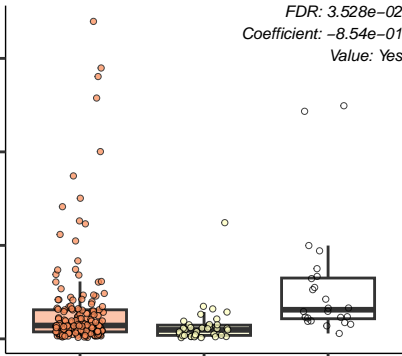
3000
2000
1000
0

No (n=157)

Yes (n=39)

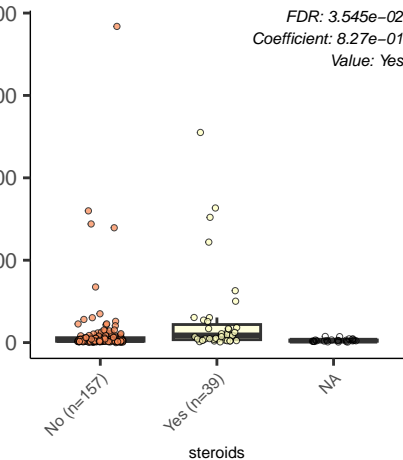
NA

steroids



HILIC.pos_Cluster_0230..carnitine

FDR: 3.545e-02
Coefficient: 8.27e-01
Value: Yes



HILIC.neg_Cluster_0182..guanine

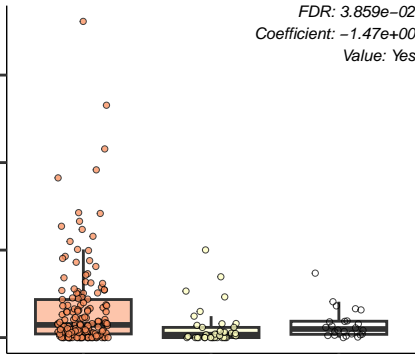
FDR: 3.859×10^{-2}
Coefficient: -1.47×10^0
Value: Yes

No (n=157)

Yes (n=39)

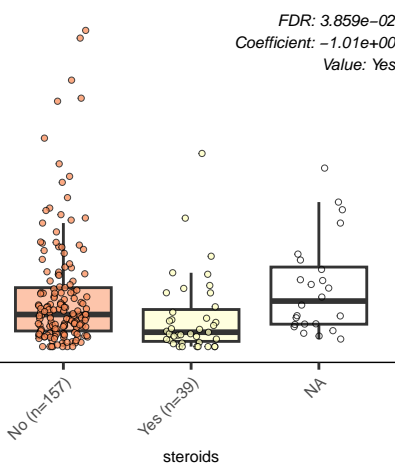
NA

steroids



ILIC.neg.Cluster_0622...1.2.3.4.tetrahydro.1.methyl.beta.carboline.3

FDR: $3.859e-02$
Coefficient: $-1.01e+00$
Value: Yes



HILIC.neg_Cluster_0299..ascorbate

FDR: $5.186e-02$
Coefficient: $-1.25e+00$
Value: Yes

20000

10000

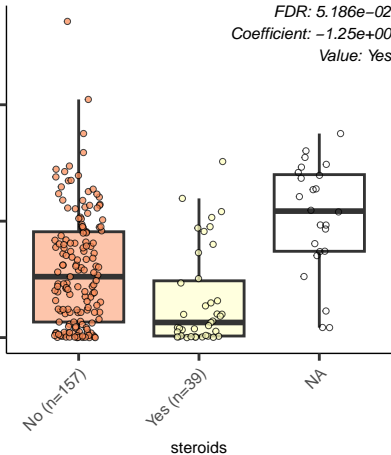
0

No (n=157)

Yes (n=39)

NA

steroids



HILIC_pos_Cluster_0184..pyridoxamine

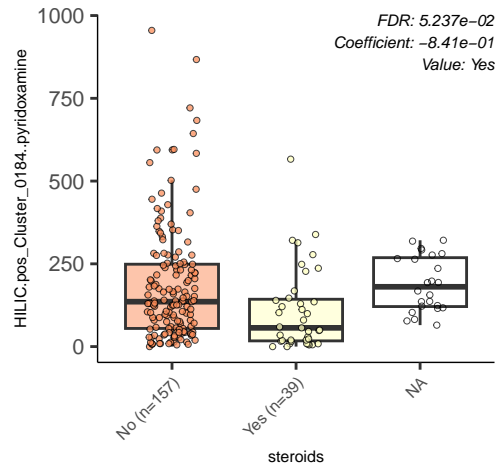
FDR: $5.237e-02$
Coefficient: $-8.41e-01$
Value: Yes

No (n=157)

Yes (n=39)

NA

steroids



HILIC.neg_Cluster_1300...riboflavin

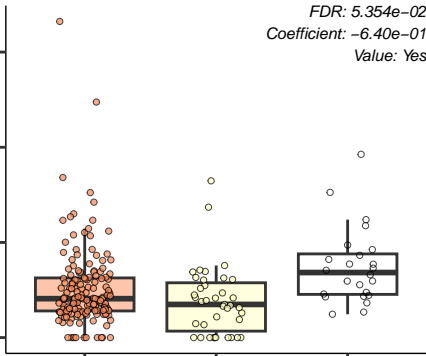
FDR: 5.354e-02
Coefficient: -6.40e-01
Value: Yes

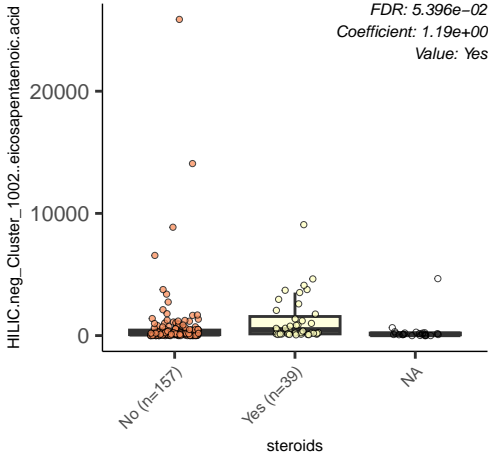
No (n=157)

Yes (n=39)

NA

steroids





C18.neg_Cluster_0045..azelate

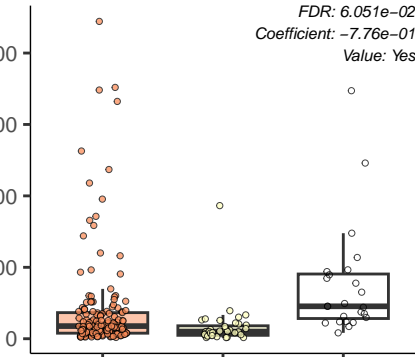
FDR: $6.051e-02$
Coefficient: $-7.76e-01$
Value: Yes

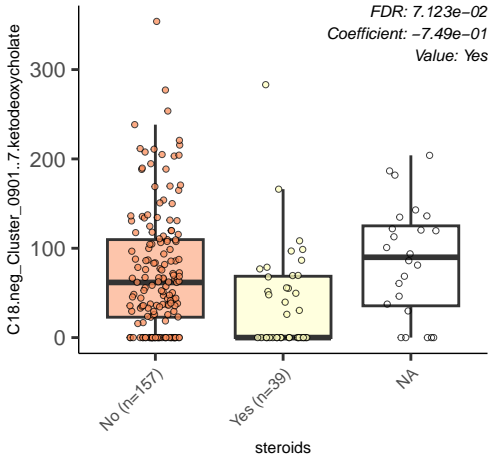
No (n=157)

Yes (n=39)

NA

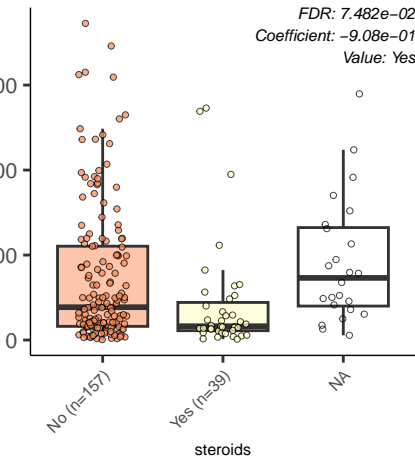
steroids

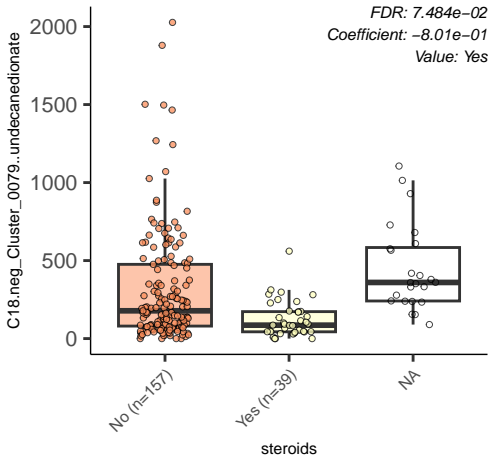


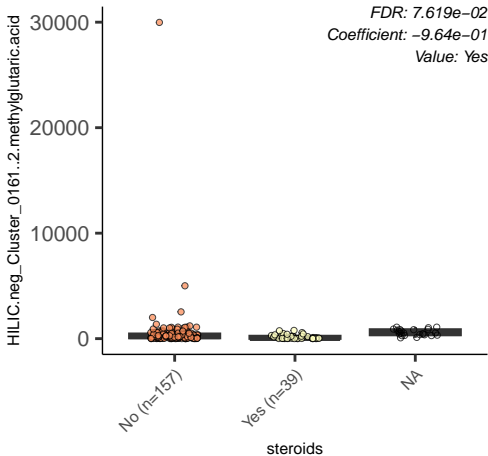


C18.neg_Cluster_0246..linoleic.acid

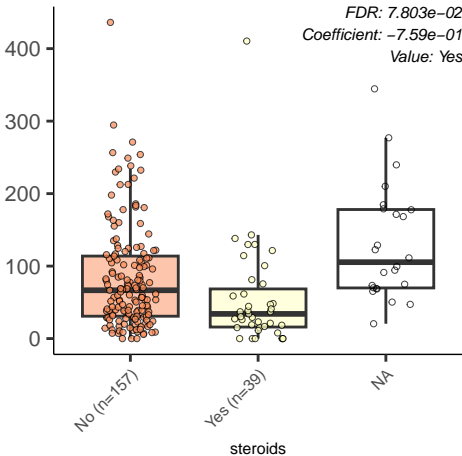
FDR: $7.482e-02$
Coefficient: $-9.08e-01$
Value: Yes



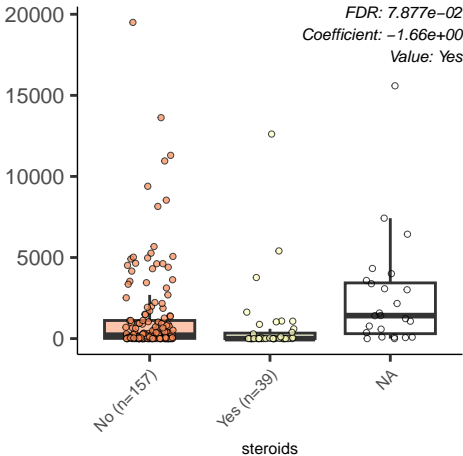




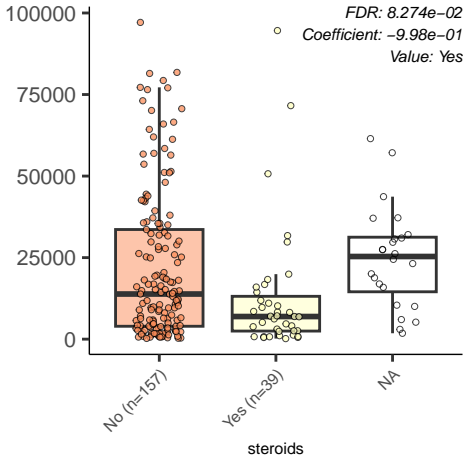
HILIC.pos_Cluster_0521..L.1.2.3.4.tetrahydro.beta.carboline.3.car

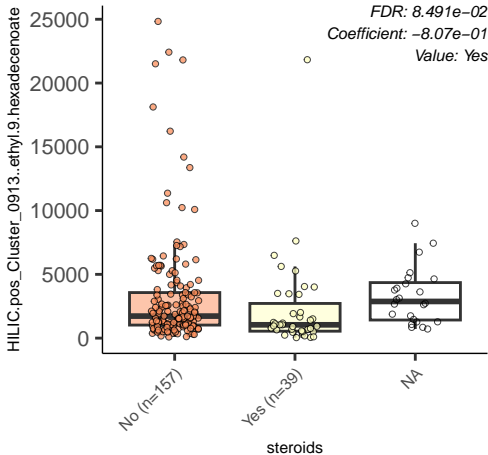


C8.pos_Cluster_1900..cholestenone



C18.neg_Cluster_0250..oleic.acid





HILIC_pos_Cluster_0268..pyridoxamine

FDR: $8.712e-02$
Coefficient: $-7.52e-01$
Value: Yes

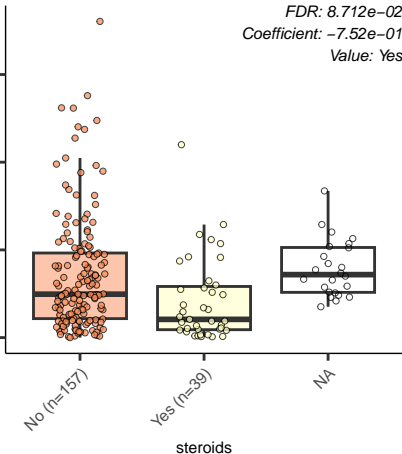
3000
2000
1000
0

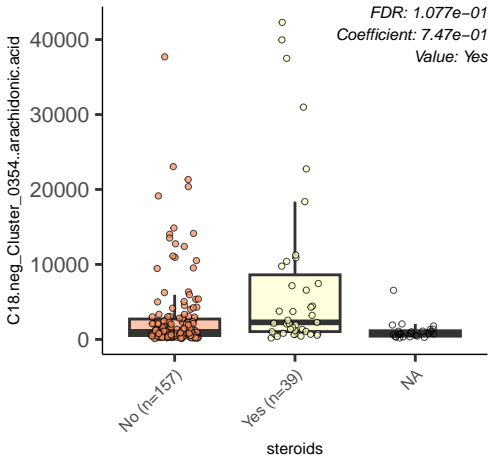
No (n=157)

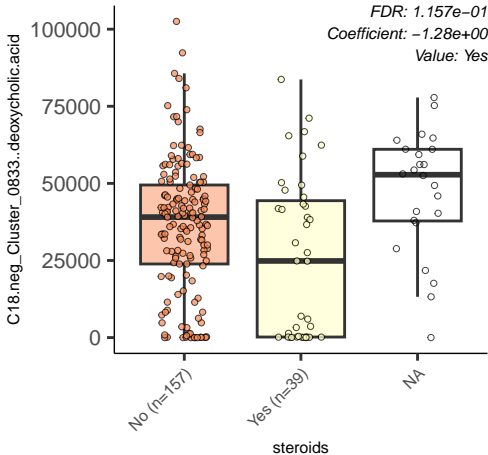
Yes (n=39)

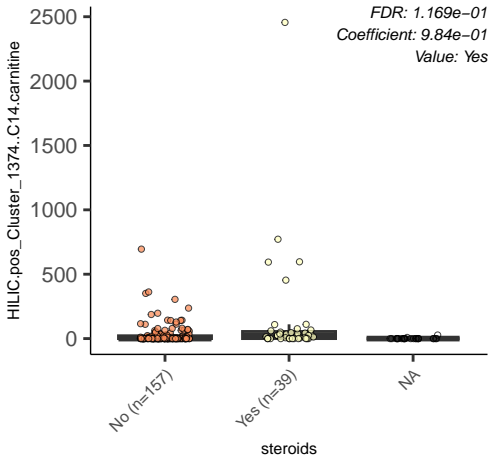
NA

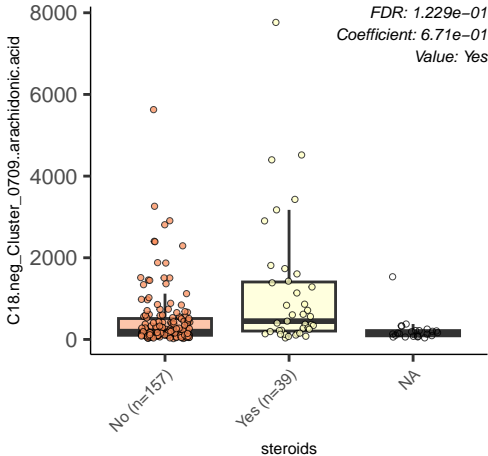
steroids











HILIC_pos_Cluster_1486..C16.carnitine

FDR: 1.267e-01
Coefficient: 1.16e+00
Value: Yes

4000

2000

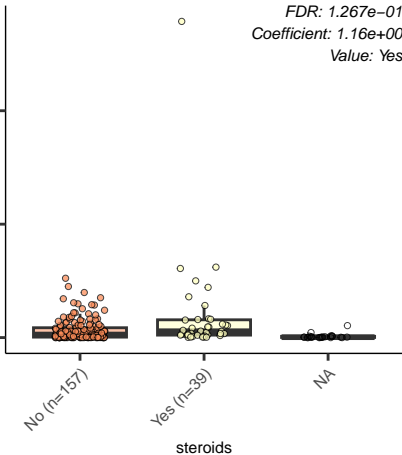
0

No (n=157)

Yes (n=39)

NA

steroids



C18.neg_Cluster_0351..eicosapentaenoic.acid

FDR: 1.272e-01
Coefficient: 8.67e-01
Value: Yes

20000

10000

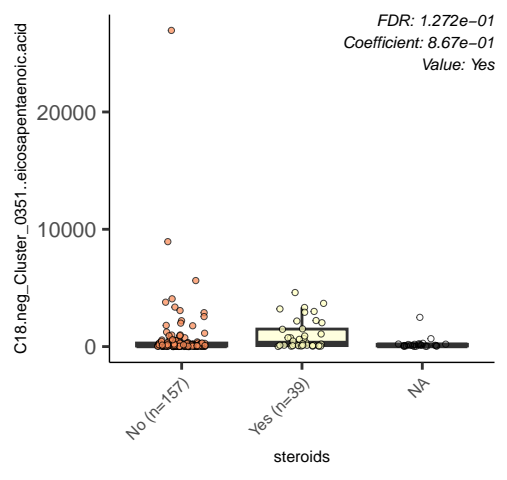
0

No (n=157)

Yes (n=39)

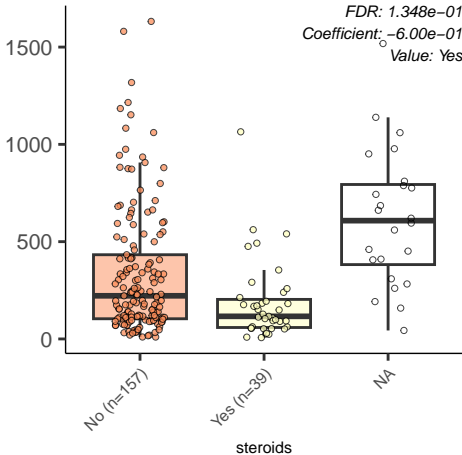
NA

steroids



HILIC.pos_Cluster_0384..N.acetylglutamic.acid

FDR: 1.348e-01
Coefficient: -6.00e-01
Value: Yes



C18.neg_Cluster_1131..arachidonic.acid

FDR: 1.354e-01
Coefficient: 5.40e-01
Value: Yes

3000

2000

1000

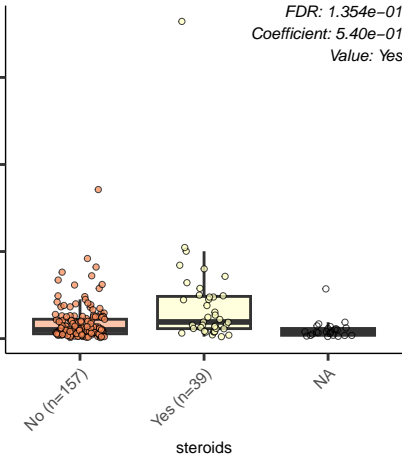
0

No (n=157)

Yes (n=39)

NA

steroids



HILIC.neg_Cluster_0677..cystine

FDR: 1.517e-01
Coefficient: 1.01e+00
Value: Yes

4000

3000

2000

1000

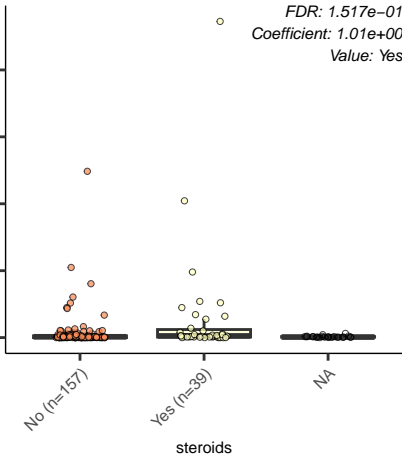
0

No (n=157)

Yes (n=39)

NA

steroids



HILIC_pos_Cluster_0177_4.hydroxy.3.methylacetophenone

FDR: $1.545e-01$
Coefficient: $-6.91e-01$
Value: Yes

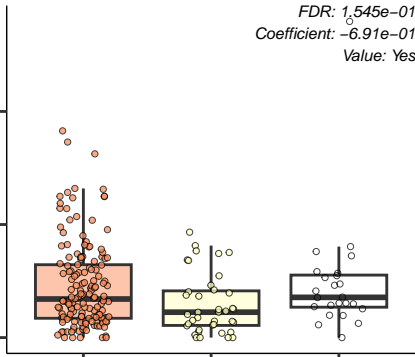
400
200
0

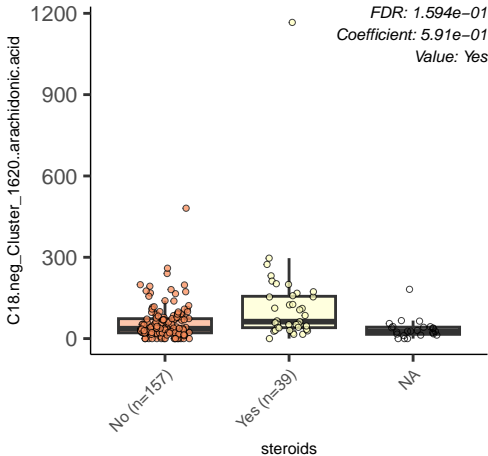
No (n=157)

Yes (n=39)

NA

steroids





HILIC.neg_Cluster_0020..lactate

FDR: 1.729e-01
Coefficient: 8.04e-01
Value: Yes

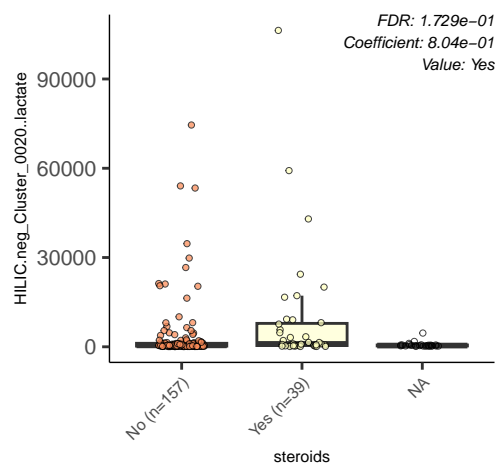
90000
60000
30000
0

No (n=157)

Yes (n=39)

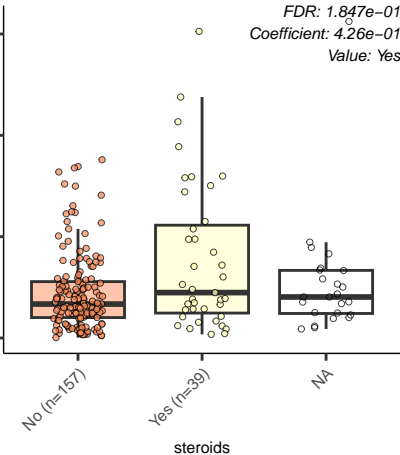
NA

steroids



HILIC.neg_Cluster_0103..acetylaniline

FDR: 1.847e-01
Coefficient: 4.26e-01
Value: Yes



C18.neg_Cluster_1621..cholate

FDR: 1.880e-01
Coefficient: 1.06e+00
Value: Yes

2000

1000

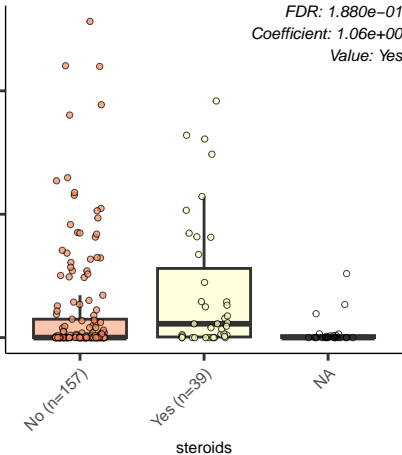
0

No (n=157)

Yes (n=39)

NA

steroids



C18.neg_Cluster_1722..cholate

FDR: 1.910e-01
Coefficient: 9.42e-01
Value: Yes

1000

500

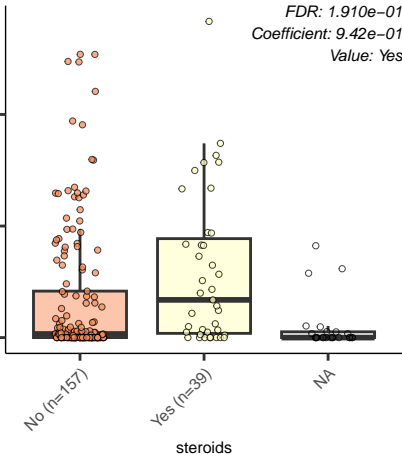
0

No (n=157)

Yes (n=39)

NA

steroids



C18.neg_Cluster_1941..arachidonic.acid

FDR: 1.910e-01
Coefficient: 5.15e-01
Value: Yes

400

200

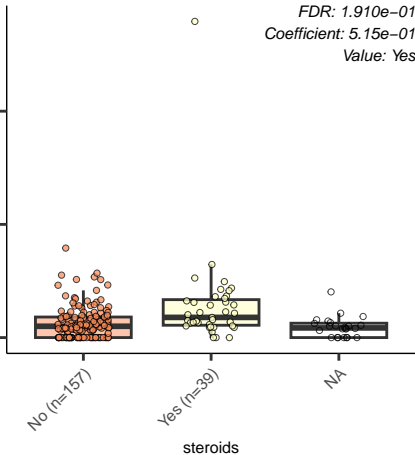
0

No (n=157)

Yes (n=39)

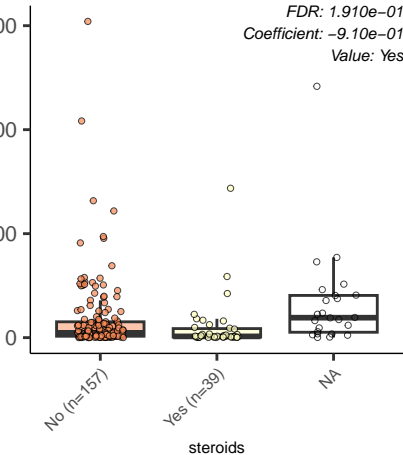
NA

steroids



C8.pos_Cluster_0478..cholestenone

FDR: $1.910e-01$
Coefficient: $-9.10e-01$
Value: Yes



C8.pos_cluster_0166...sphingosine

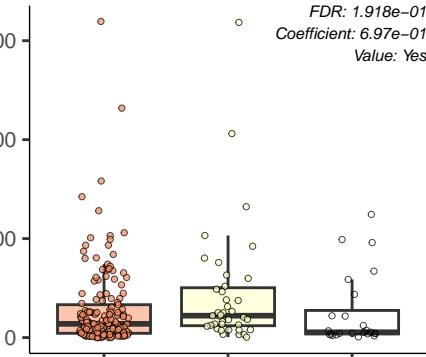
FDR: 1.918e-01
Coefficient: 6.97e-01
Value: Yes

No (n=157)

Yes (n=39)

NA

steroids



HILIC.pos_Cluster_1370..5alpha.cholestanol

FDR: 1.918e-01
Coefficient: -1.33e+00
Value: Yes

400

200

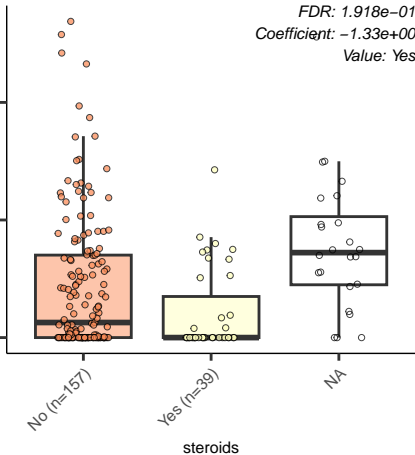
0

No (n=157)

Yes (n=39)

NA

steroids



C18.neg_Cluster_0930..cholate

FDR: 2.008e-01
Coefficient: 9.10e-01
Value: Yes

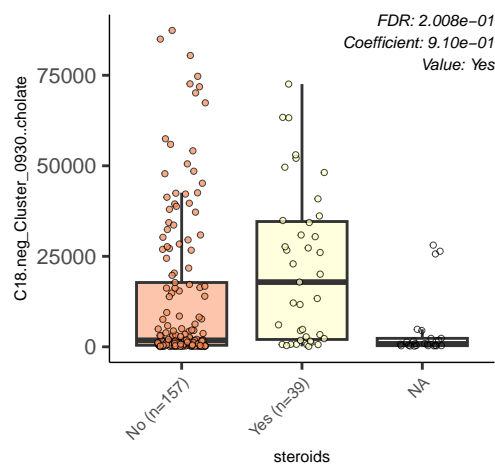
75000
50000
25000
0

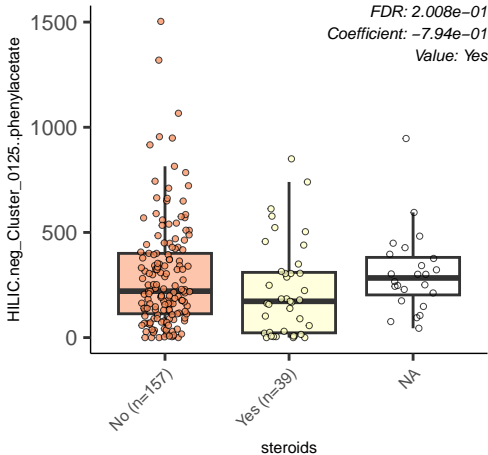
No (n=157)

Yes (n=39)

NA

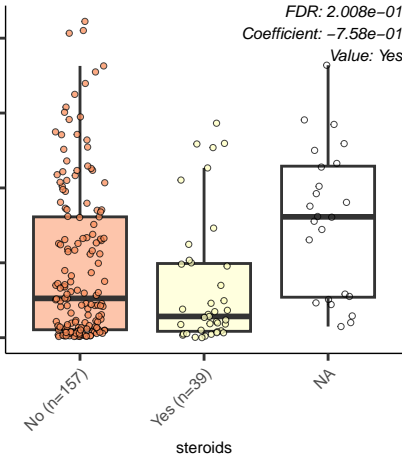
steroids





HILIC.neg_Cluster_0203...orotate

FDR: 2.008e-01
Coefficient: -7.58e-01
Value: Yes



C18.neg_Cluster_0244..alpha.linolenic.acid

FDR: $2.044e-01$
Coefficient: $-8.62e-01$
Value: Yes

$1e+05$

$5e+04$

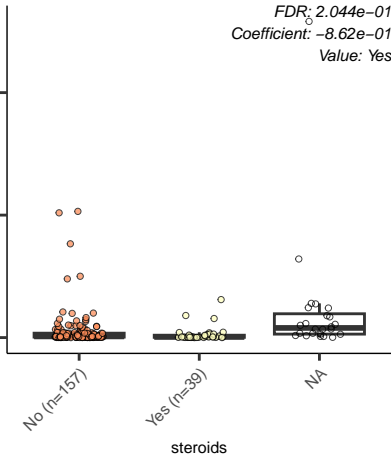
$0e+00$

No (n=157)

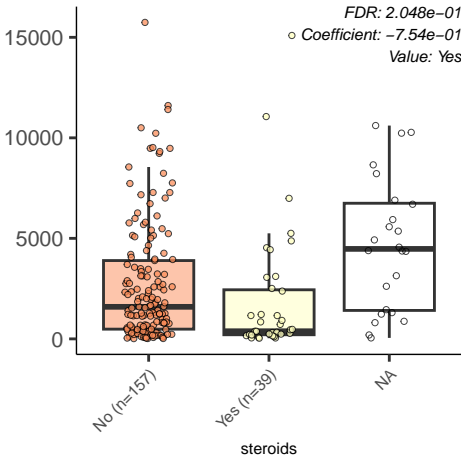
Yes (n=39)

NA

steroids



C8.pos_Cluster_0554..cholestenone



C18.neg_Cluster_0591..eicosatrienoic.acid

FDR: 2.053e-01
Coefficient: 6.96e-01
Value: Yes

400

200

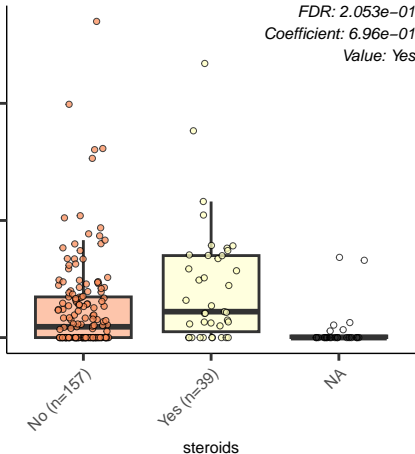
0

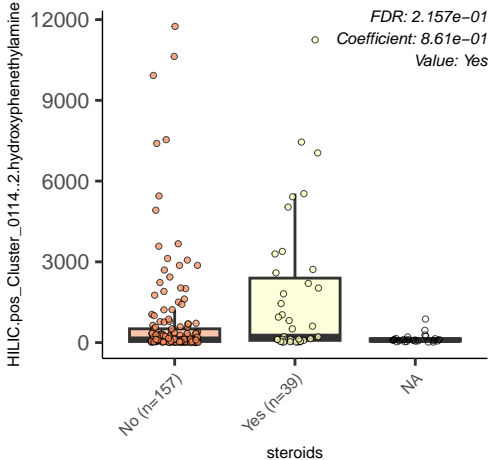
No (n=157)

Yes (n=39)

NA

steroids





C18.neg_Cluster_1275..oleanolic.acid

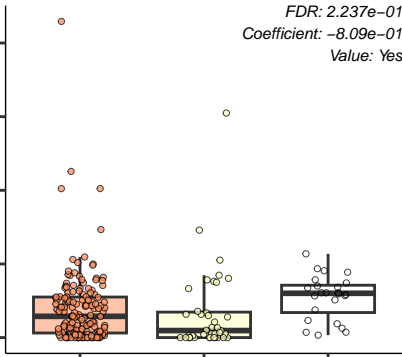
FDR: 2.237e-01
Coefficient: -8.09e-01
Value: Yes

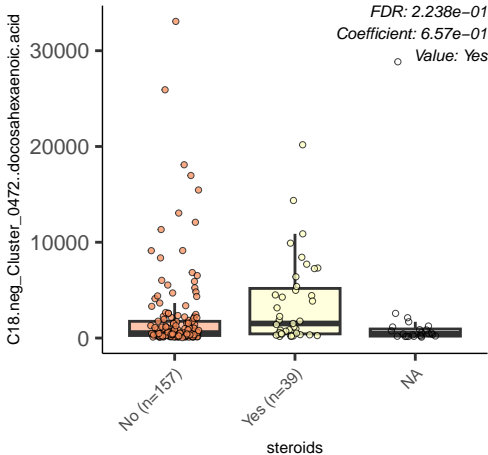
No (n=157)

Yes (n=39)

NA

steroids





HILIC.pos_Cluster_0540..pantothenate

FDR: 2.273e-01
Coefficient: -4.25e-01
Value: Yes

10000

5000

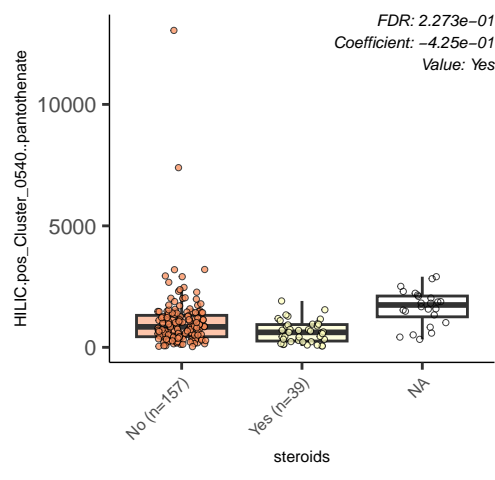
0

No (n=157)

Yes (n=39)

NA

steroids



C18.neg_Cluster_1258..cholate

FDR: 2.369e-01
Coefficient: 8.71e-01
Value: Yes

1e+05

5e+04

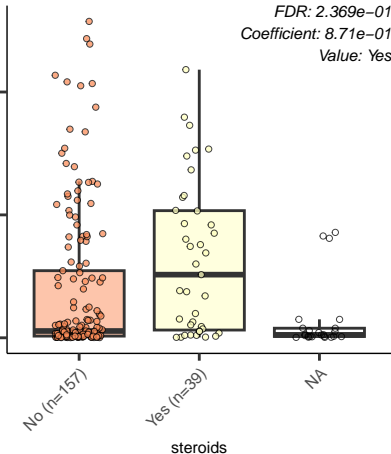
0e+00

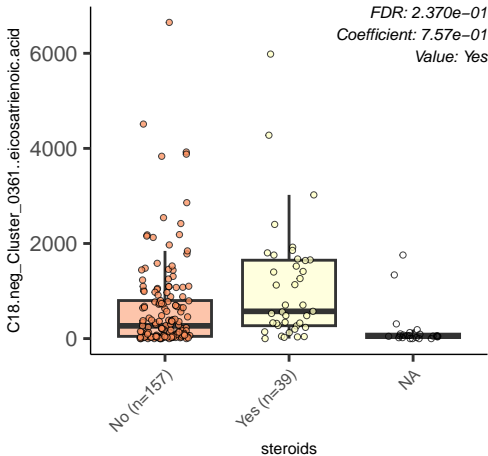
No (n=157)

Yes (n=39)

NA

steroids





HILIC.neg_Cluster_0372..N.acetylglutamate

FDR: $2.397e-01$
Coefficient: $-4.15e-01$
Value: Yes

