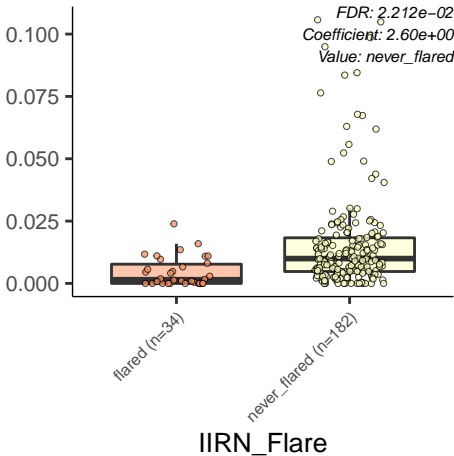


Thymidine\_241.1



Oleic.acid\_281.2

30

20

10

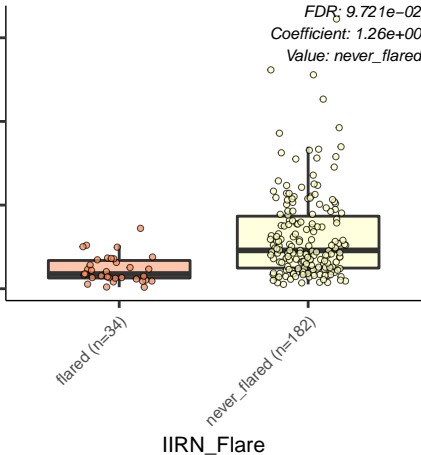
0

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

FDR:  $9.721e-02$   
Coefficient:  $1.26e+00$   
Value: never\_flared



Succinic.Acid\_117

FDR:  $9.721e-02$

Coefficient:  $-1.65e+00$

Value: never\_flared

10

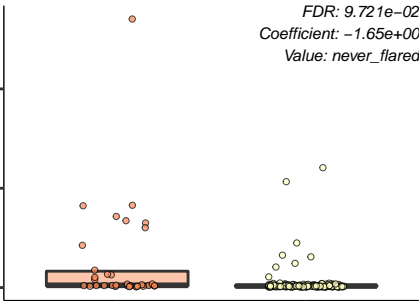
5

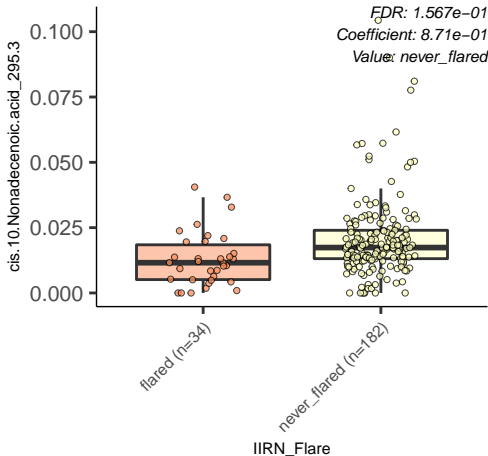
0

flared (n=34)

never\_flared (n=182)

IIRN\_Flare





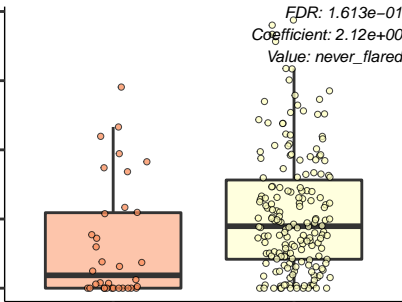
Benzyl.Alcohol\_107.1

FDR: 1.613e-01  
Coefficient: 2.12e+00  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare



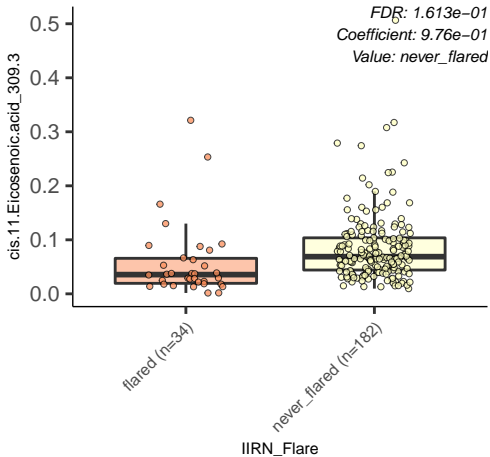
cis.11.Eicosenoic.acid\_309.3

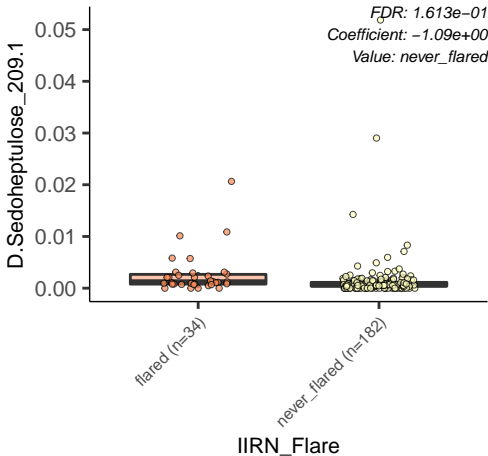
*FDR: 1.613e-01*  
*Coefficient: 9.76e-01*  
*Value: never\_flared*

flared (n=34)

never\_flared (n=182)

IIRN\_Flare





Malonate\_103

*FDR: 1.613e-01*

*Coefficient: -6.13e-01*

*Value: never\_flared*

0.3

0.2

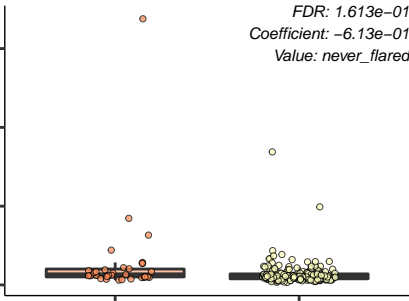
0.1

0.0

flared (n=34)

never\_flared (n=182)

IIRN\_Flare





Methylguanidine\_74.1

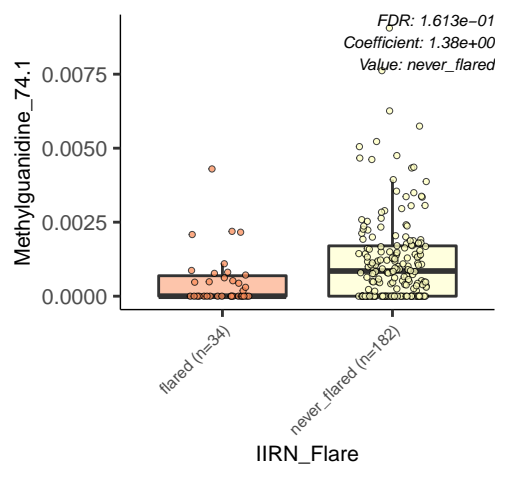
FDR: 1.613e-01  
Coefficient: 1.38e+00  
Value: never\_flared

flared (n=34)

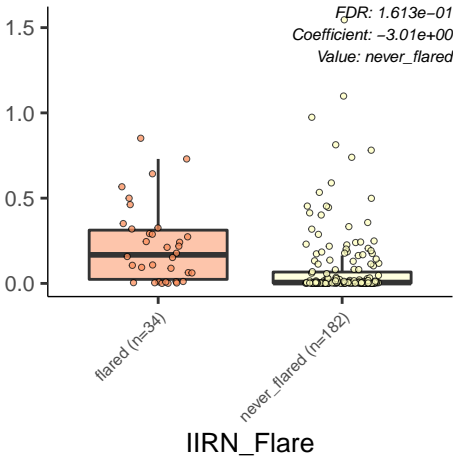
never\_flared (n=182)

IIRN\_Flare

0.0075  
0.0050  
0.0025  
0.0000



Taurine\_124



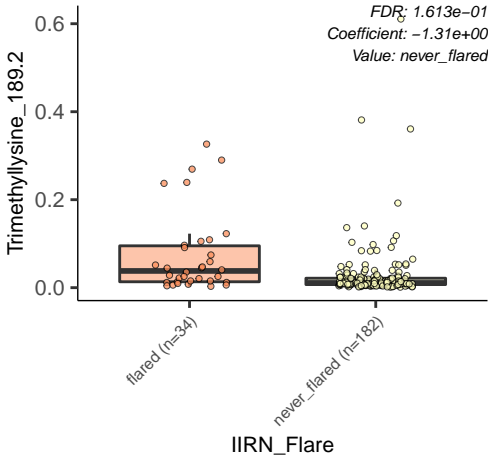
Trimethyllysine\_189.2

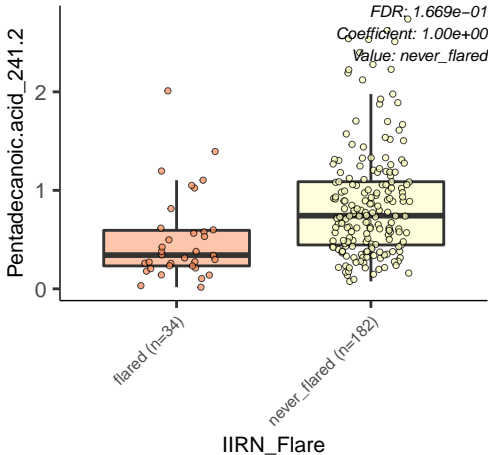
FDR: 1.613e-01  
Coefficient: -1.31e+00  
Value: never\_flared

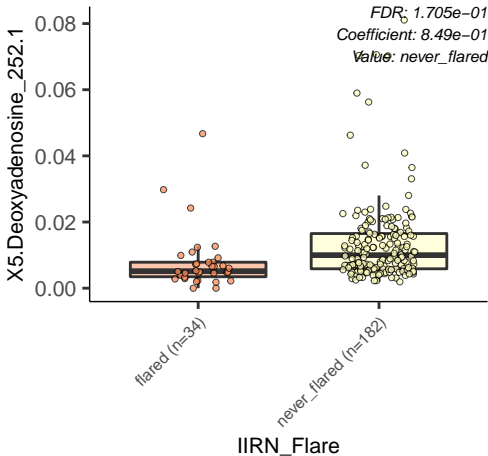
flared (n=34)

never\_flared (n=182)

IIRN\_Flare







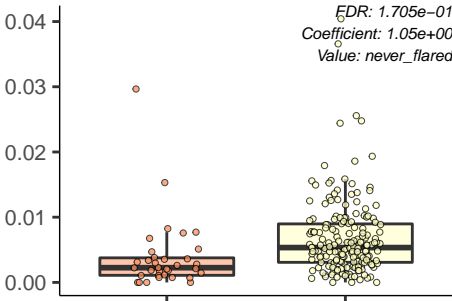
Kynurenate\_188

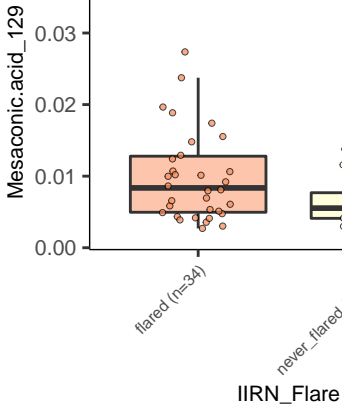
FDR: 1.705e-01  
Coefficient: 1.05e+00  
Value: never\_flared

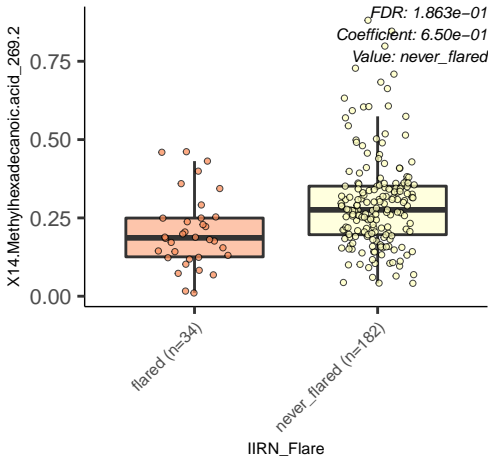
flared (n=34)

never\_flared (n=182)

IIRN\_Flare









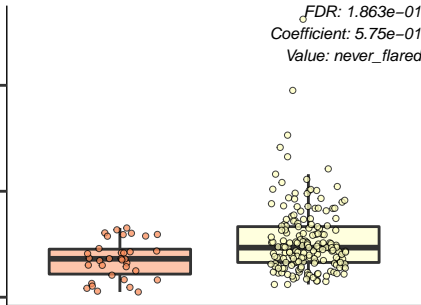
X4.Acetamidobutanoate\_146.1

FDR: 1.863e-01  
Coefficient: 5.75e-01  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare



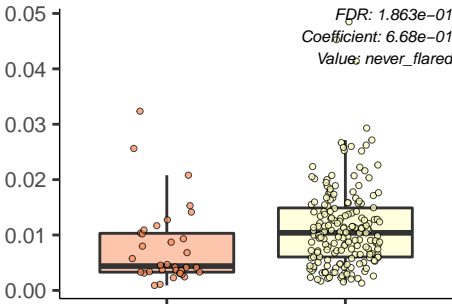
Biotin\_245.1

FDR: 1.863e-01  
Coefficient: 6.68e-01  
Value: never\_flared

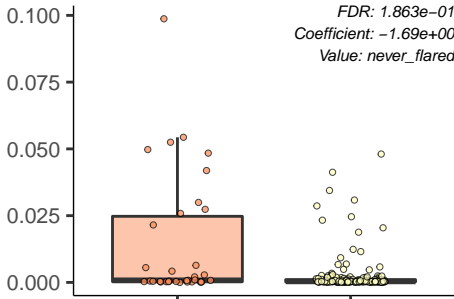
flared (n=34)

never\_flared (n=182)

IIRN\_Flare



Creatine\_130.1



FDR: 1.863e-01  
Coefficient: -1.69e+00  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

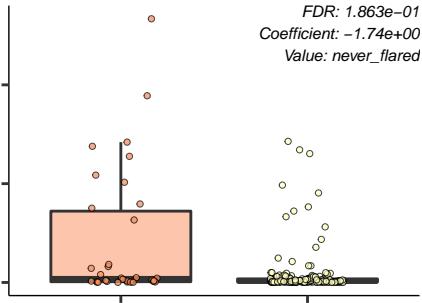
Creatine\_132.1

FDR: 1.863e-01  
Coefficient: -1.74e+00  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

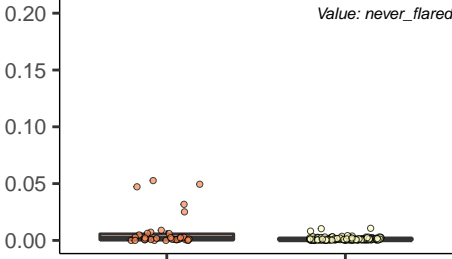




FDR: 1.863e-01

*Coefficient: -8.75e-01*

Value: never\_flared



flared (n=34)

never\_flared (n=182)

IIRN\_Flare

Palmitoleic.acid\_253.2

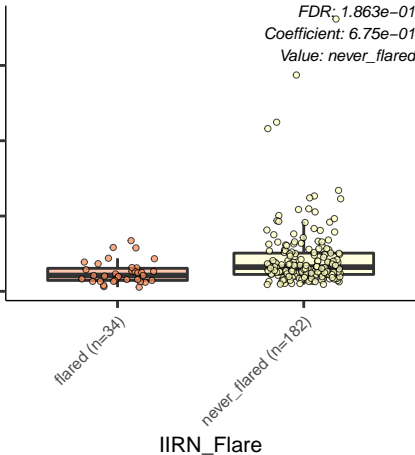
*FDR: 1.863e-01*  
*Coefficient: 6.75e-01*  
*Value: never\_flared*

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

1.5  
1.0  
0.5  
0.0



Pentanoate\_101.1

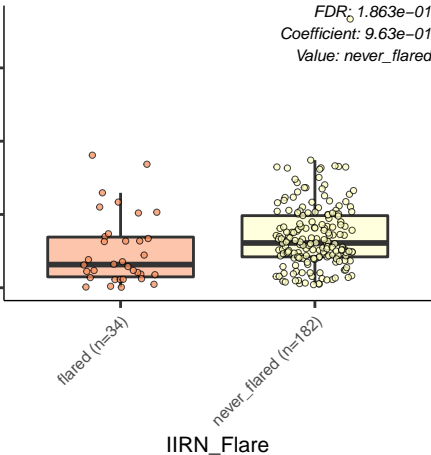
FDR: 1.863e-01  
Coefficient: 9.63e-01  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

6  
4  
2  
0



Pipecolate\_130.1

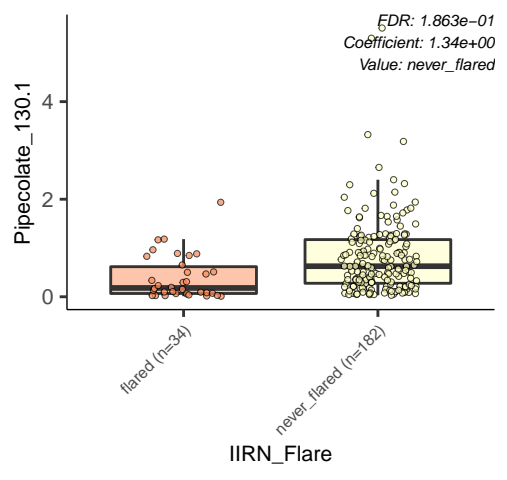
EDR: 1.863e-01  
Coefficient: 1.34e+00  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

4  
2  
0





Raffinose\_503.2

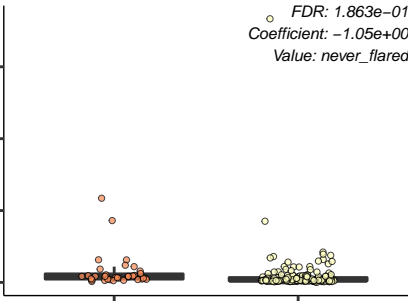
FDR: 1.863e-01  
Coefficient: -1.05e+00  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

0.3  
0.2  
0.1  
0.0



Thymine\_125

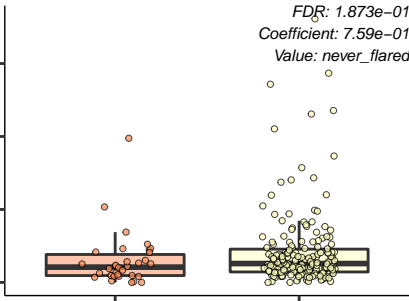
*FDR: 1.873e-01*  
*Coefficient: 7.59e-01*  
*Value: never\_flared*

0.6  
0.4  
0.2  
0.0

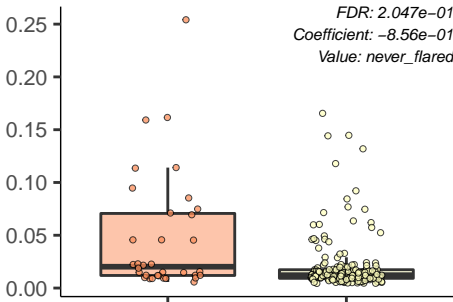
flared (n=34)

never\_flared (n=182)

IIRN\_Flare



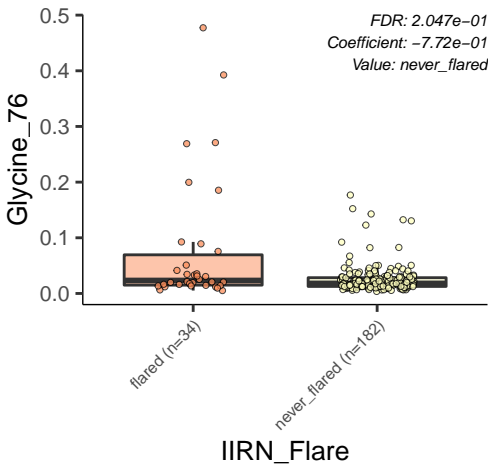
Fructose\_179.1



flared (n=34)

never\_flared (n=182)

IIRN\_Flare



Myo.Inositol\_179.1

*FDR: 2.047e-01*  
*Coefficient: -8.43e-01*  
*Value: never\_flared*

0.10

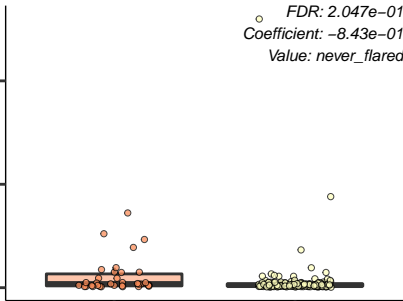
0.05

0.00

flared (n=34)

never\_flared (n=182)

IIRN\_Flare



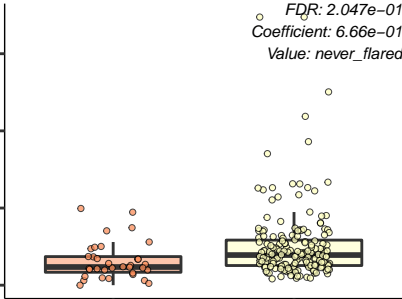
N.Acetylmethionine\_192.1

FDR: 2.047e-01  
Coefficient: 6.66e-01  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare



Quinolinate\_166

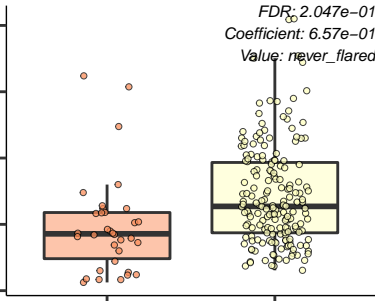
0.0100  
0.0075  
0.0050  
0.0025  
0.0000

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

FDR: 2.047e-01  
Coefficient: 6.57e-01  
Value: never\_flared



Stachyose\_665.2

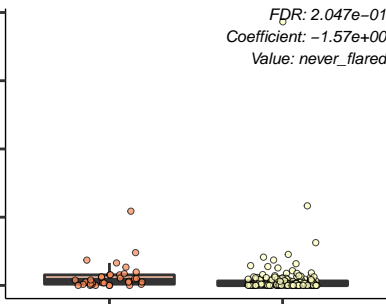
0.100  
0.075  
0.050  
0.025  
0.000

*FDR: 2.047e-01*  
*Coefficient: -1.57e+00*  
*Value: never\_flared*

flared (n=34)

never\_flared (n=182)

IIRN\_Flare





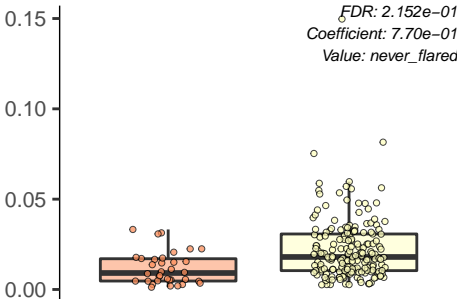
X4.Pyridoxate\_184.1

FDR: 2.152e-01  
Coefficient: 7.70e-01  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare



Ascorbic.acid\_175

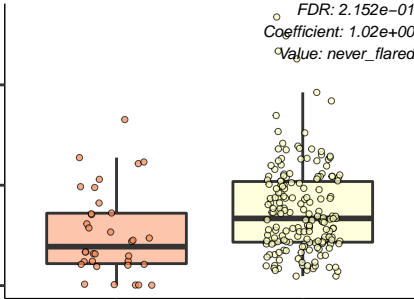
FDR: 2.152e-01  
Coefficient: 1.02e+00  
Value: never\_flared

flared (n=34)

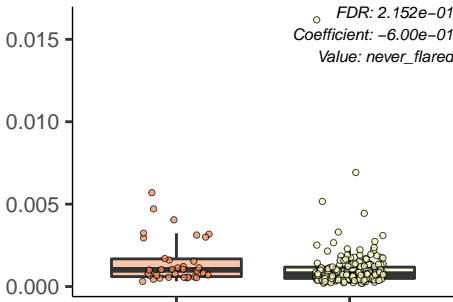
never\_flared (n=182)

IIRN\_Flare

1.0  
0.5  
0.0



Hypotaurnine\_110



flared (n=34)

never\_flared (n=182)

IIRN\_Flare

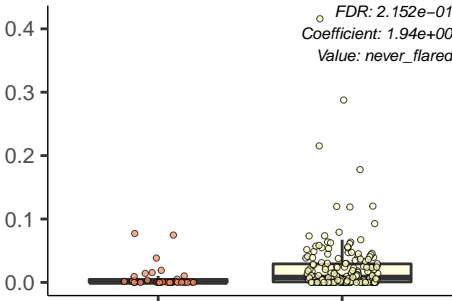
Melatonin\_233.1

FDR: 2.152e-01  
Coefficient: 1.94e+00  
Value: never\_flared

flared (n=34)

never\_flared (n=182)

IIRN\_Flare



Oxoglutarate\_145

*FDR: 2.152e-01*  
*Coefficient: 9.78e-01*  
*Value: never\_flared*

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

0.4

0.2

0.0

Stachydrine\_144.1

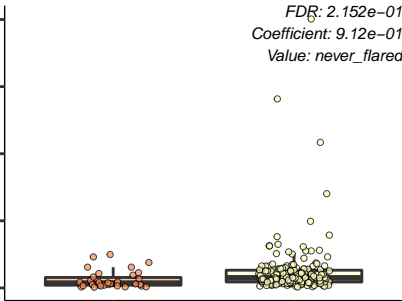
10.0  
7.5  
5.0  
2.5  
0.0

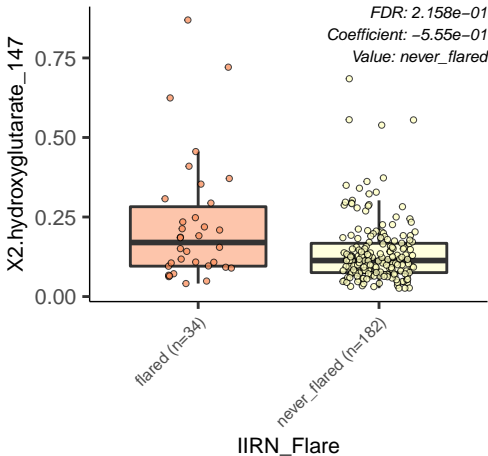
*FDR: 2.152e-01*  
*Coefficient: 9.12e-01*  
*Value: never\_flared*

flared (n=34)

never\_flared (n=182)

IIRN\_Flare





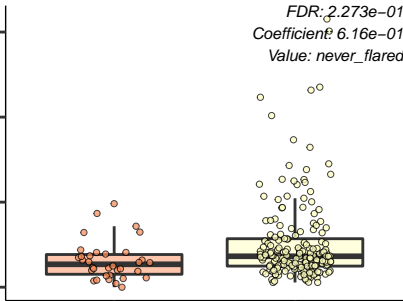
Deoxyguanosine\_268.1

*FDR: 2.273e-01*  
*Coefficient: 6.16e-01*  
*Value: never\_flared*

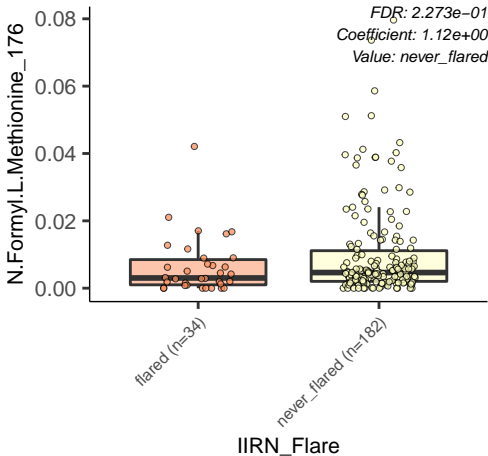
flared (n=34)

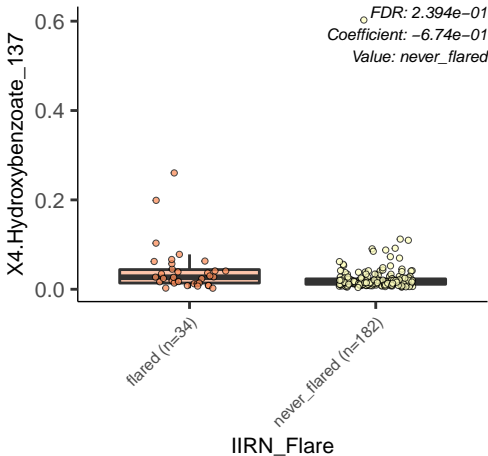
never\_flared (n=182)

IIRN\_Flare

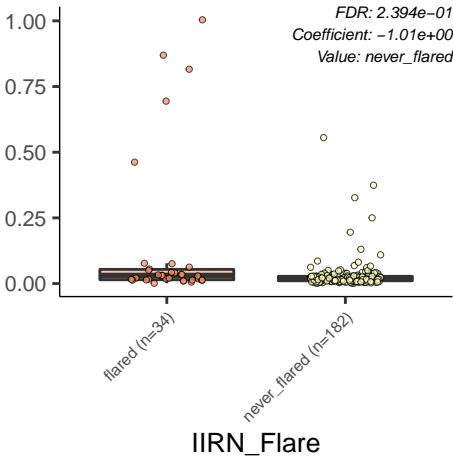








Histidine\_156.1



Erucic.acid\_337.3

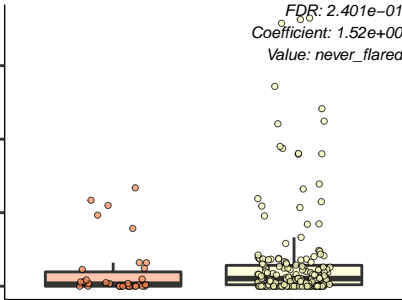
*FDR: 2.401e-01*  
*Coefficient: 1.52e+00*  
*Value: never\_flared*

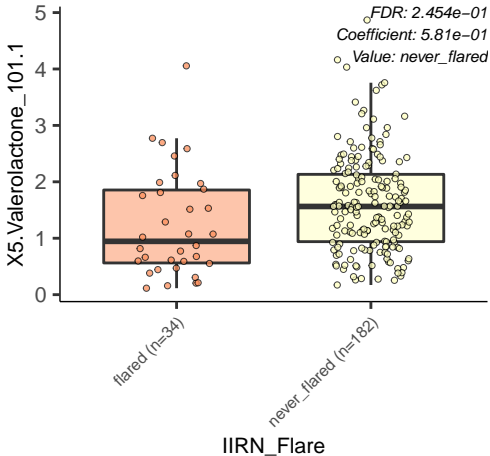
flared (n=34)

never\_flared (n=182)

IIRN\_Flare

0.00  
0.05  
0.10  
0.15





Uridine\_245.1

FDR:  $2.454e-01$   
Coefficient:  $5.61e-01$   
Value: never\_flared

0.002

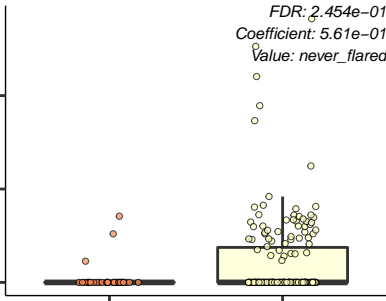
0.001

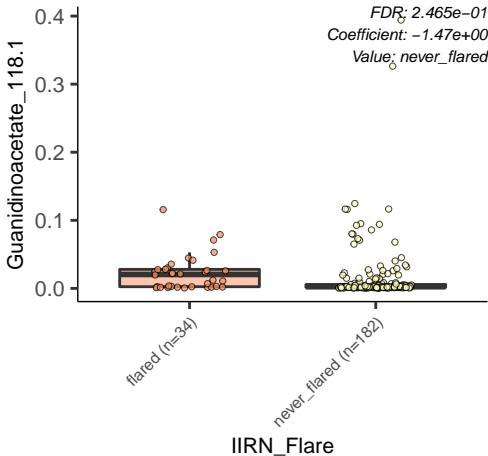
0.000

flared (n=34)

never\_flared (n=182)

IIRN\_Flare





Trehalose\_341.1

*FDR: 2.465e-01*

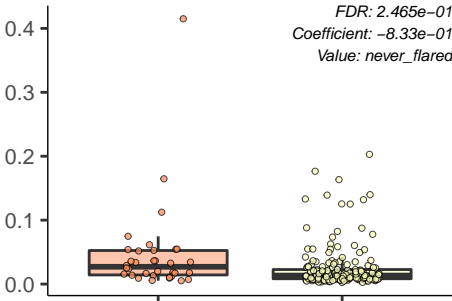
*Coefficient: -8.33e-01*

*Value: never\_flared*

flared (n=34)

never\_flared (n=182)

IIRN\_Flare





Urocanate\_139.1

*FDR: 2.465e-01*  
*Coefficient: 8.60e-01*  
*Value: never\_flared*

flared (n=34)

never\_flared (n=182)

IIRN\_Flare

