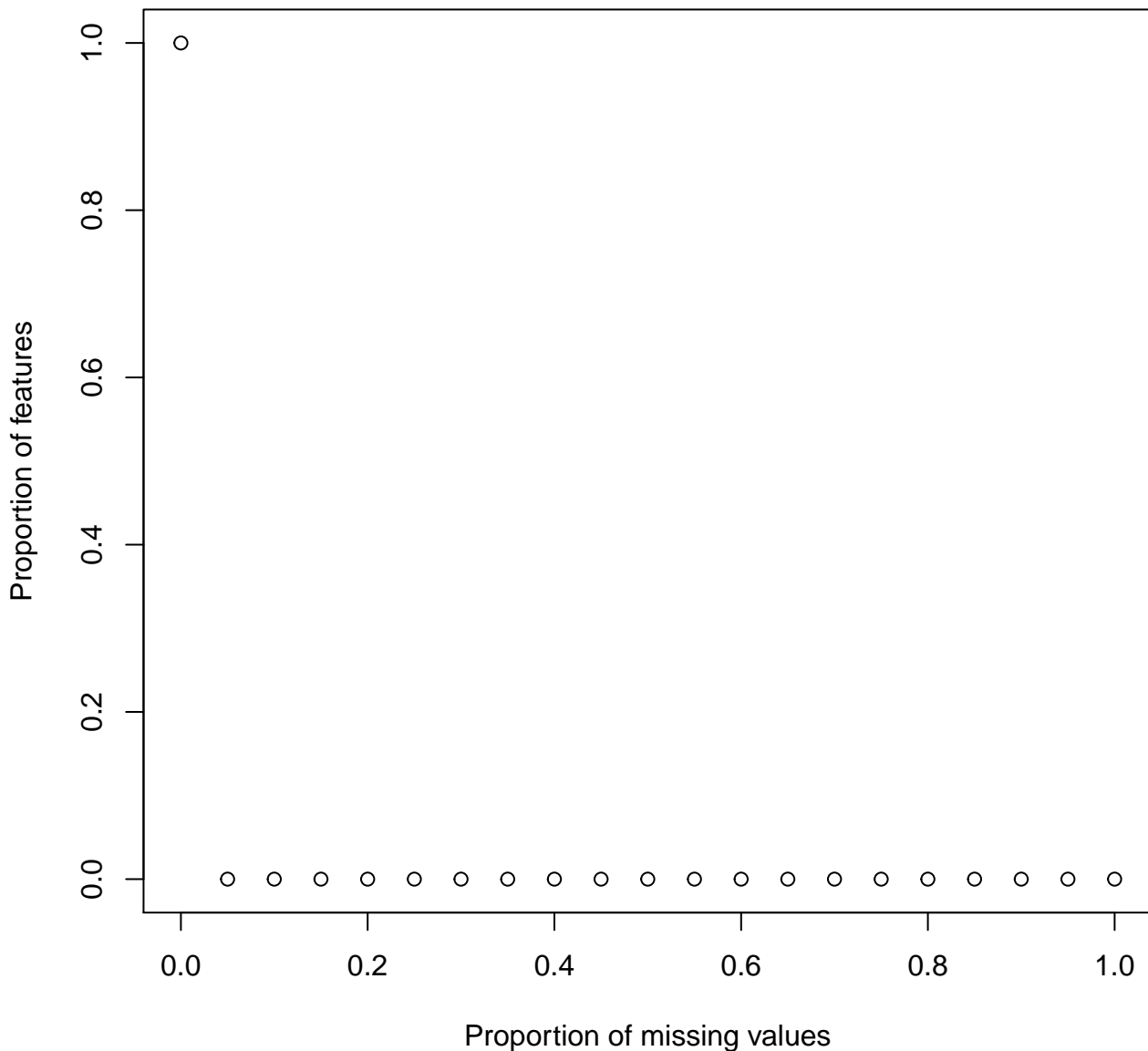
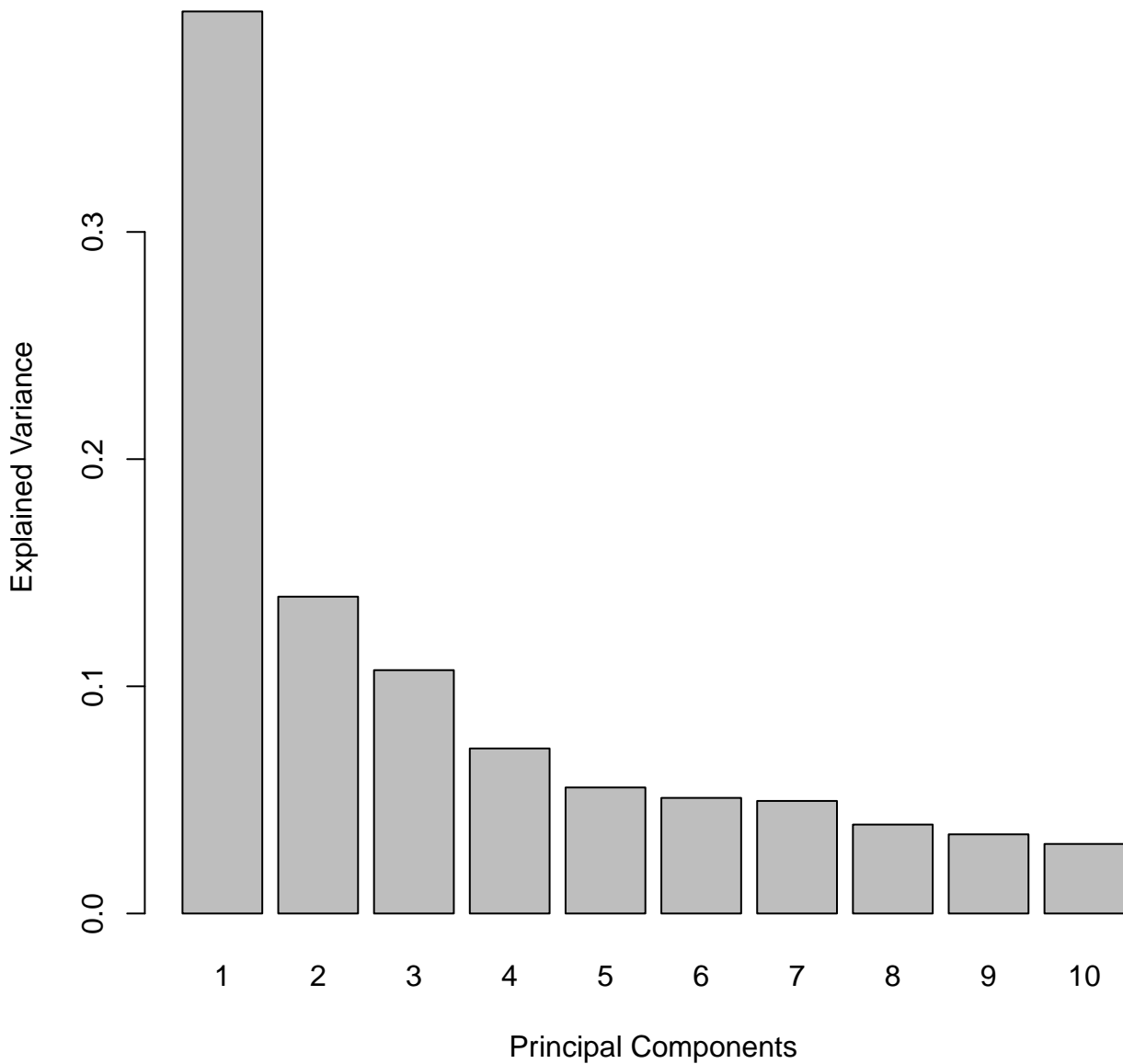


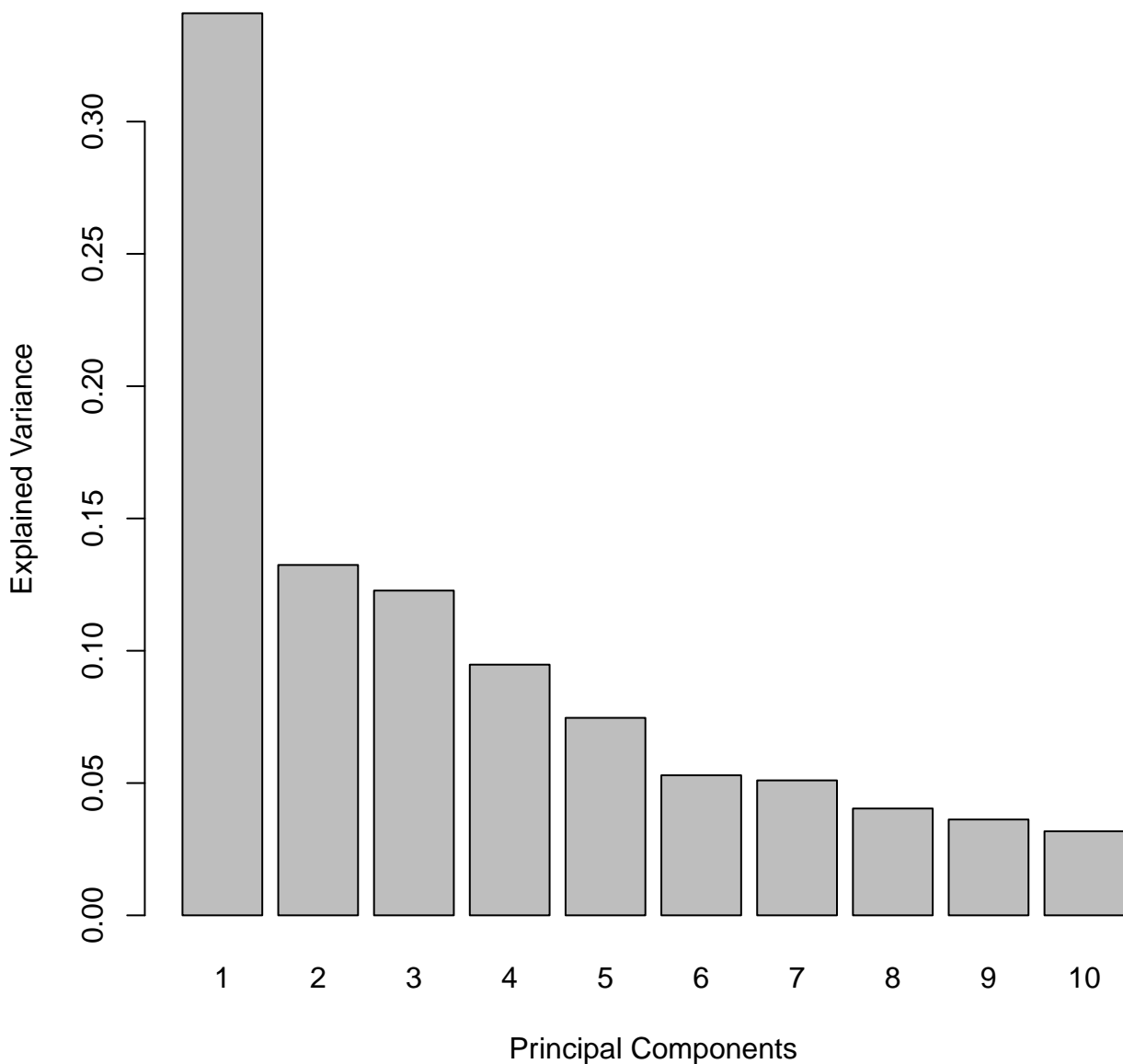
# RNA\_Seq missing value proportions for unfiltered data



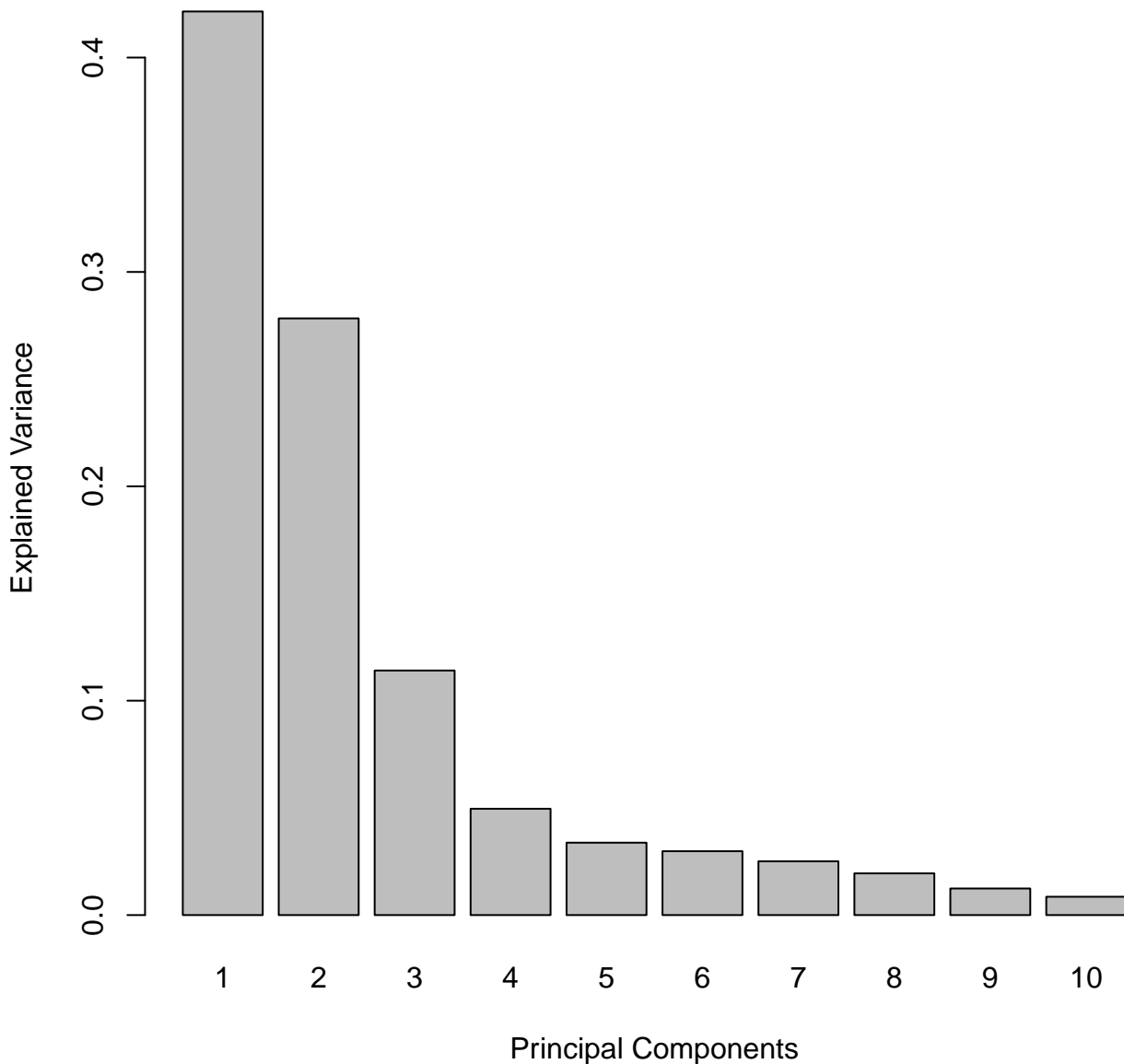
# Metabolomics screeplot



# Proteomics screeplot

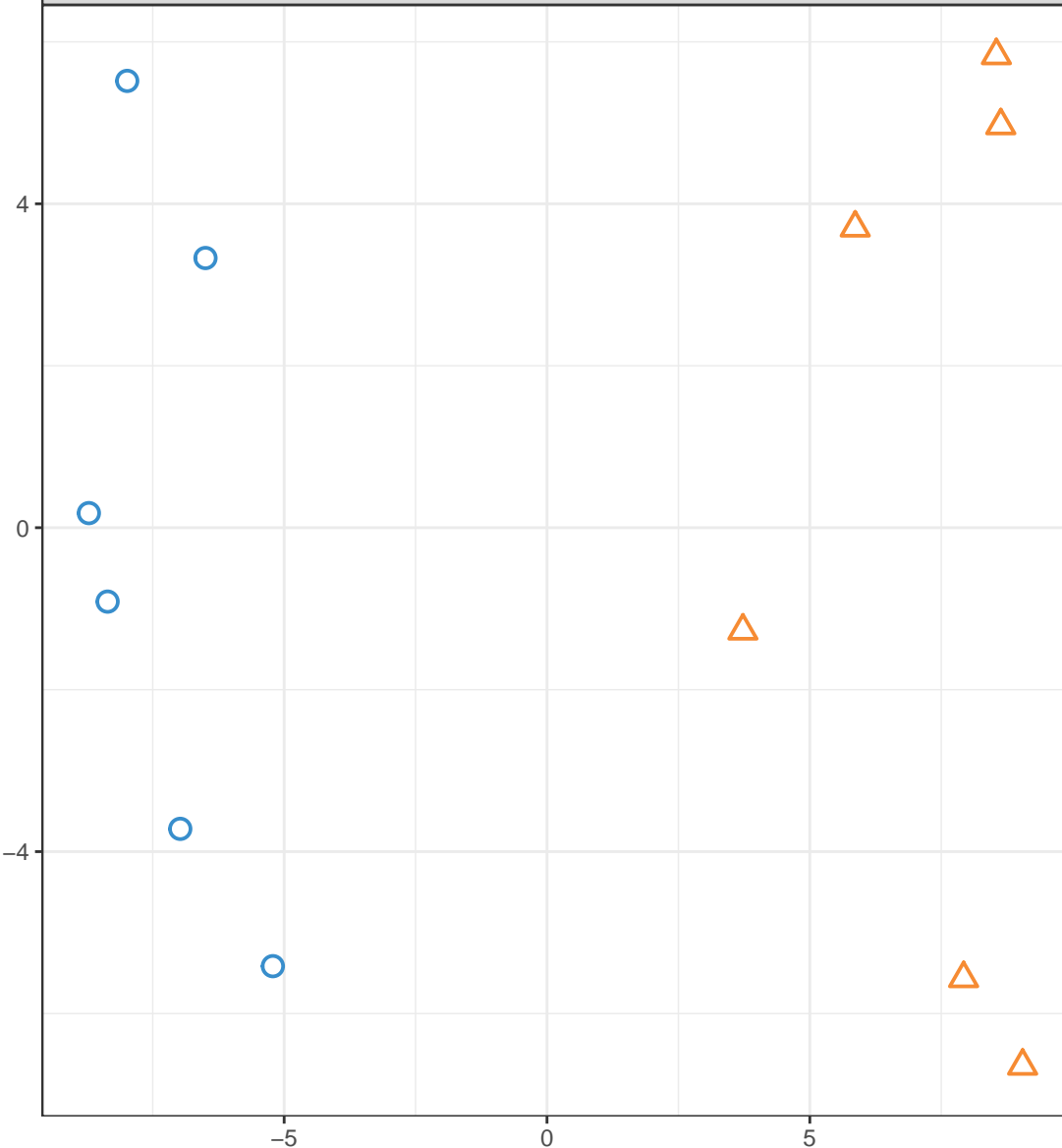


# RNA\_Seq screeplot



**No Impute n\_PCs = 10**  
**Metabolomics PCs (1,2)**

PC2: 14% expl. var

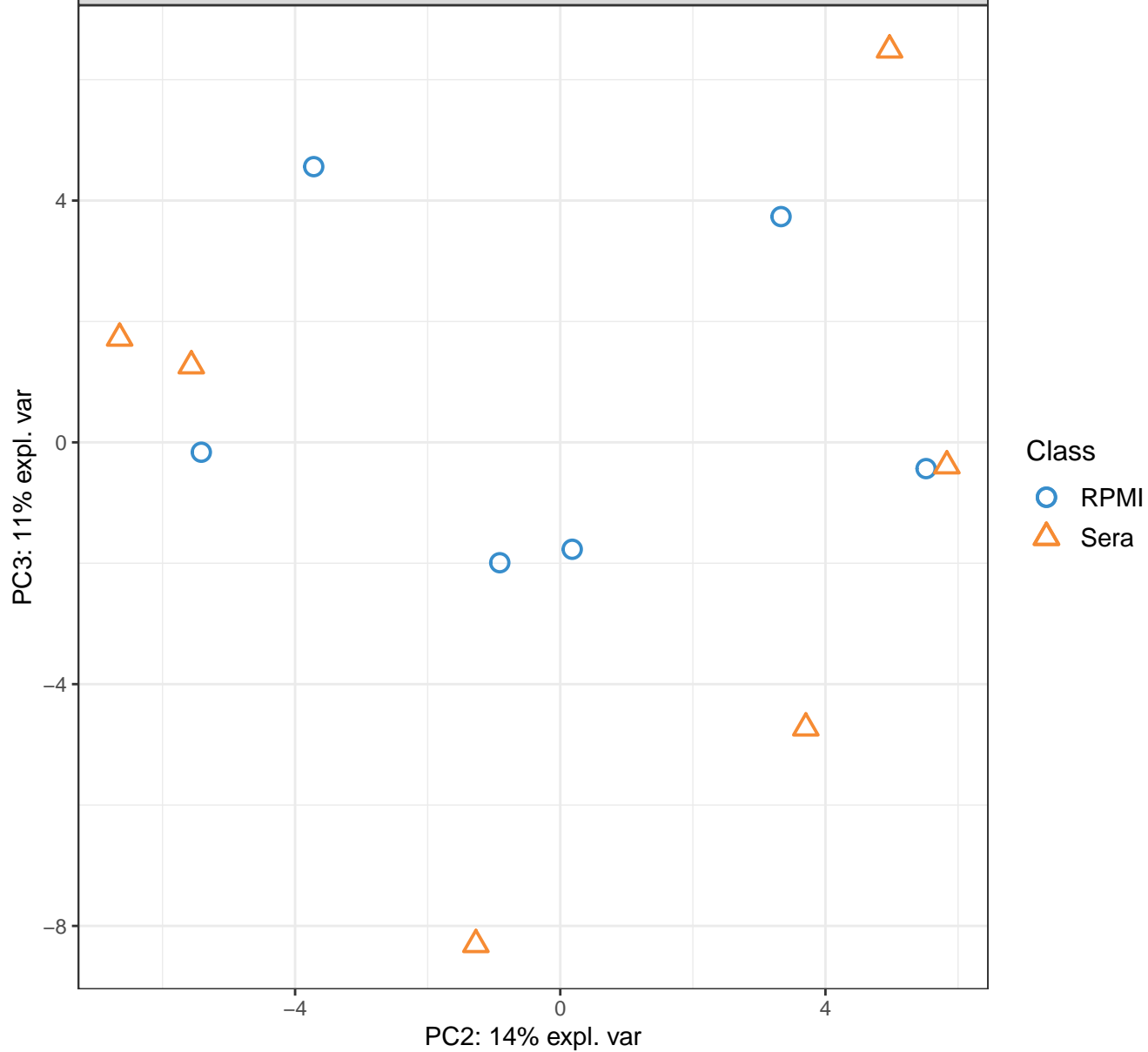


Class

○ RPMI  
△ Sera

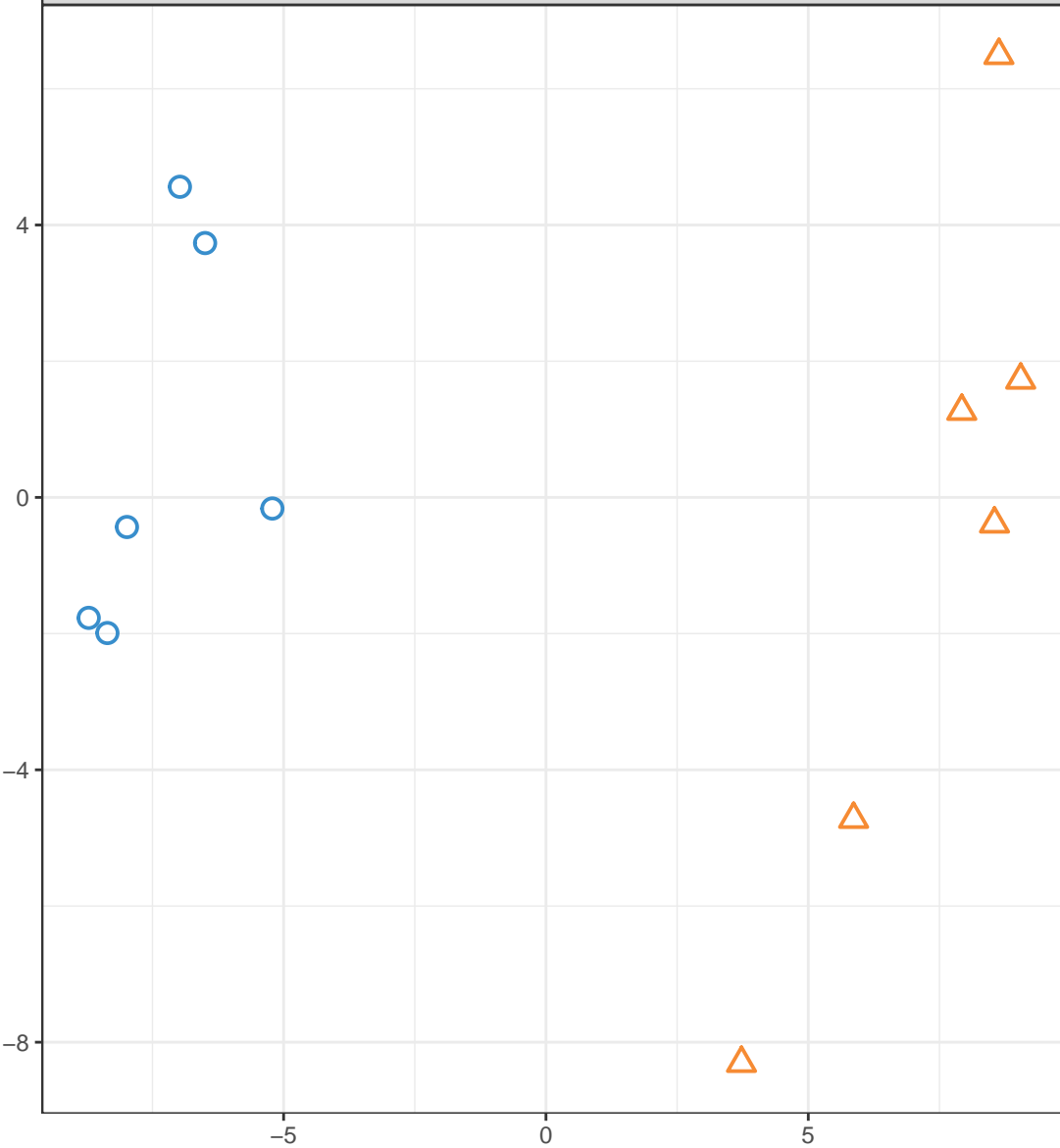
PC1: 40% expl. var

**No Impute n\_PCs = 10**  
**Metabolomics PCs (2,3)**



**No Impute n\_PCs = 10**  
**Metabolomics PCs (1,3)**

PC3: 11% expl. var

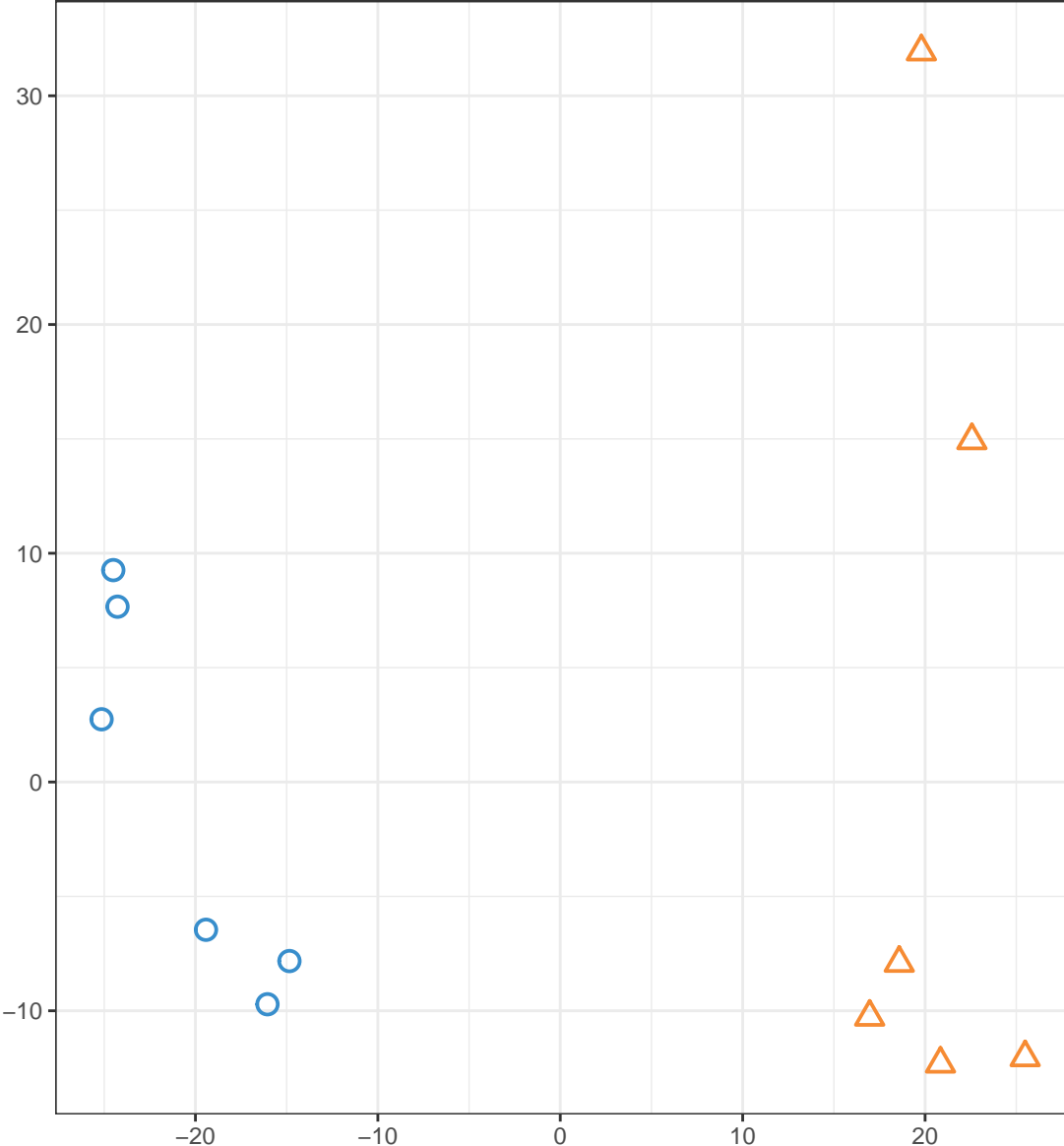


Class

○ RPMI  
△ Sera

**No Impute n\_PCs = 10**  
**Proteomics PCs (1,2)**

PC2: 13% expl. var



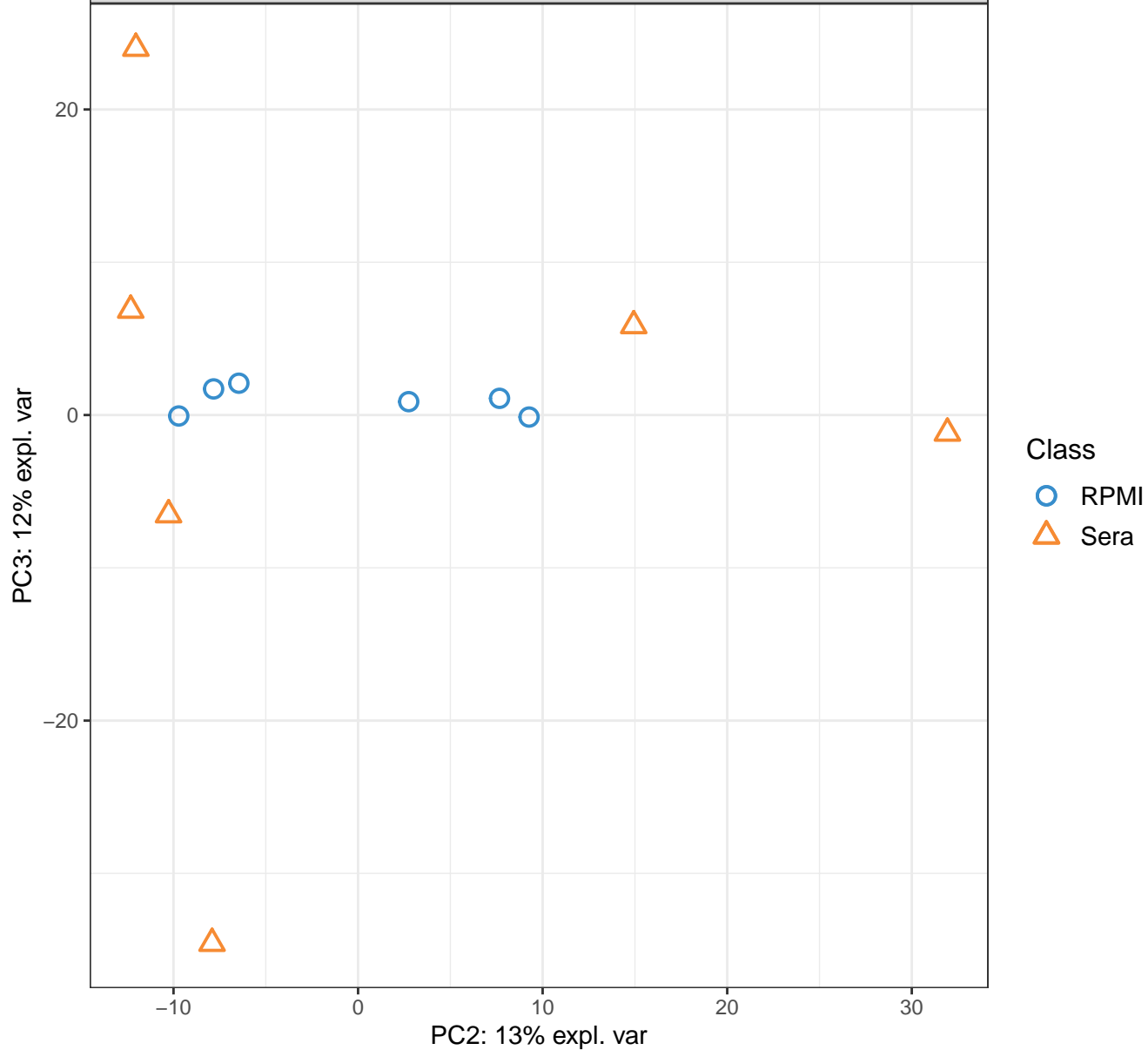
Class

○ RPMI  
△ Sera

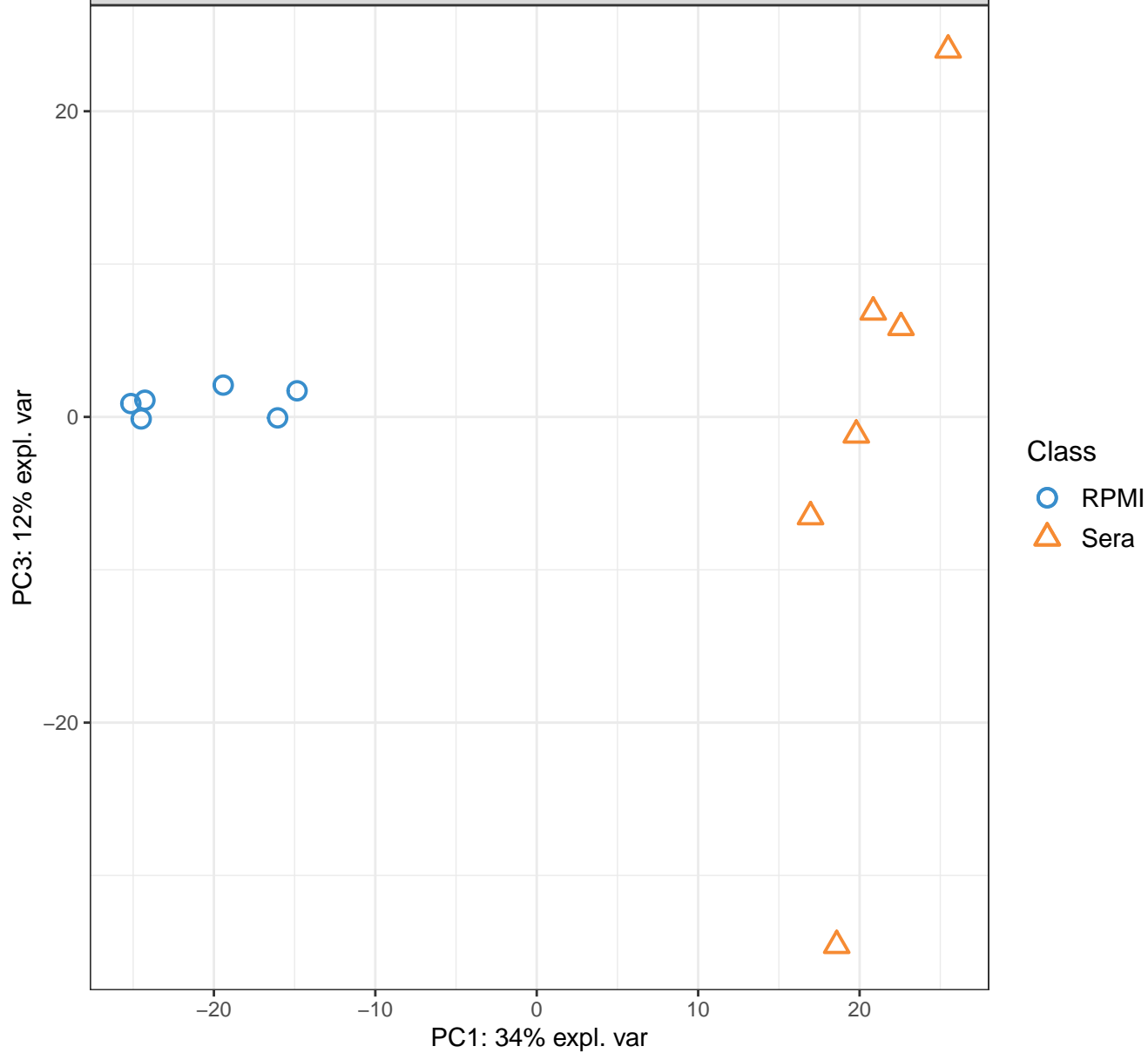
PC1: 34% expl. var



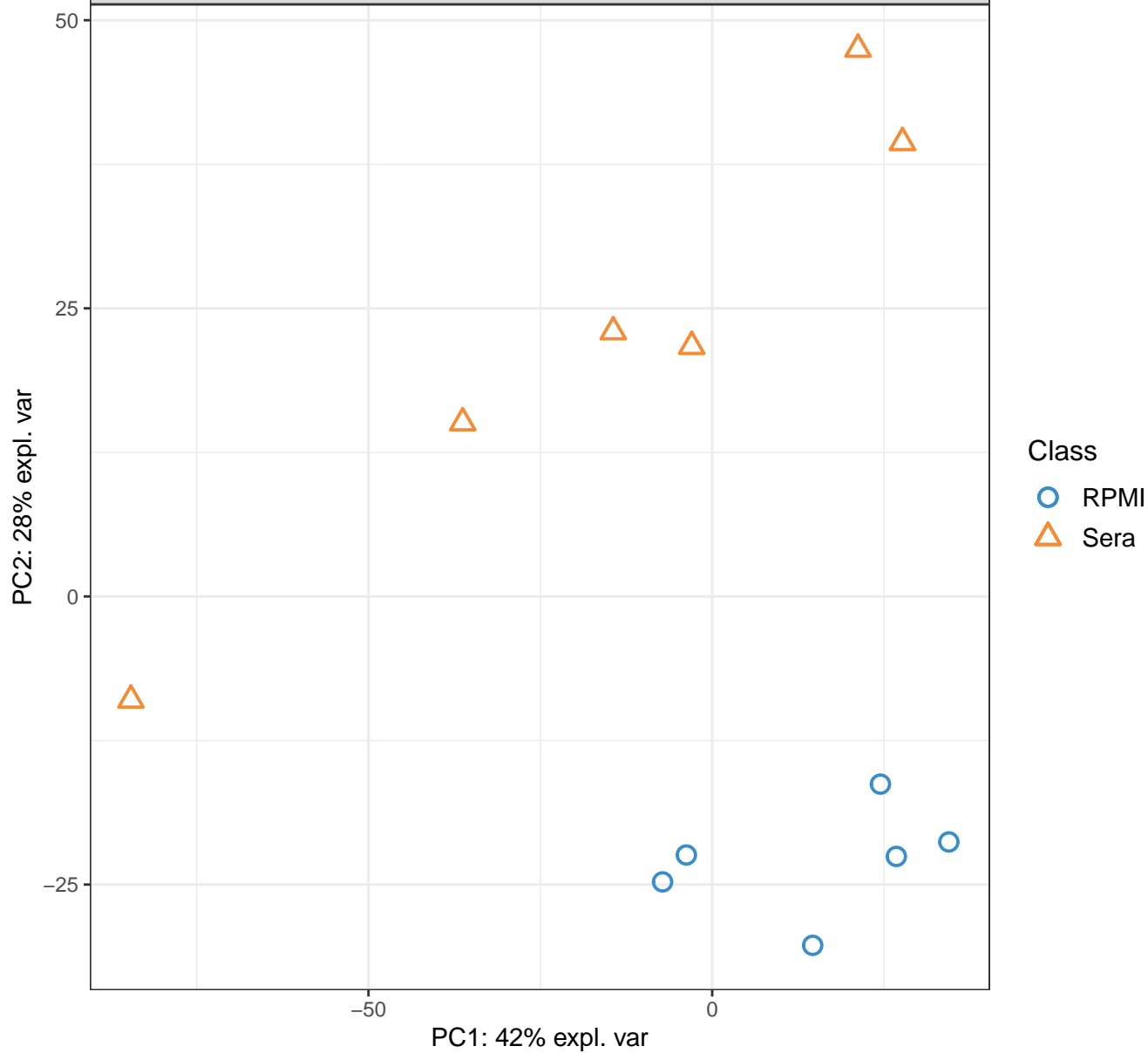
**No Impute n\_PCs = 10**  
**Proteomics PCs (2,3)**



**No Impute n\_PCs = 10**  
**Proteomics PCs (1,3)**

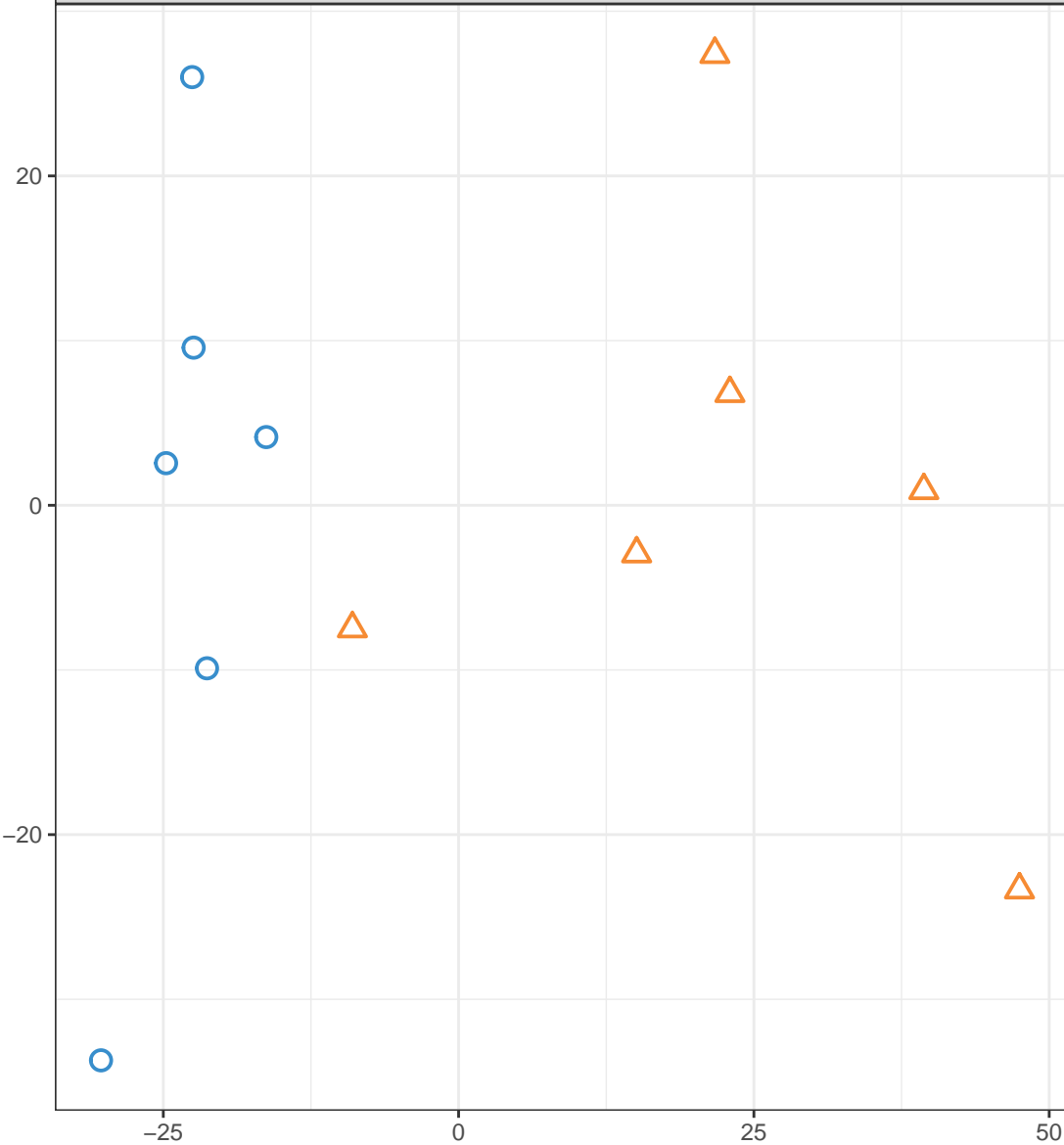


No Impute n\_PCs = 10  
RNA\_Seq PCs (1,2)



No Impute n\_PCs = 10  
RNA\_Seq PCs (2,3)

PC3: 11% expl. var



Class

○ RPMI  
△ Sera

No Impute n\_PCs = 10  
RNA\_Seq PCs (1,3)

PC3: 11% expl. var

20

0

-20

-50

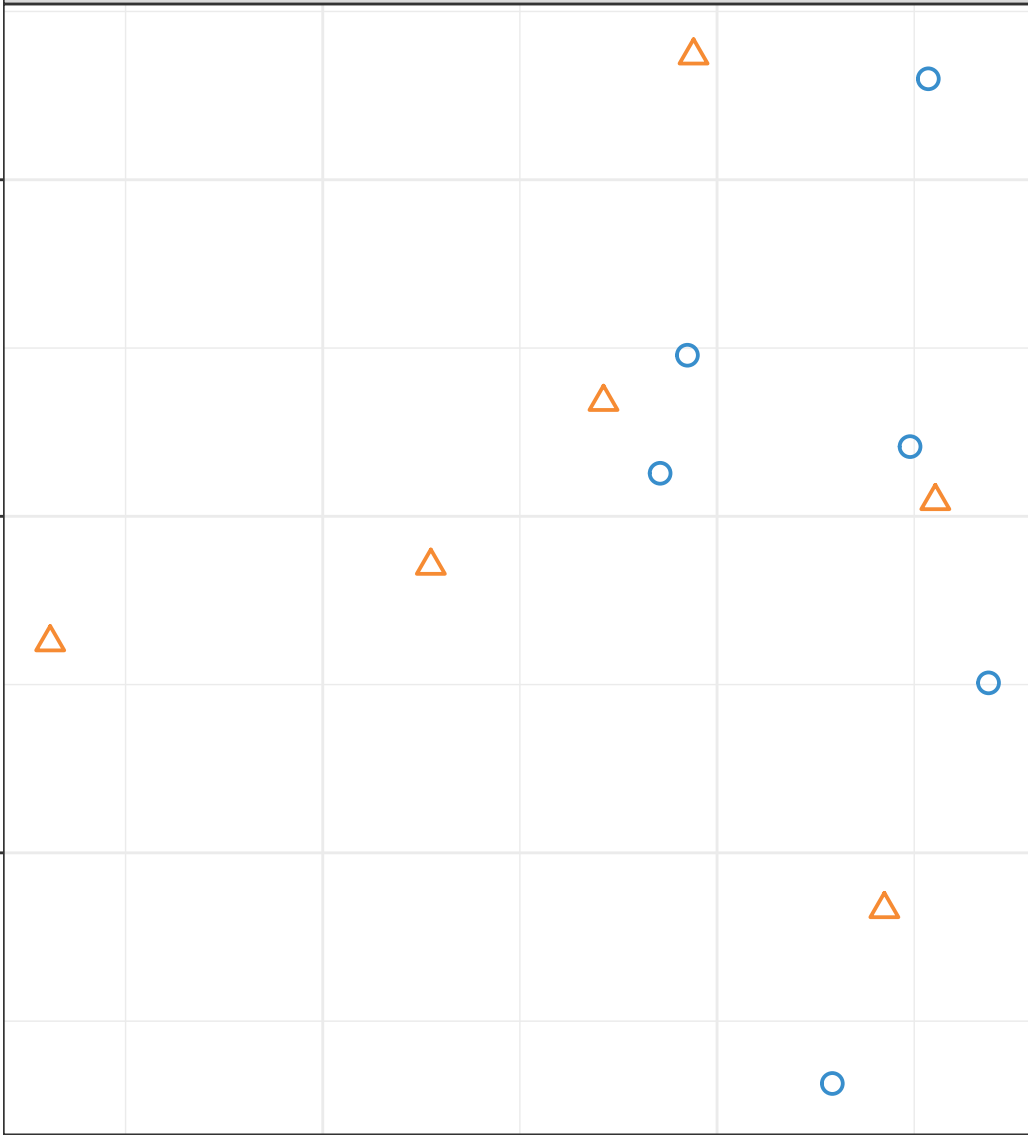
0

PC1: 42% expl. var

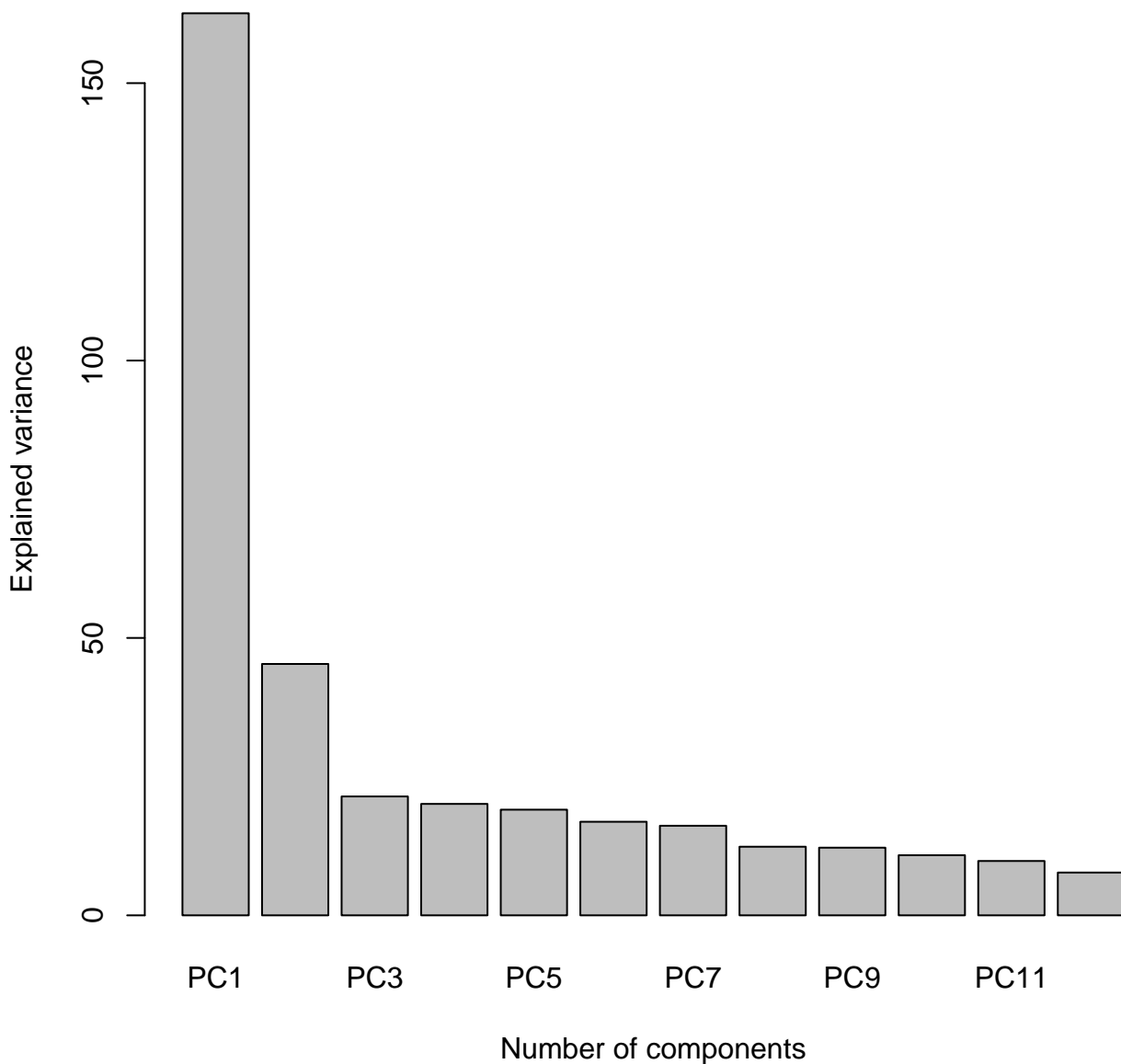
Class

○ RPMI

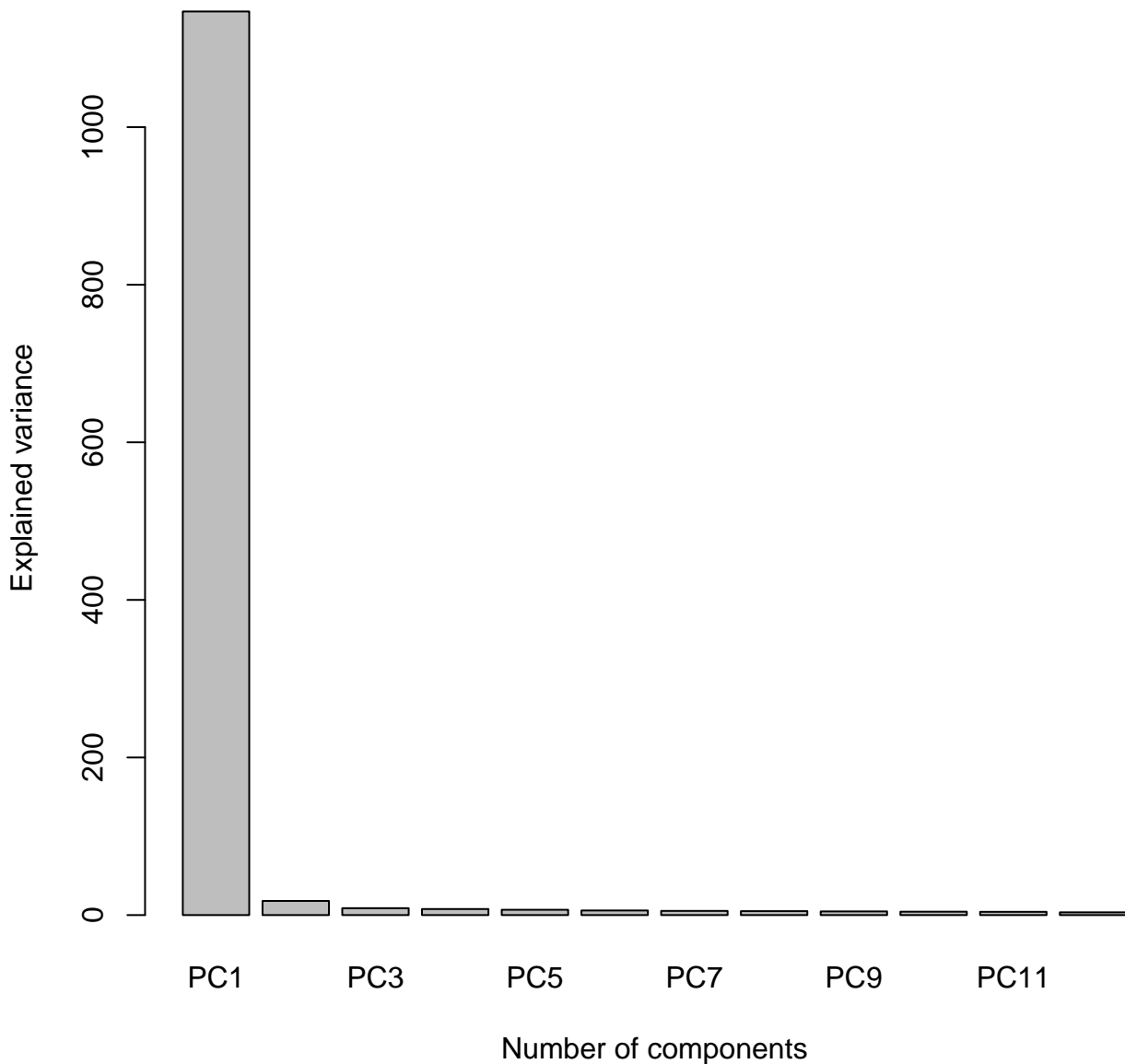
△ Sera



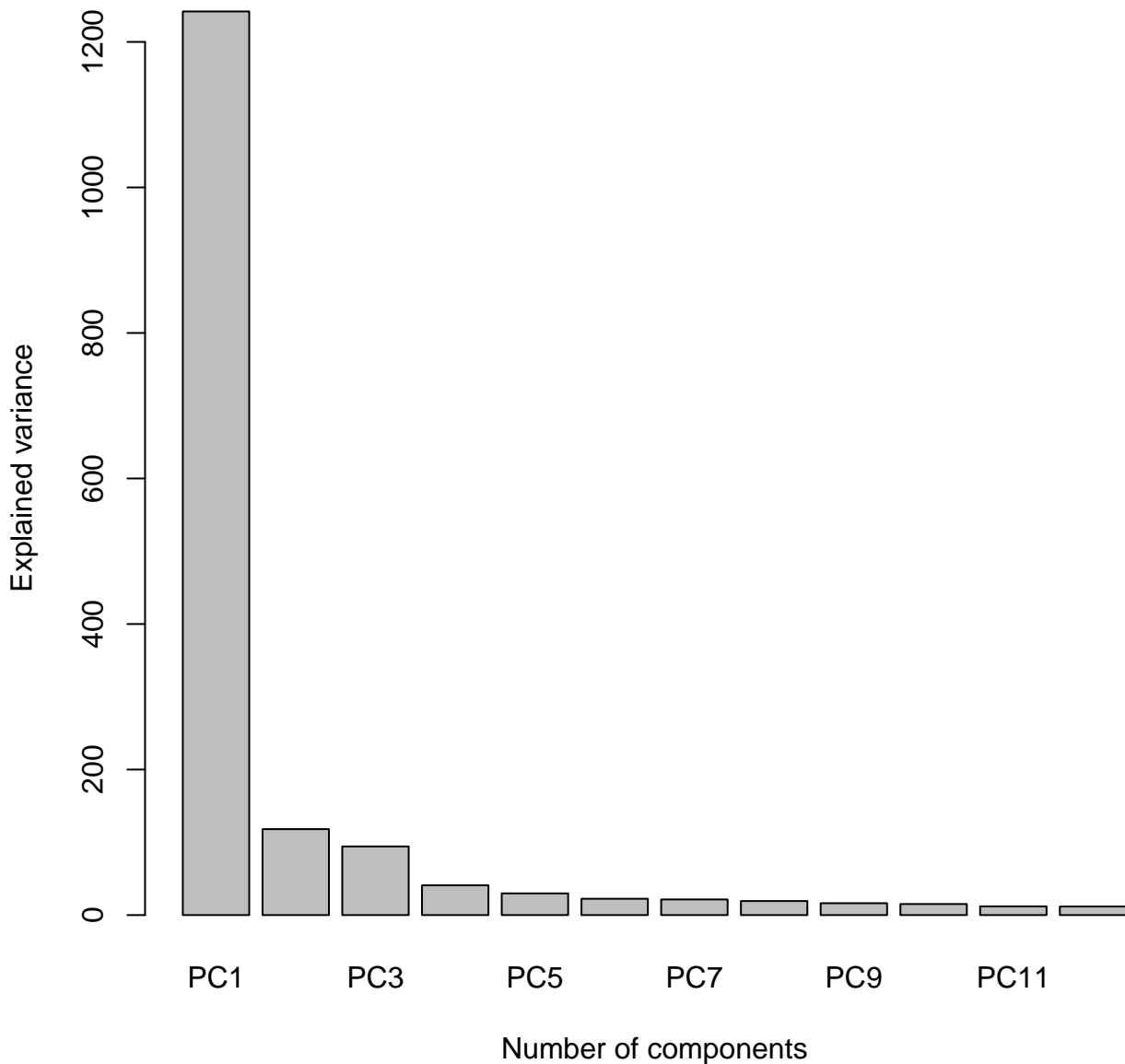
# Metabolomics Screeplot (nipals imputed)



**Proteomics Screeplot (nipals imputed)**

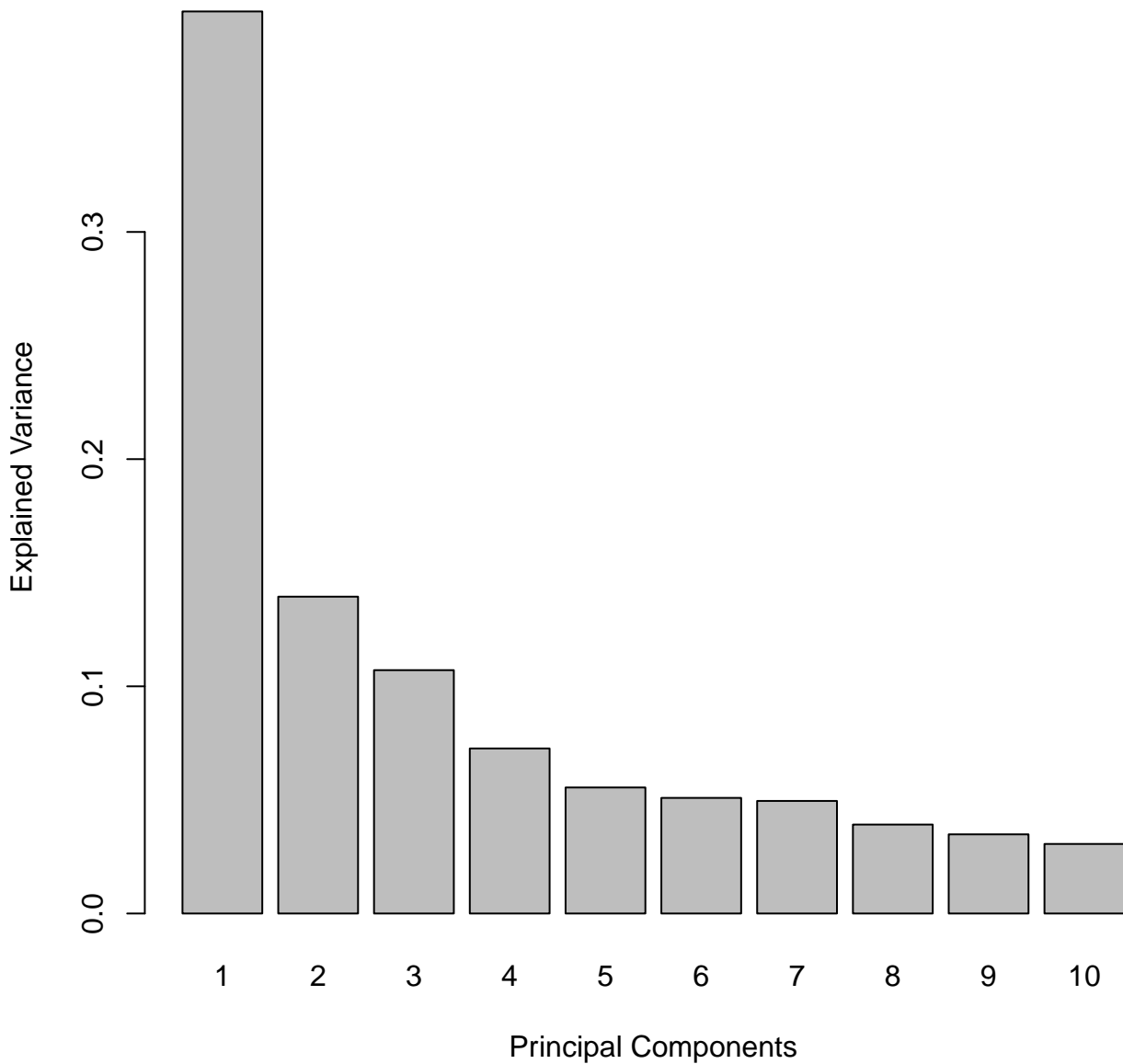


## RNA\_Seq Screeplot (nipals imputed)

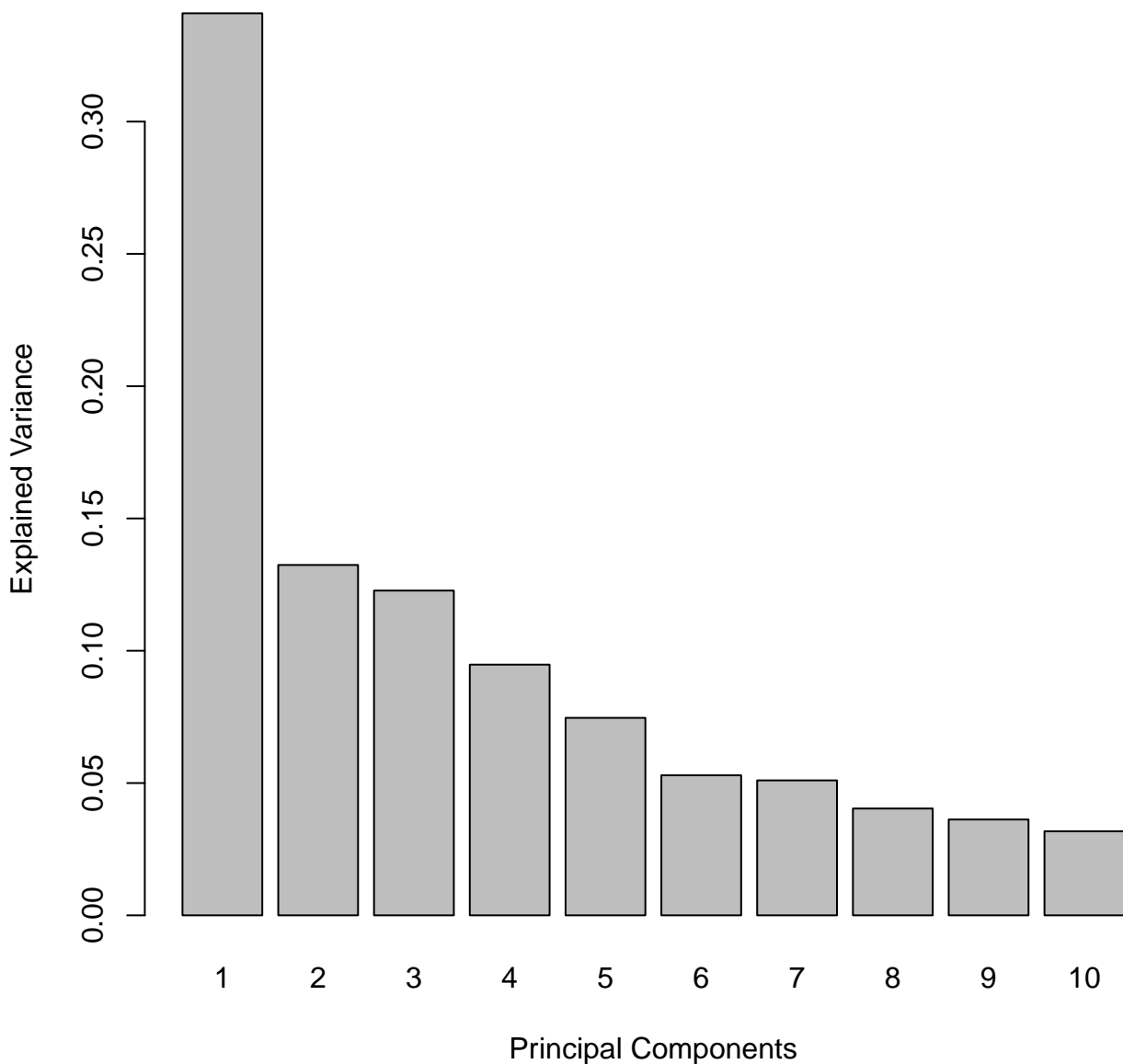




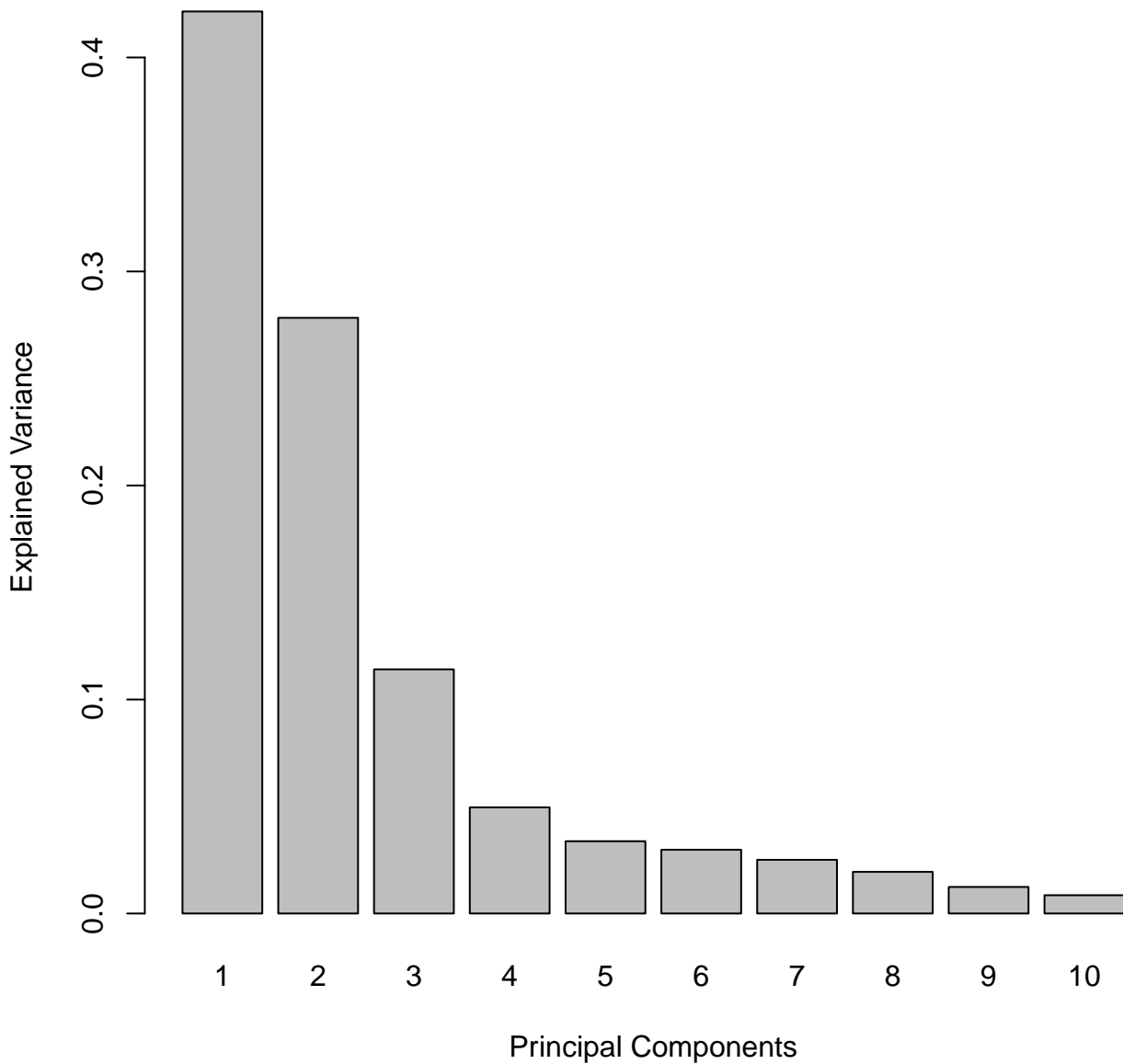
# Metabolomics screeplot



# Proteomics screeplot

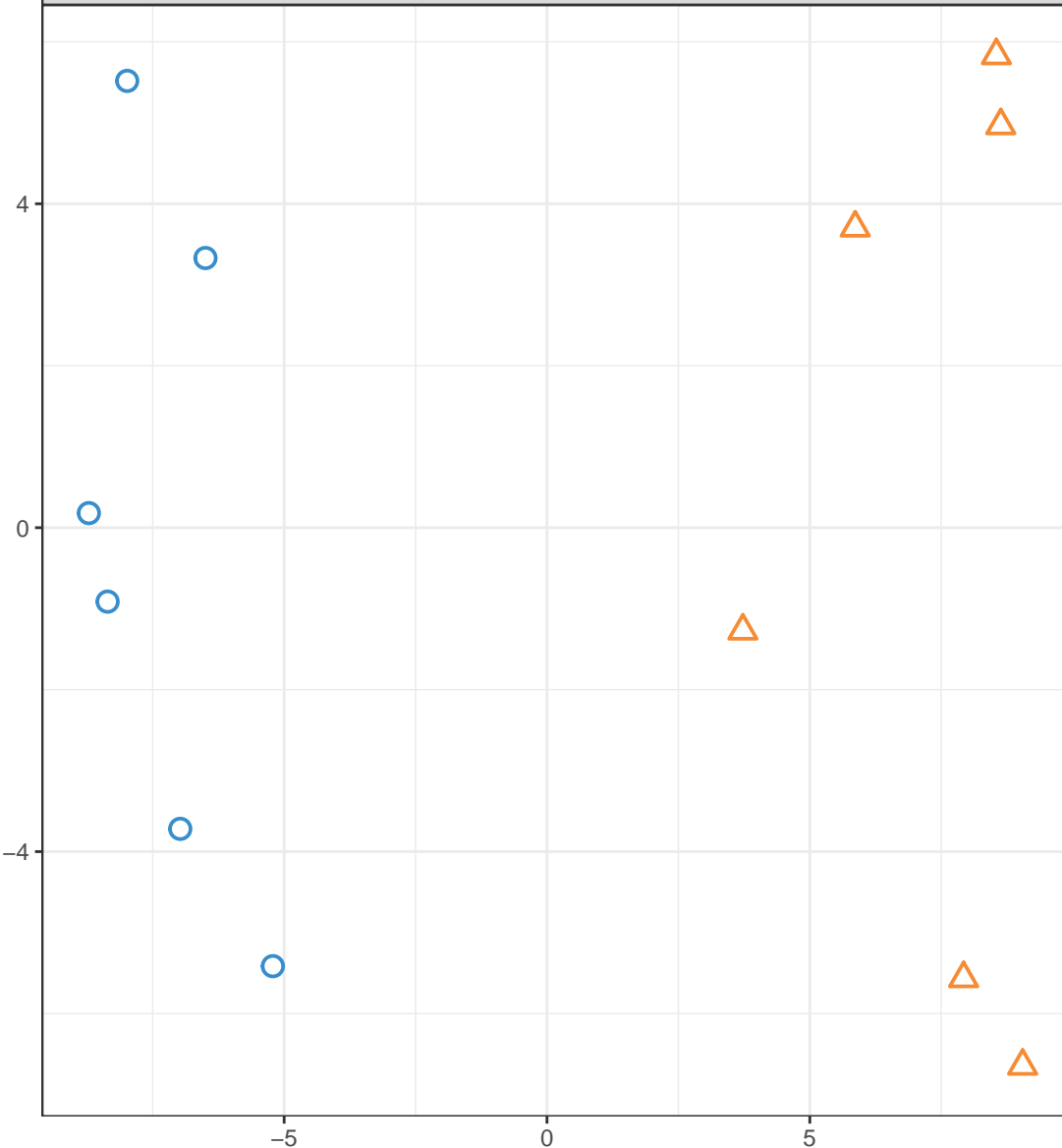


# RNA\_Seq screeplot



**Imputed n\_PCs = 10 IC: 12**  
**Metabolomics PCs (1,2)**

PC2: 14% expl. var



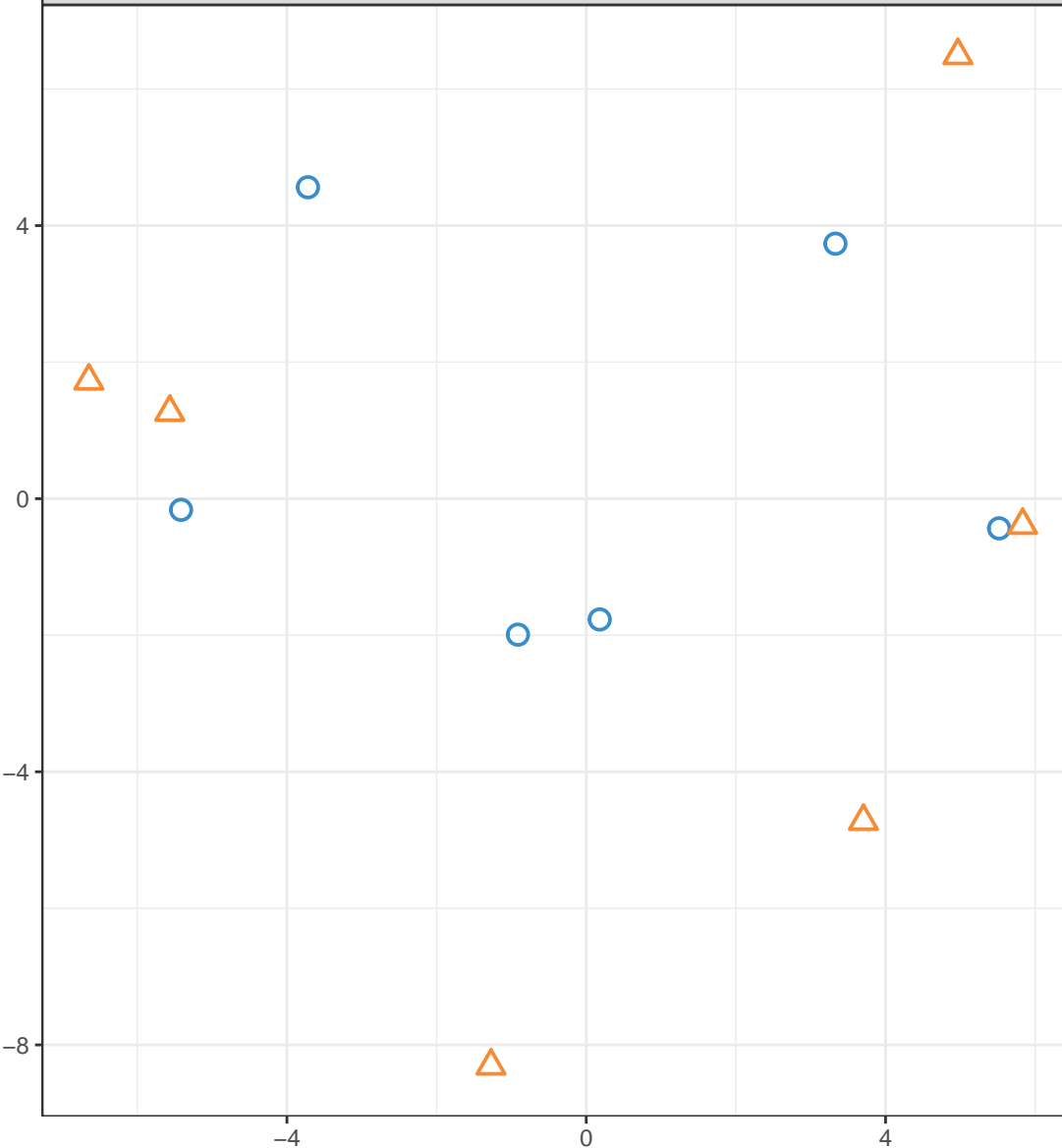
Class

○ RPMI  
△ Sera

PC1: 40% expl. var

**Imputed n\_PCs = 10 IC: 12**  
**Metabolomics PCs (2,3)**

PC3: 11% expl. var



Class

○ RPMI  
△ Sera

PC2: 14% expl. var

**Imputed n\_PCs = 10 IC: 12**  
**Metabolomics PCs (1,3)**

PC3: 11% expl. var

PC1: 40% expl. var

Class

○ RPMI  
△ Sera

4

0

-4

-8

-5

0

5

6

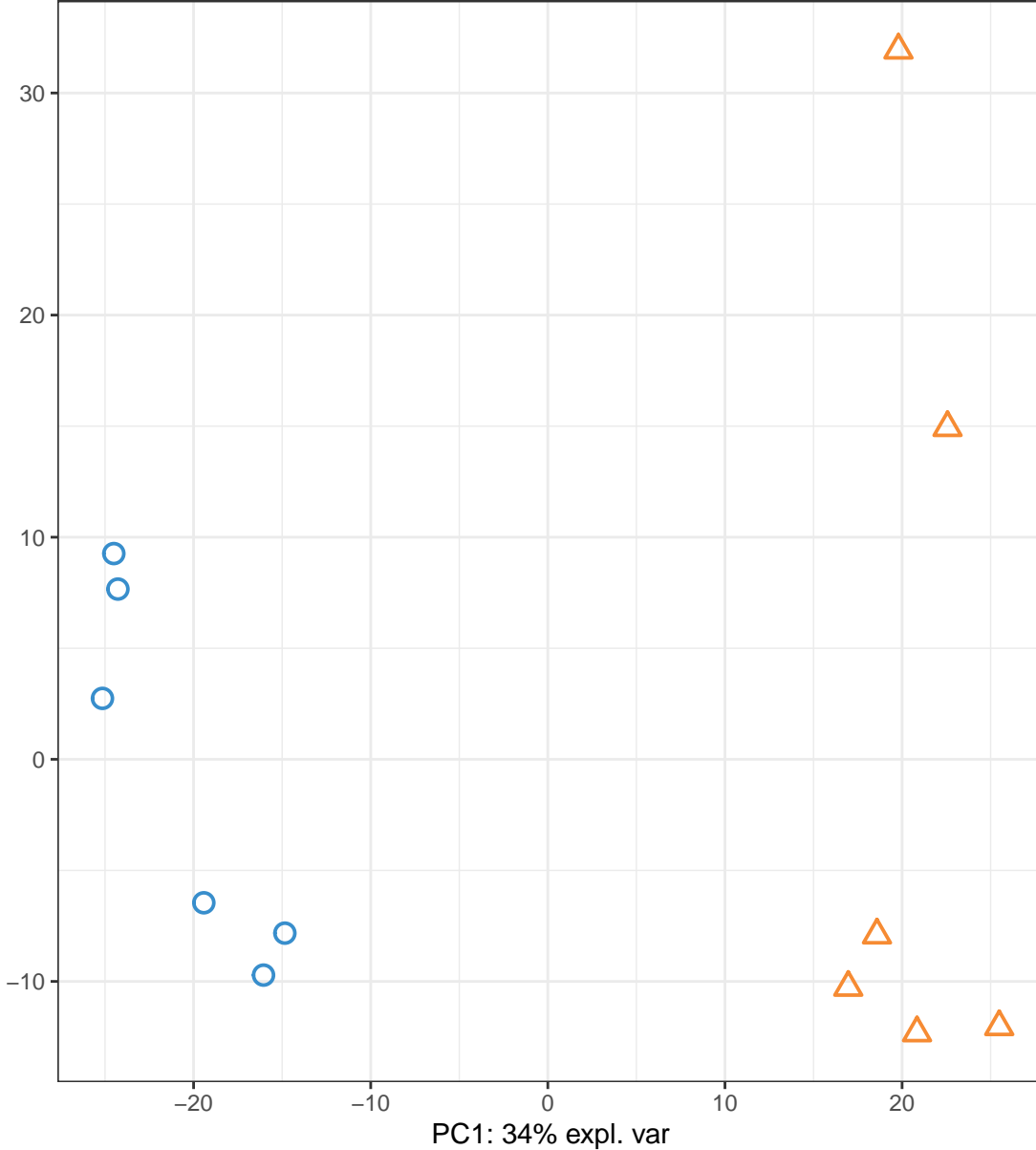
2

-2

-6

**Imputed n\_PCs = 10 IC: 12**  
**Proteomics PCs (1,2)**

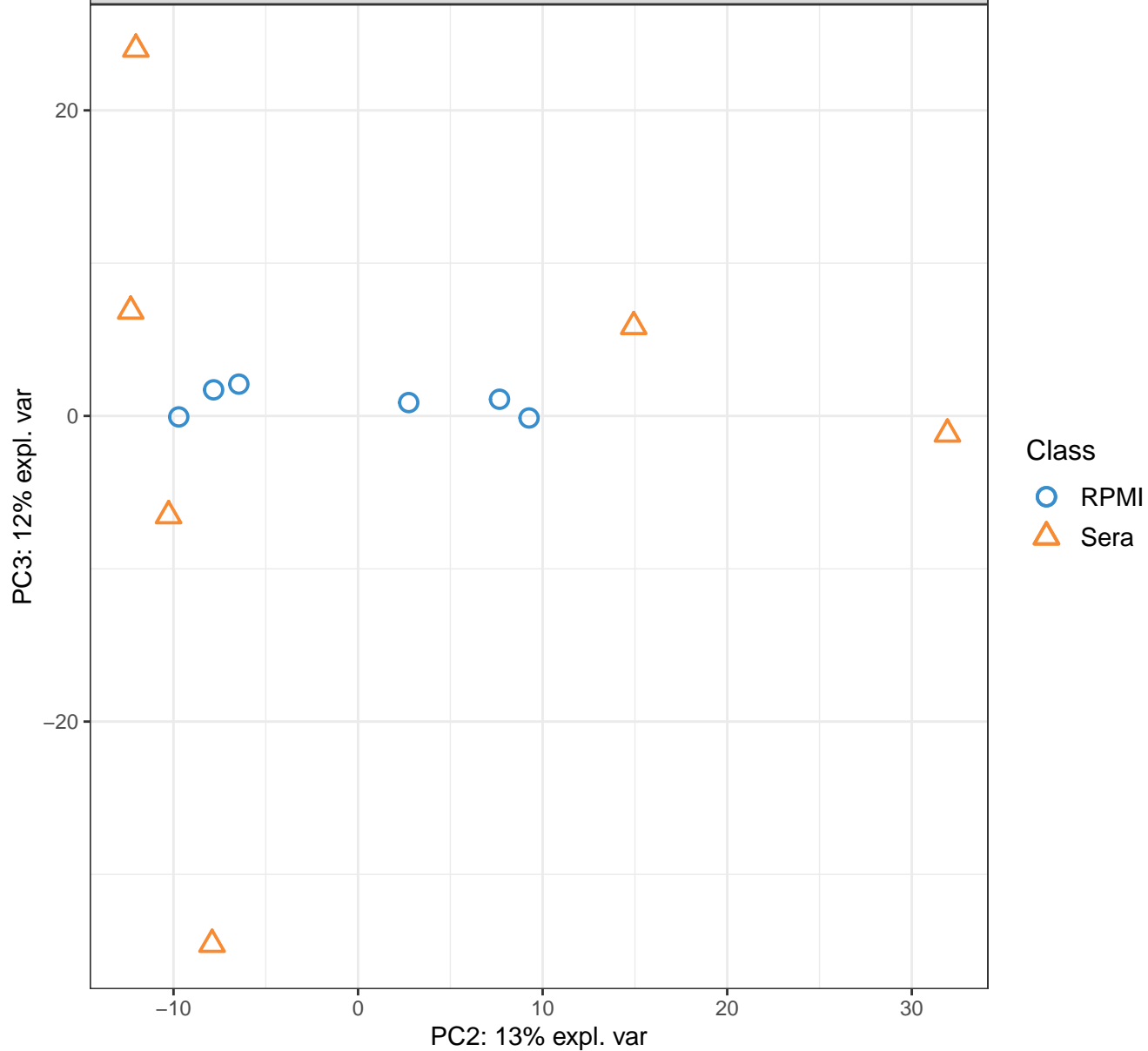
PC2: 13% expl. var



Class

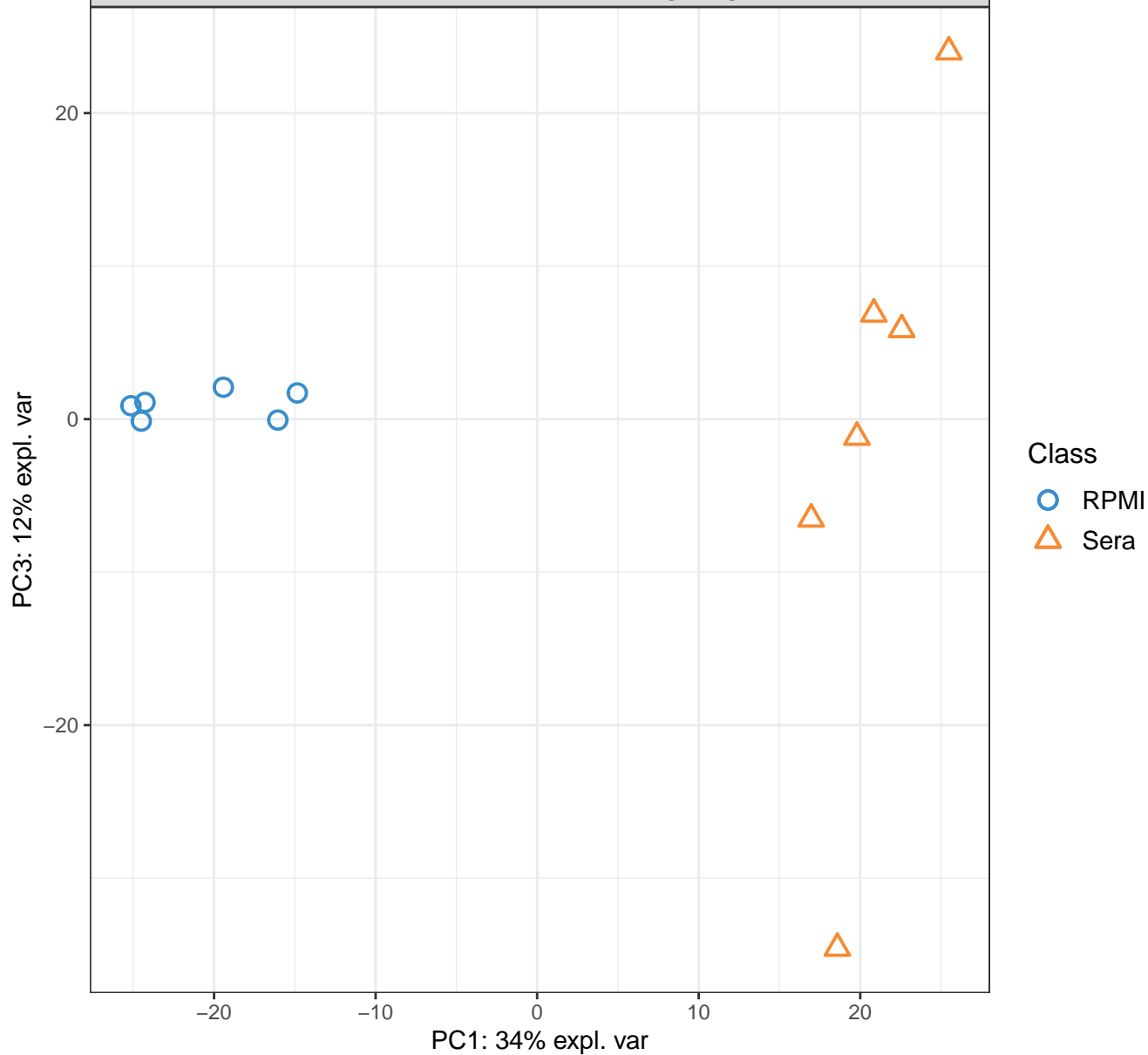
○ RPMI  
△ Sera

**Imputed n\_PCs = 10 IC: 12**  
**Proteomics PCs (2,3)**





**Imputed n\_PCs = 10 IC: 12**  
**Proteomics PCs (1,3)**



Imputed n\_PCs = 10 IC: 12  
RNA\_Seq PCs (1,2)

PC2: 28% expl. var

50

25

0

-25

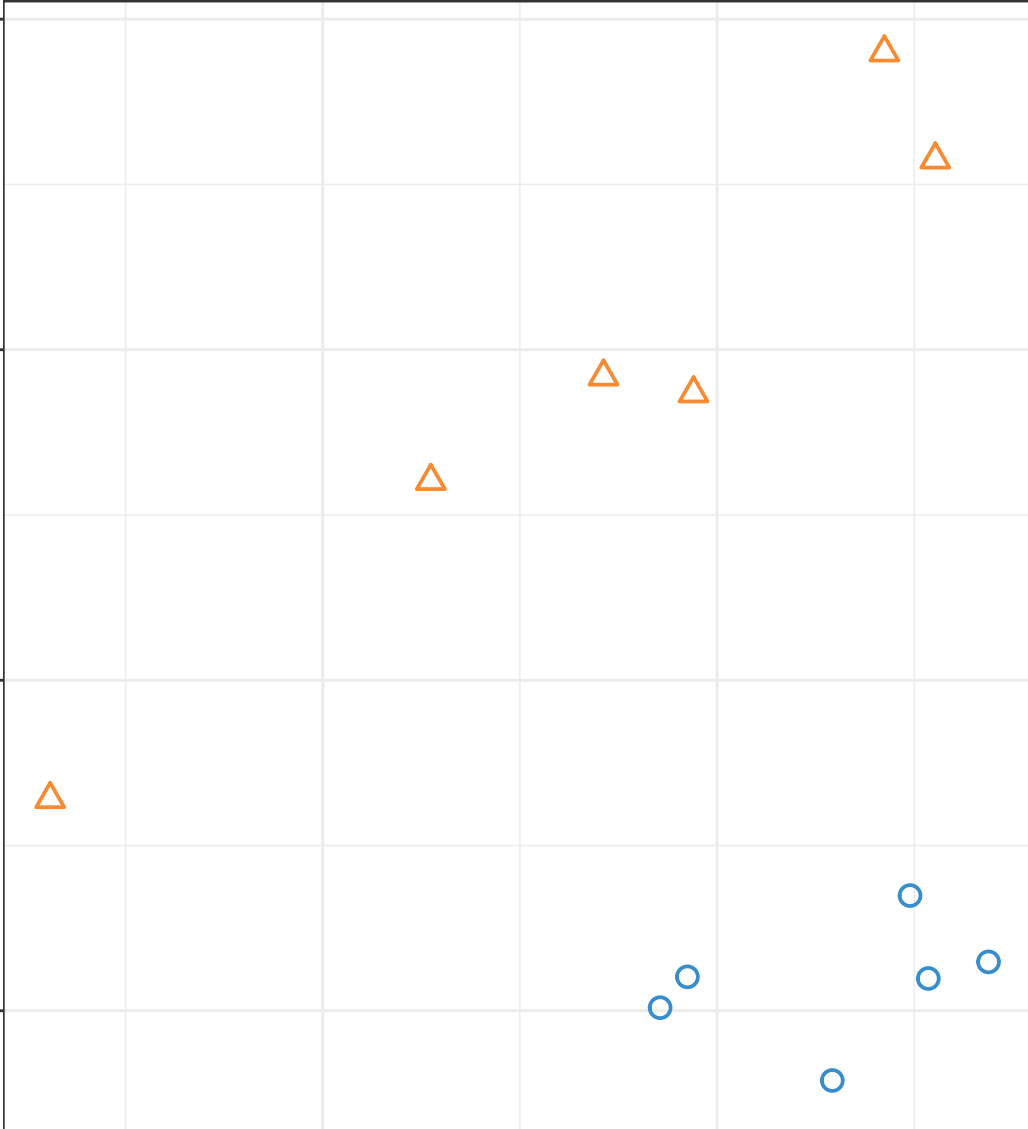
-50

0

PC1: 42% expl. var

Class

○ RPMI  
△ Sera



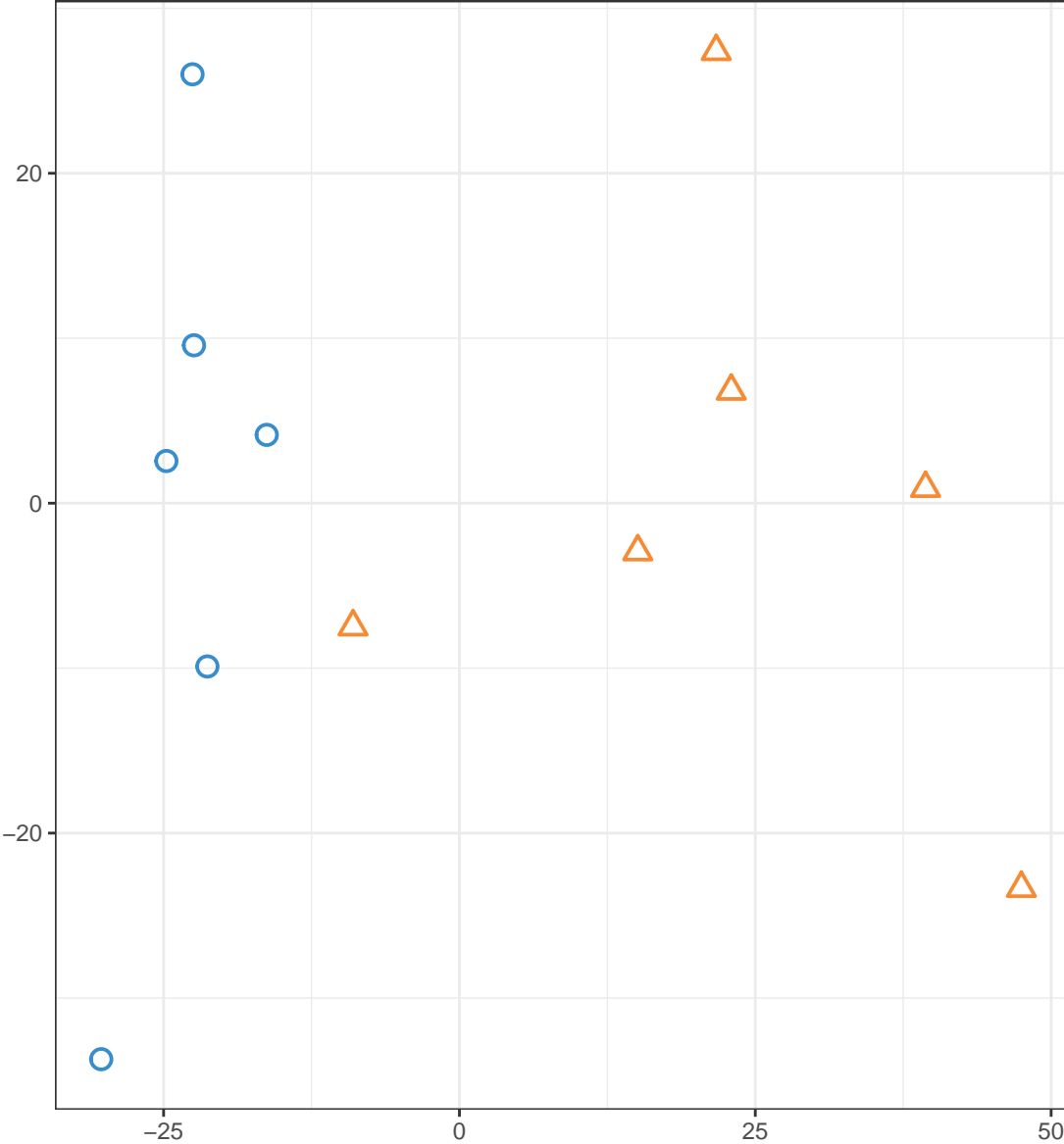
Imputed n\_PCs = 10 IC: 12  
RNA\_Seq PCs (2,3)

PC3: 11% expl. var

PC2: 28% expl. var

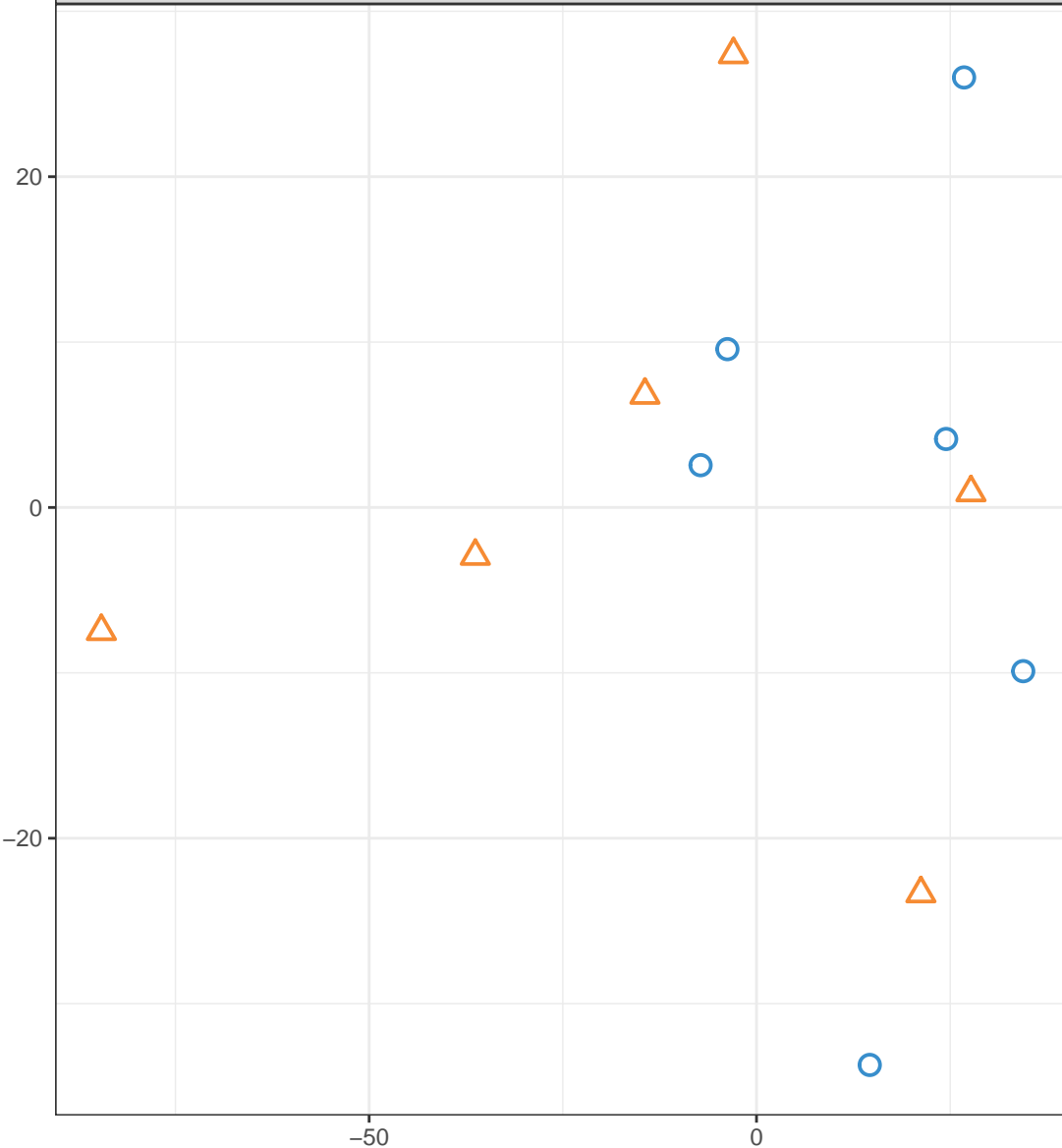
Class

○ RPMI  
△ Sera



Imputed n\_PCs = 10 IC: 12  
RNA\_Seq PCs (1,3)

PC3: 11% expl. var

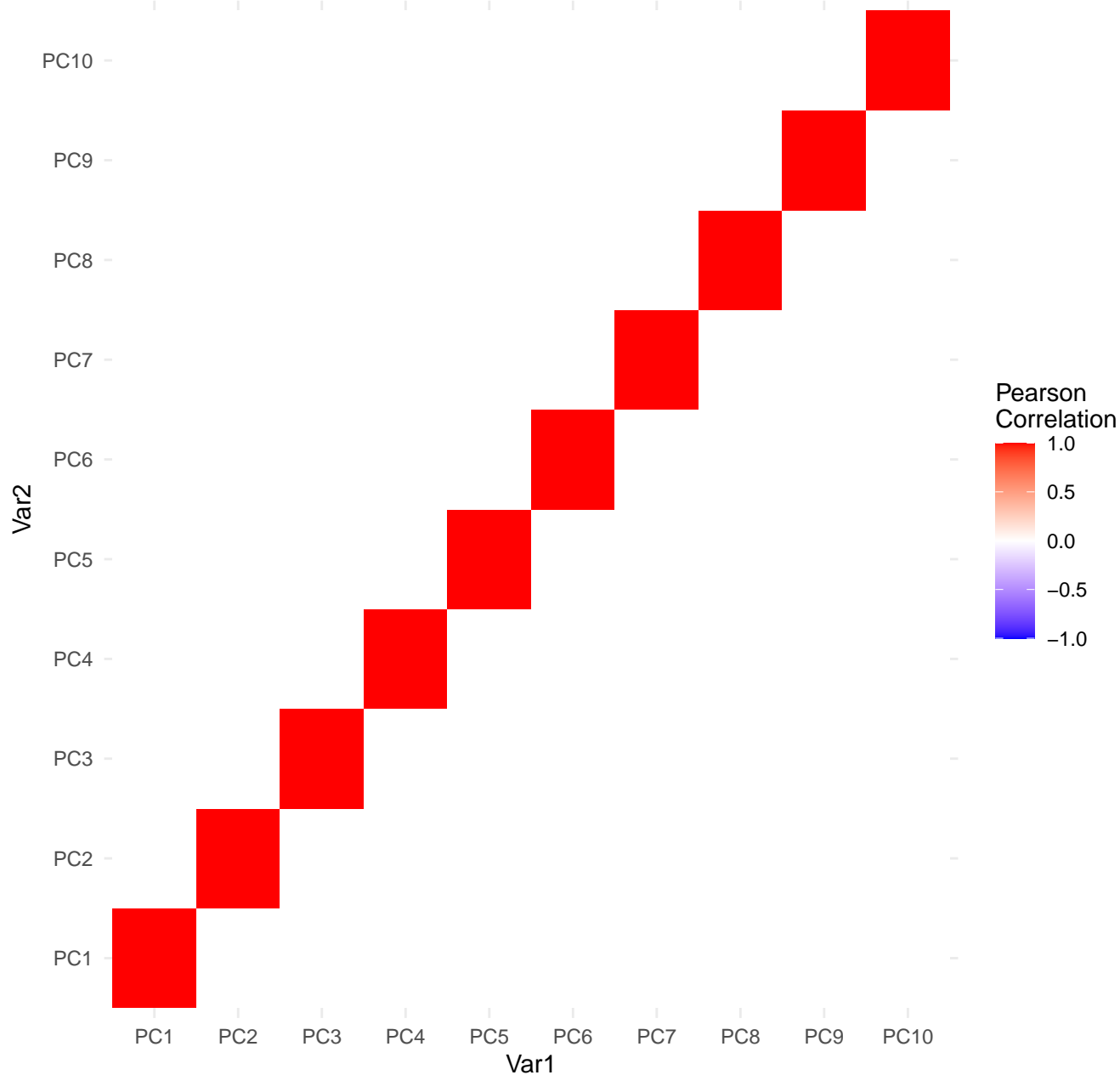


Class

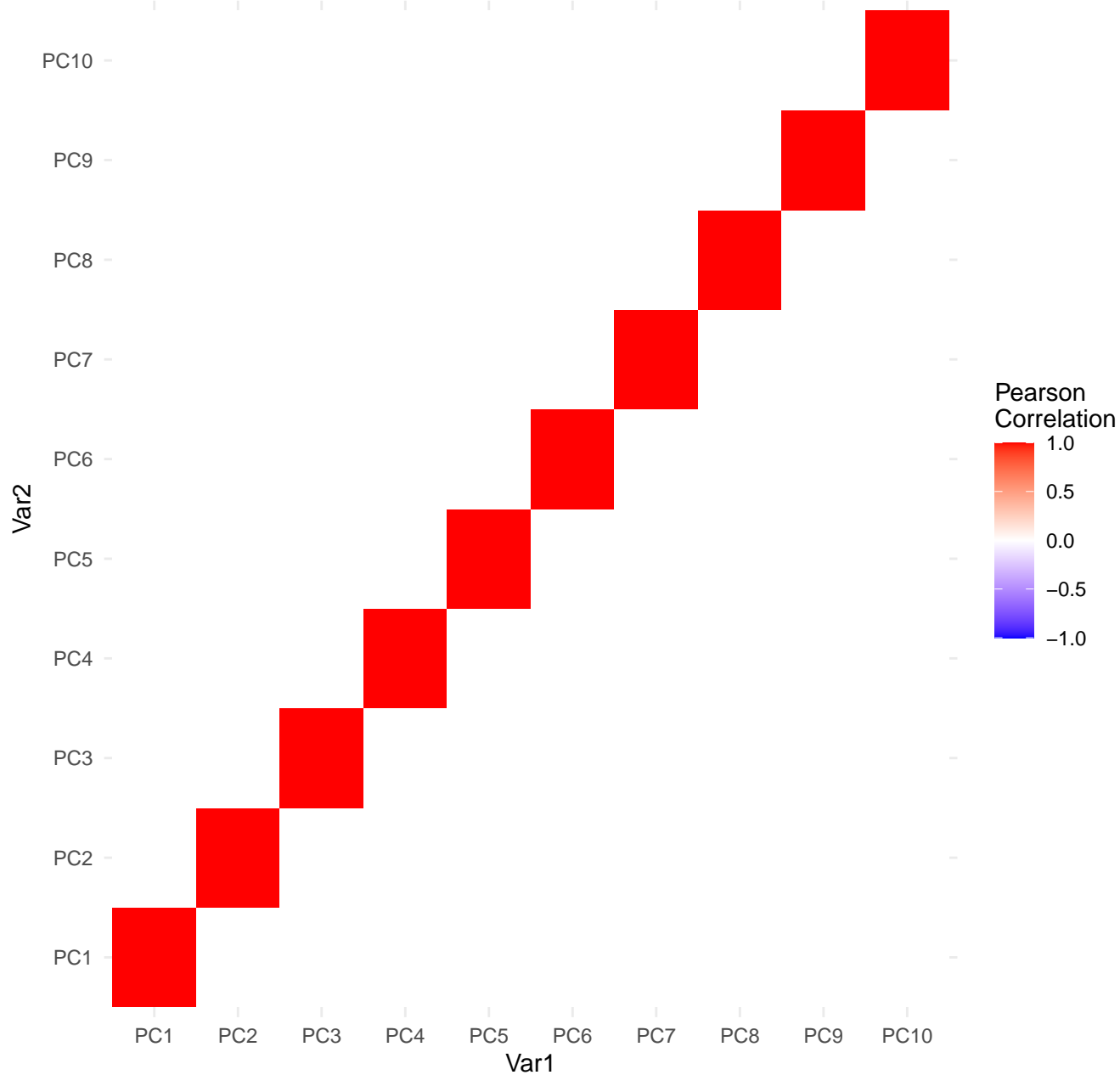
○ RPMI  
△ Sera

PC1: 42% expl. var

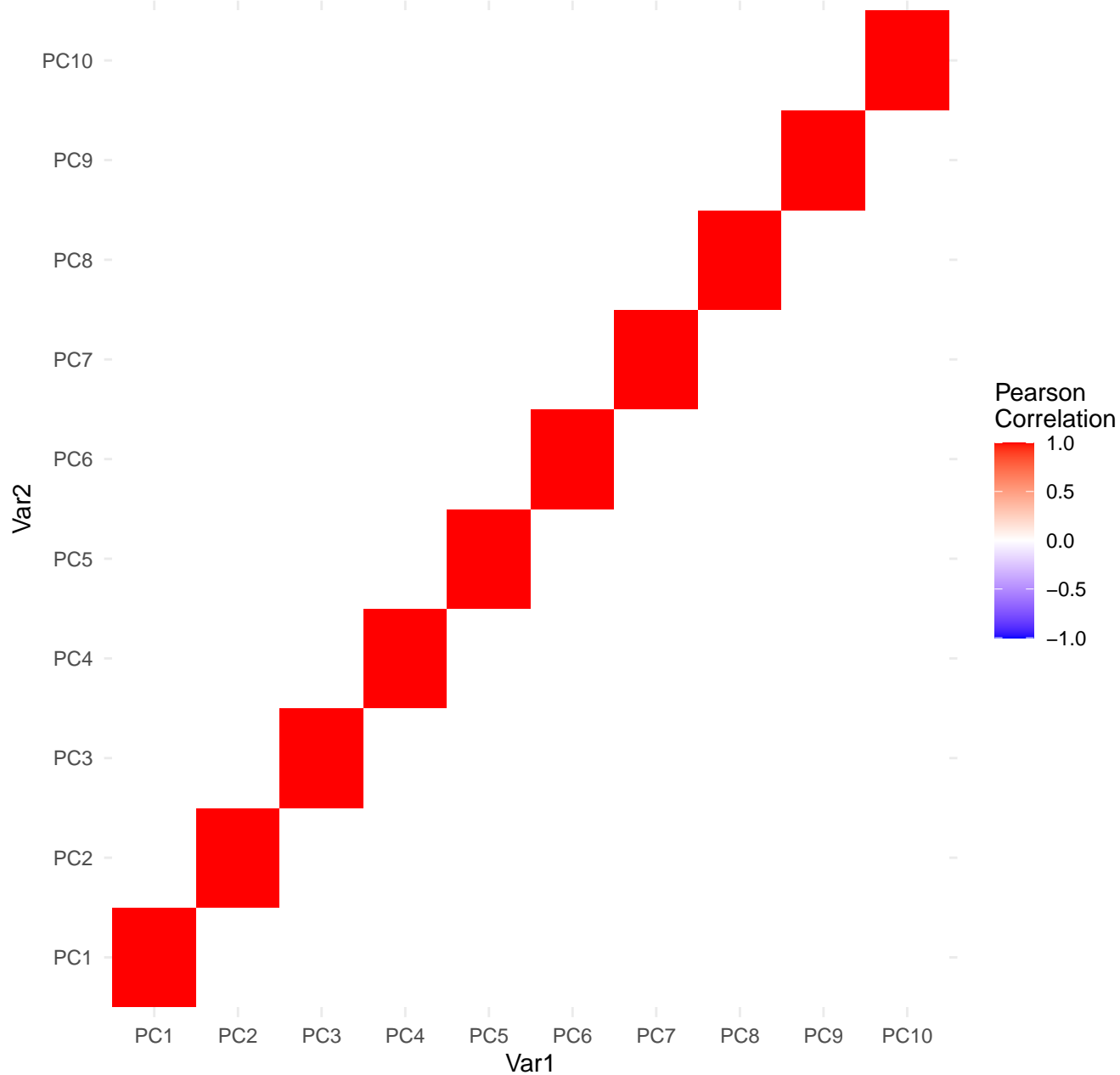
## Metabolomics Correlation between imputed and unimputed data



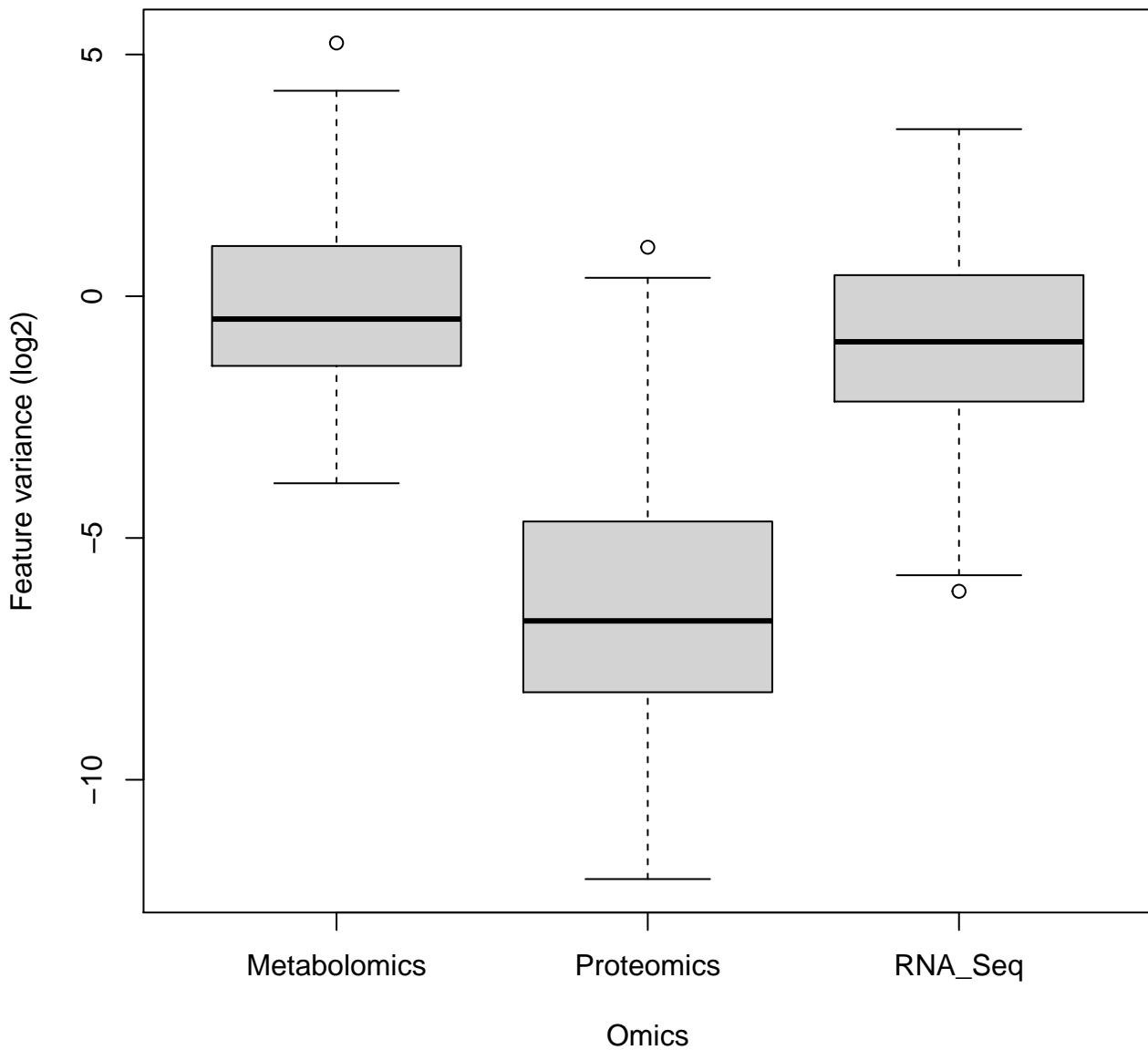
## Proteomics Correlation between imputed and unimputed data



## RNA\_Seq Correlation between imputed and unimputed data



**Feature variances (log2) per omics**





# Metabolomics PLSDA single 1/2

X-variate 2: 10% expl. var

10  
5  
0  
-5  
-10

X-variate 1: 40% expl. var

-10

-5

0

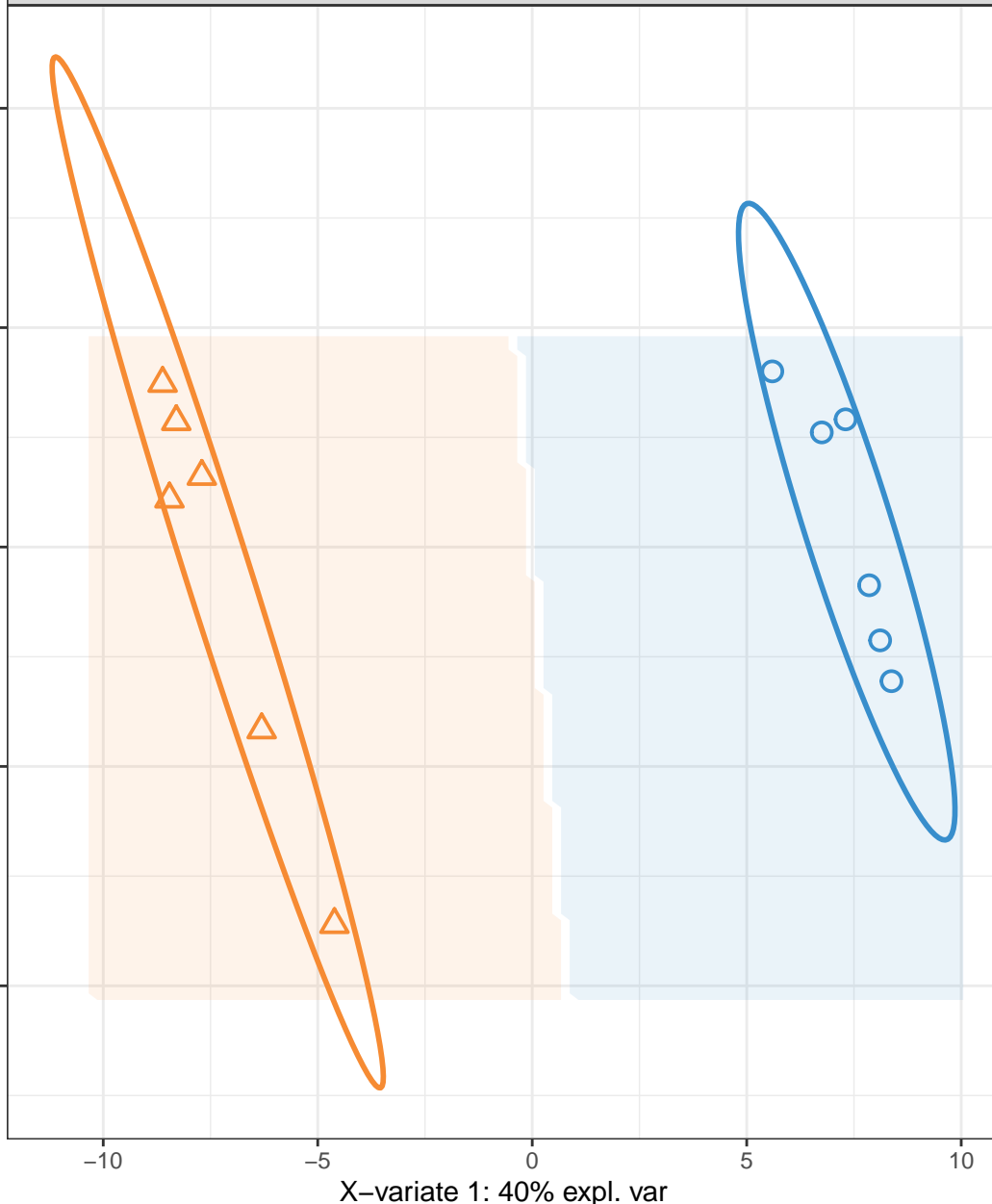
5

10

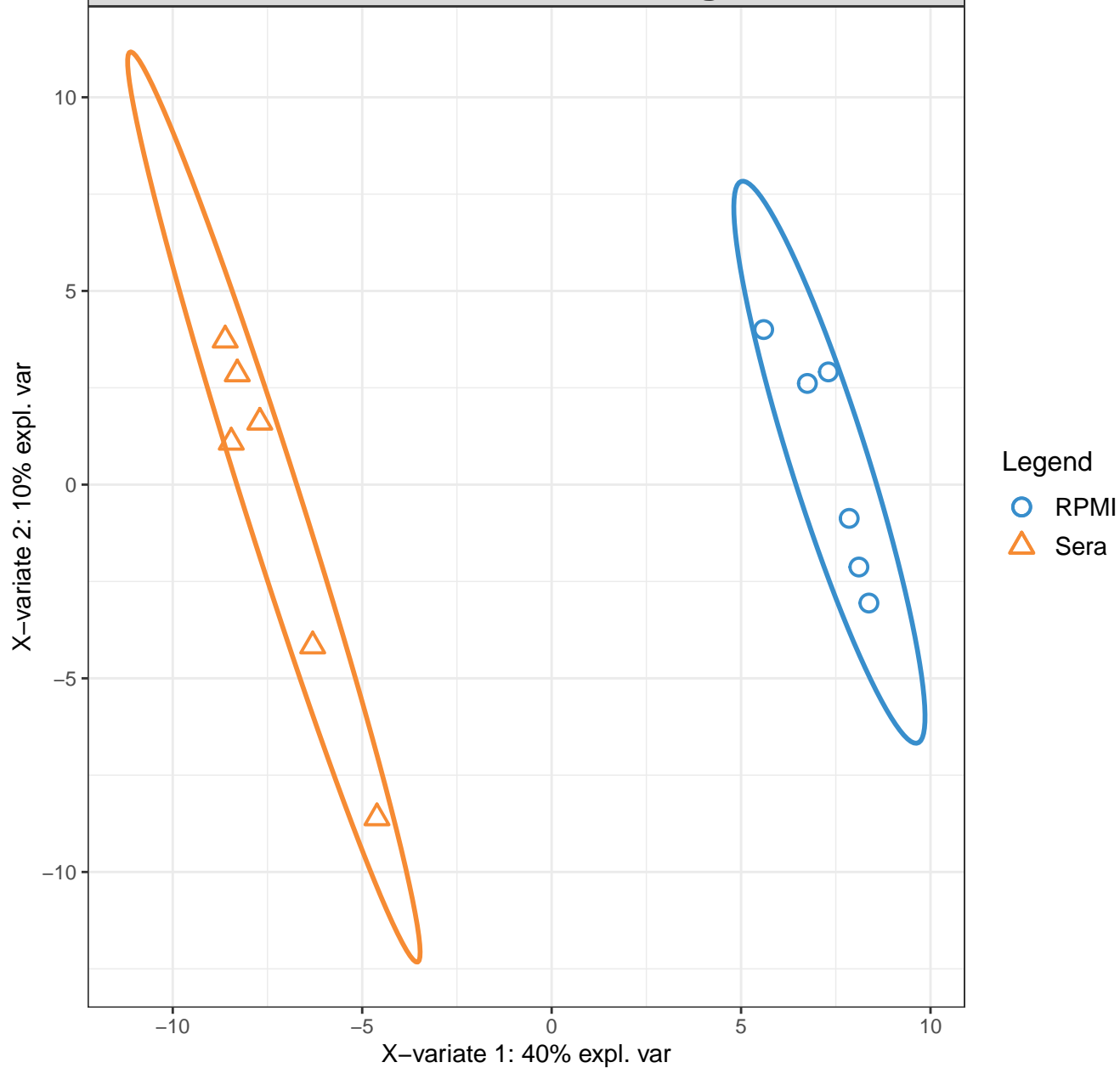
Legend

○ RPMI

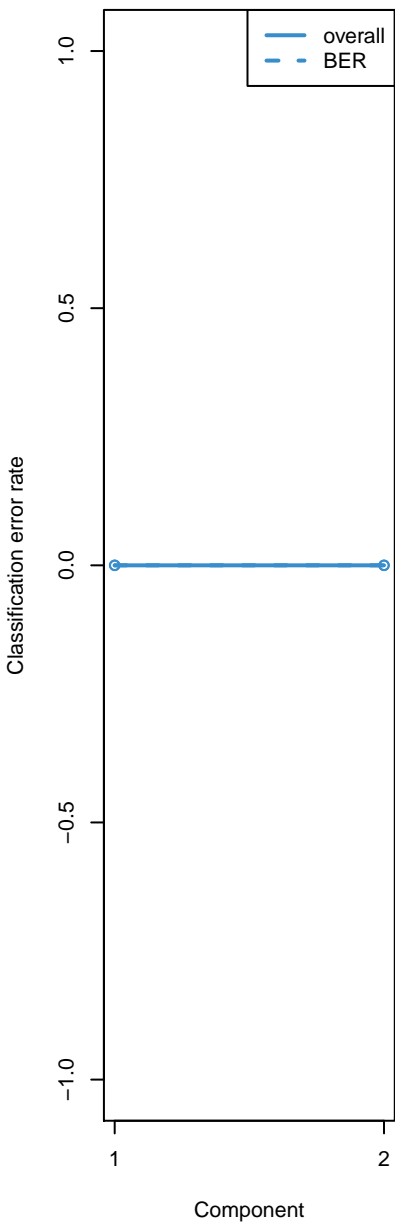
△ Sera



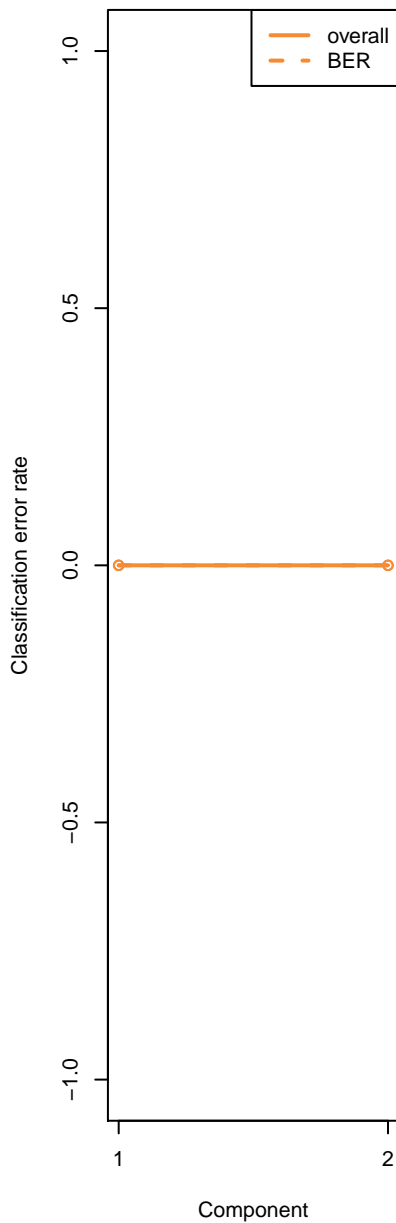
# Metabolomics PLSDA single 1/2



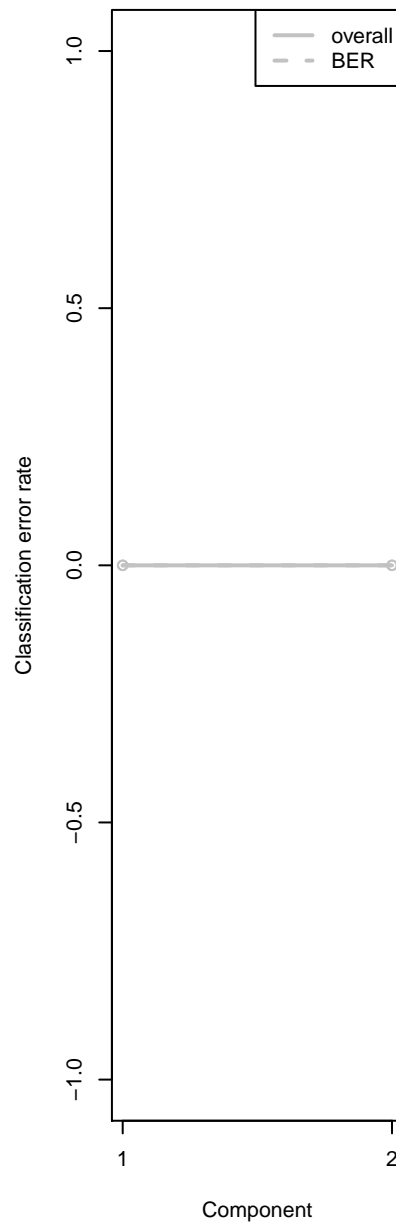
max.dist



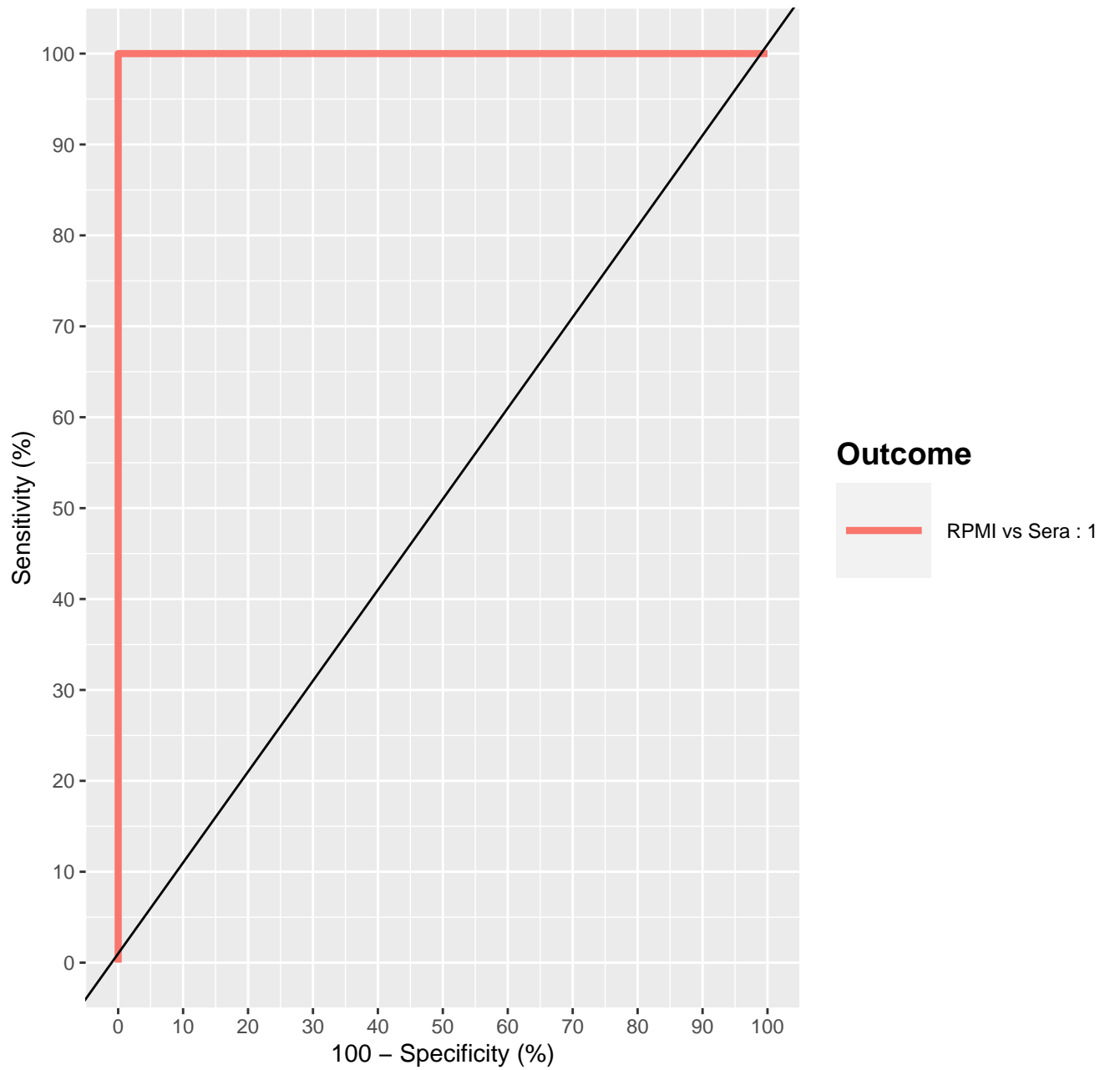
centroids.dist



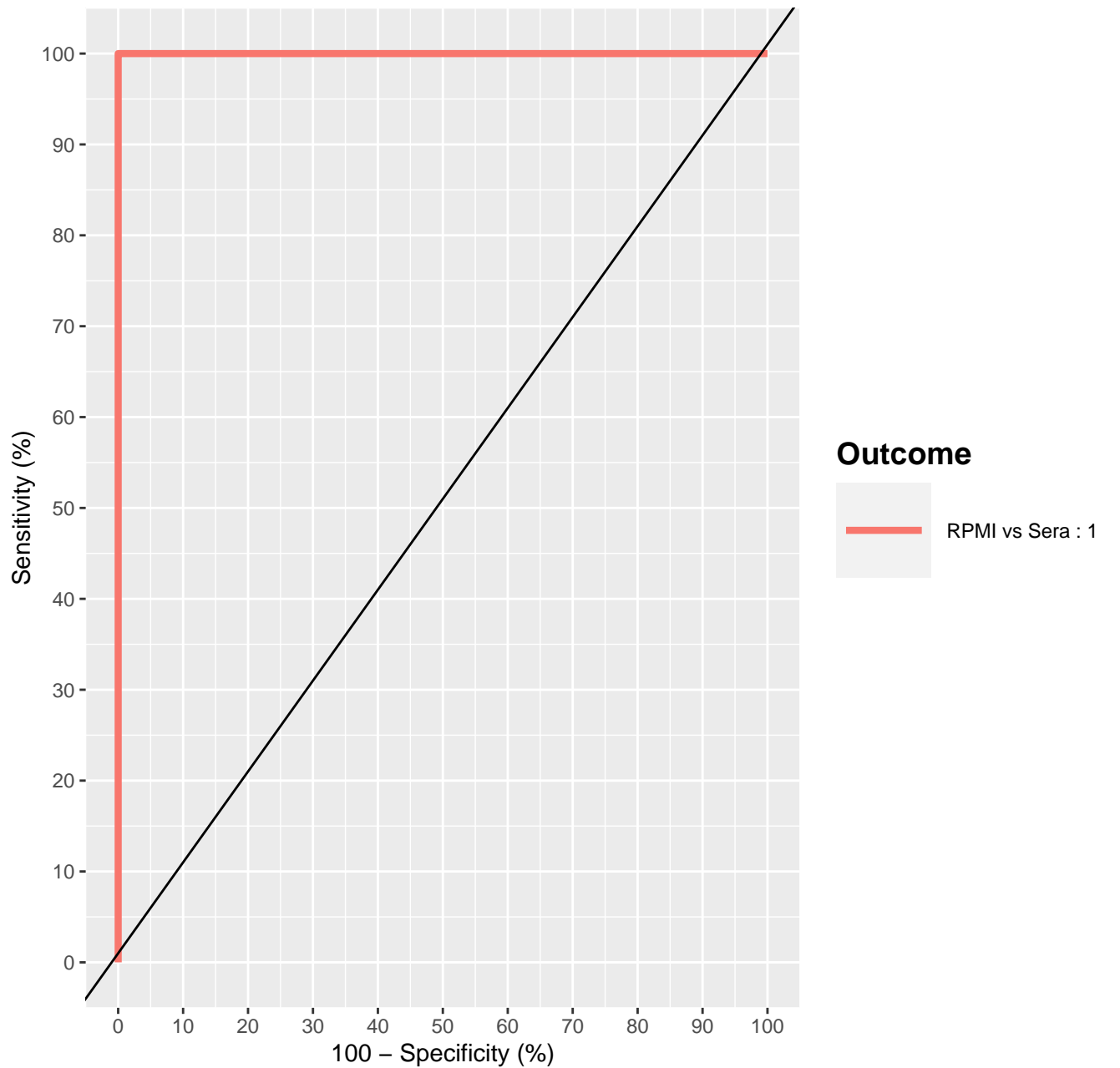
mahalanobis.dist



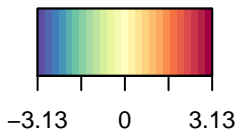
**ROC Curve Comp 1**



## ROC Curve Comp 2



Color key

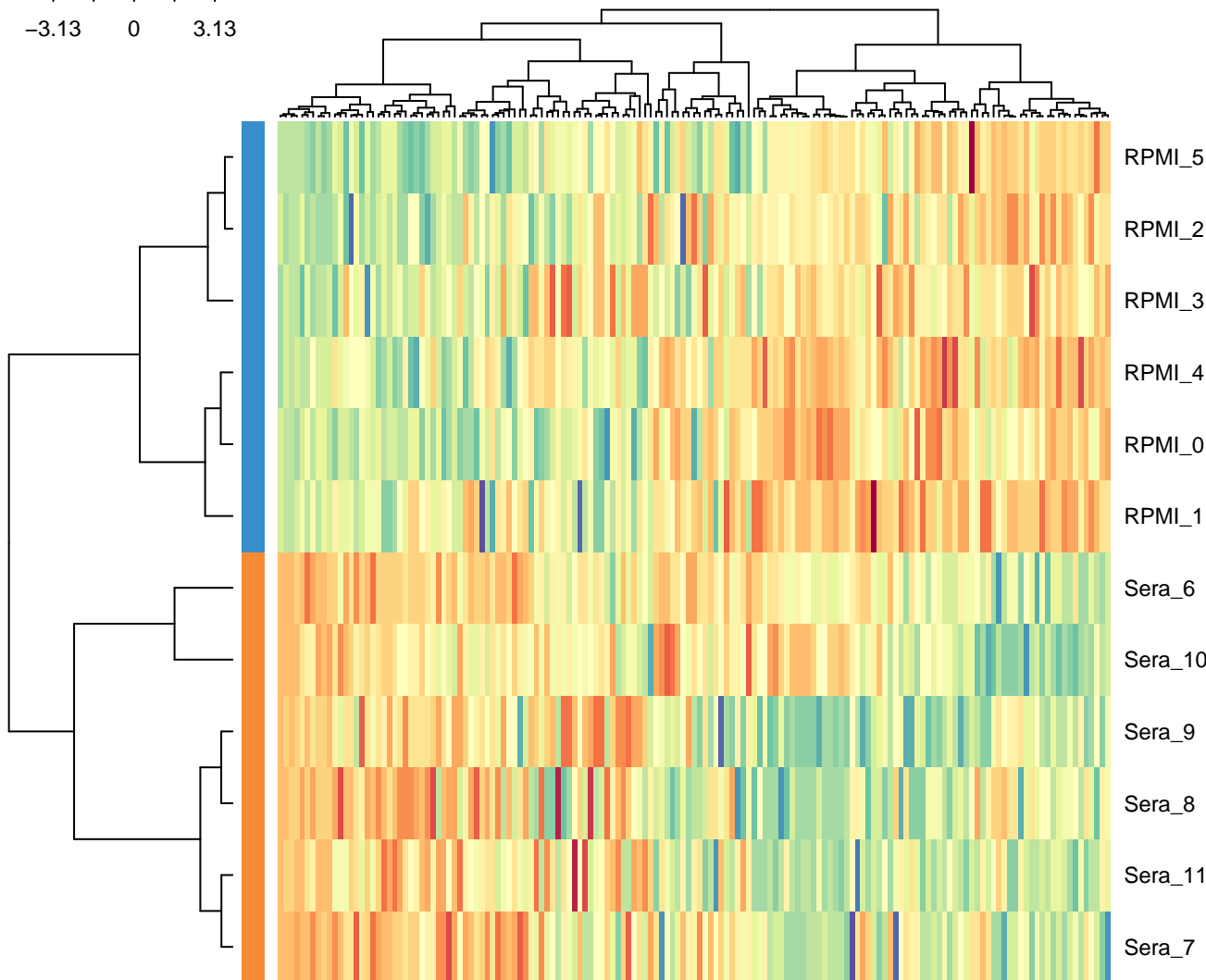


PLSDA

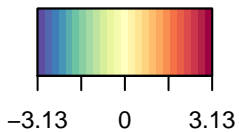
Status

RPMI

Sera



Color key

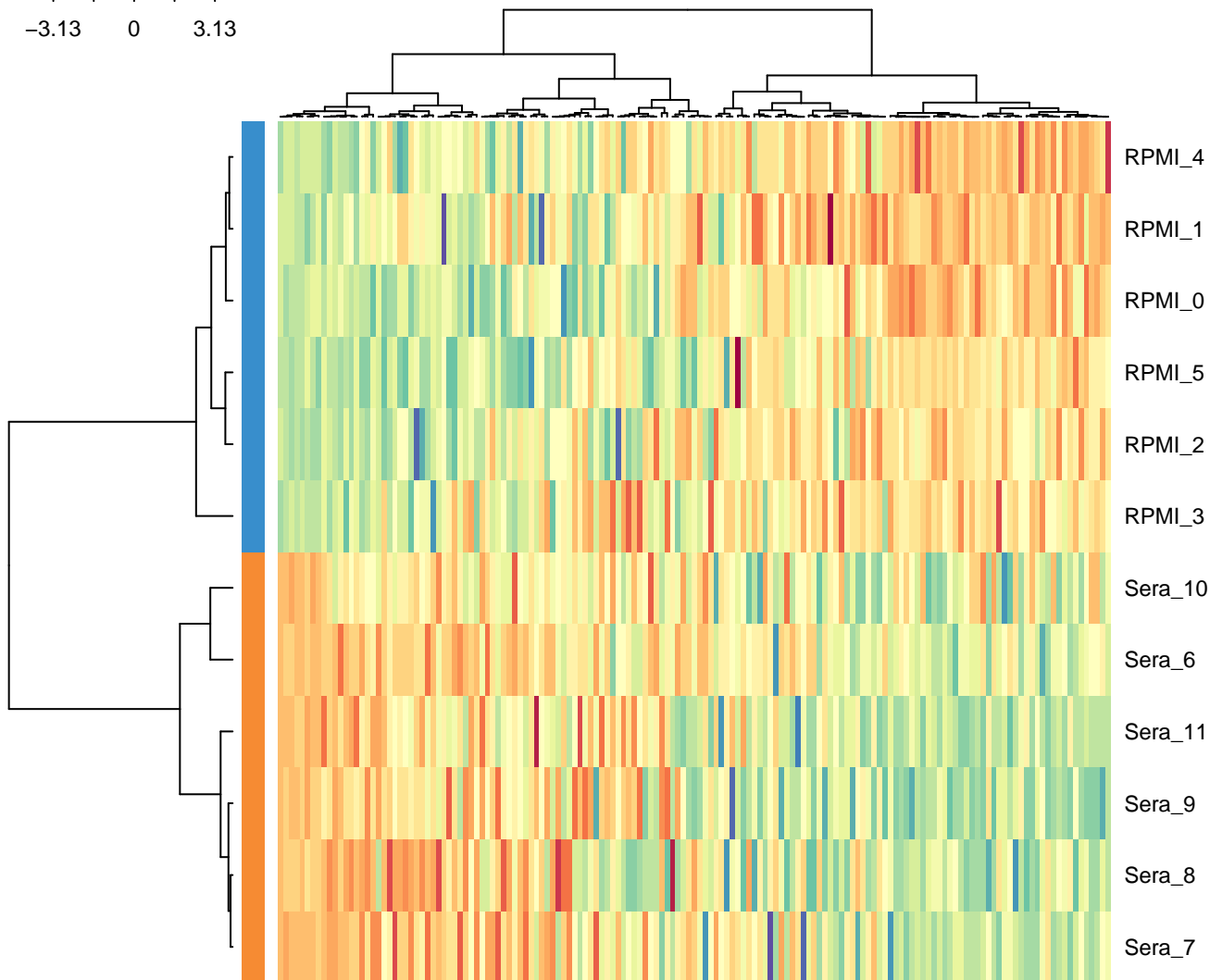


# PLSDA Component 1

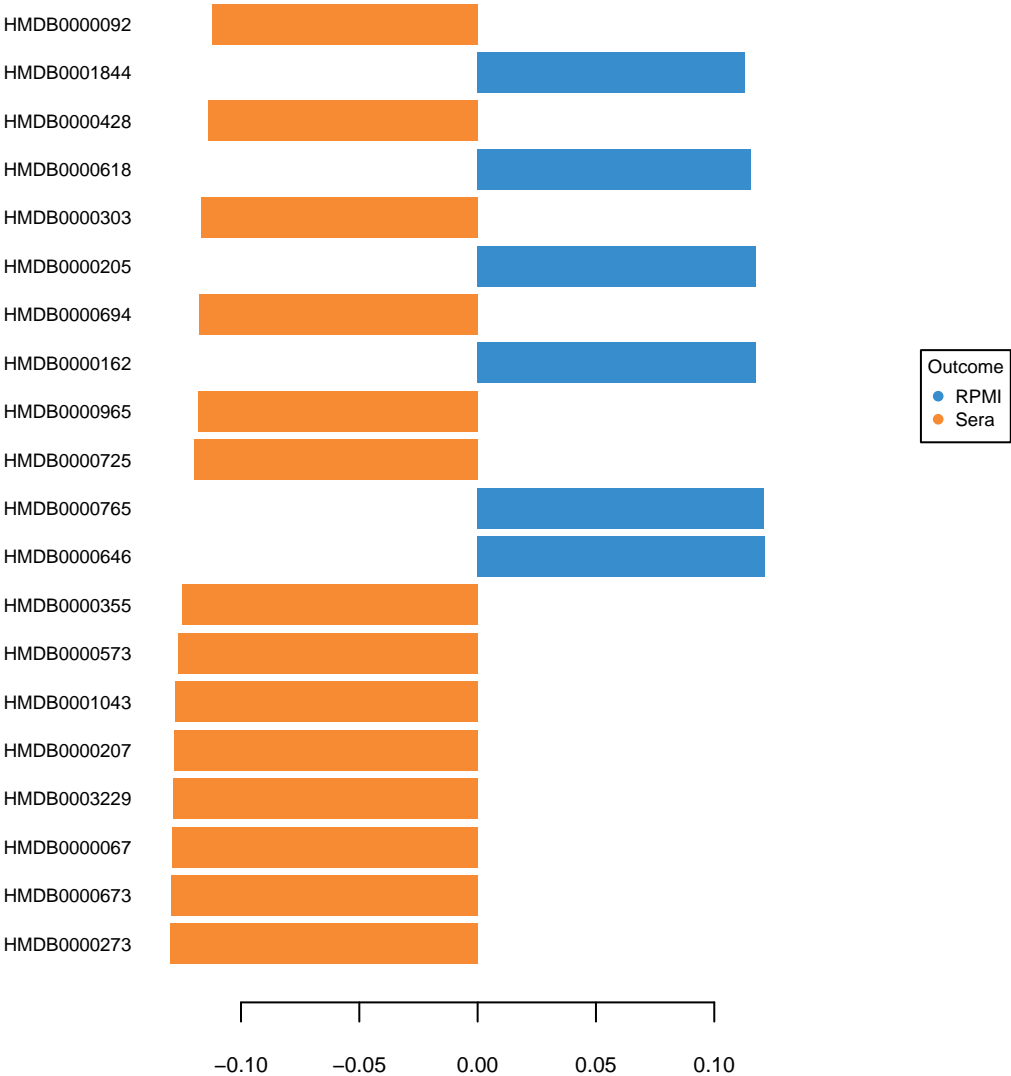
Status

■ RPMI

■ Sera

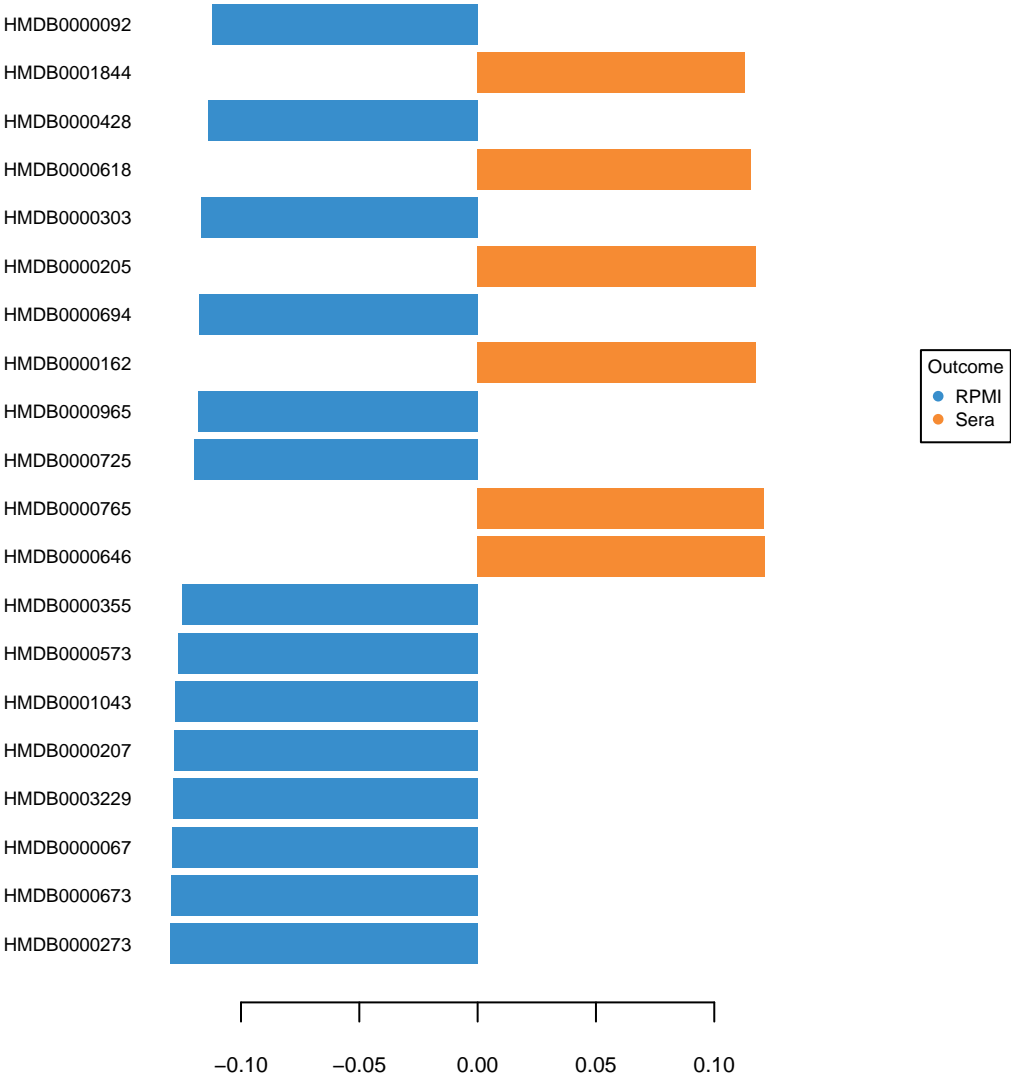


# Metabolomics 1 PLSDA max load

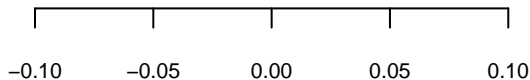
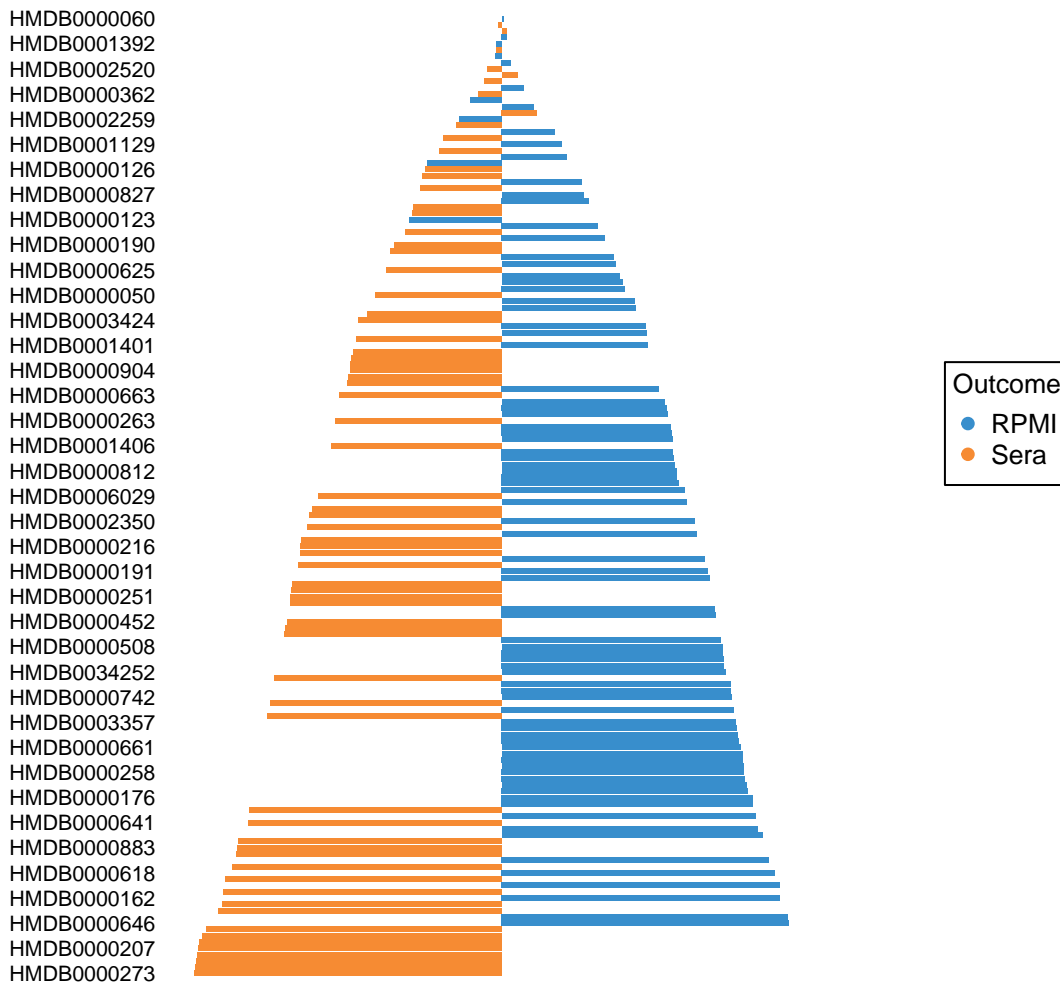




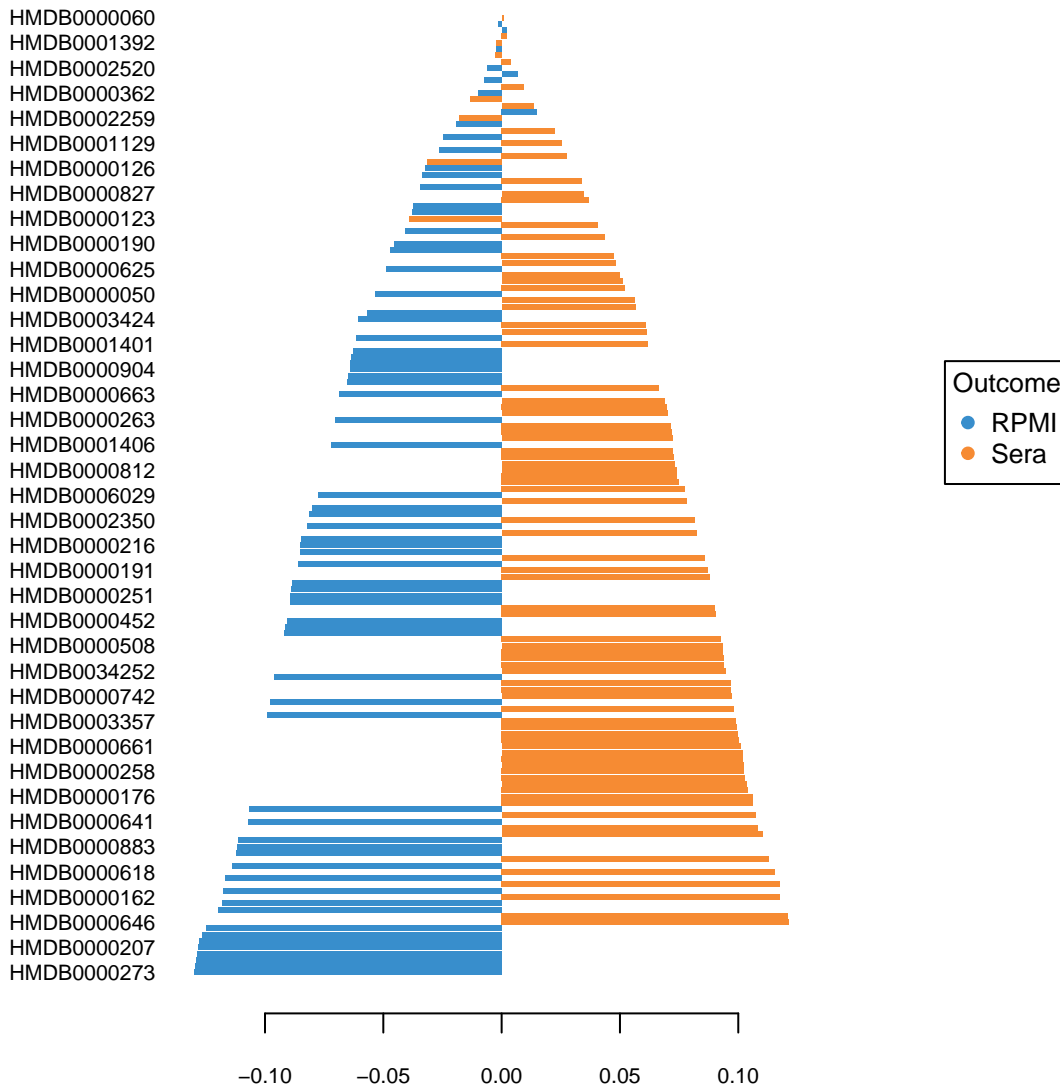
# Metabolomics 1 PLSDA min load



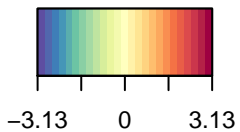
# Contribution on comp 1



# Contribution on comp 1



Color key

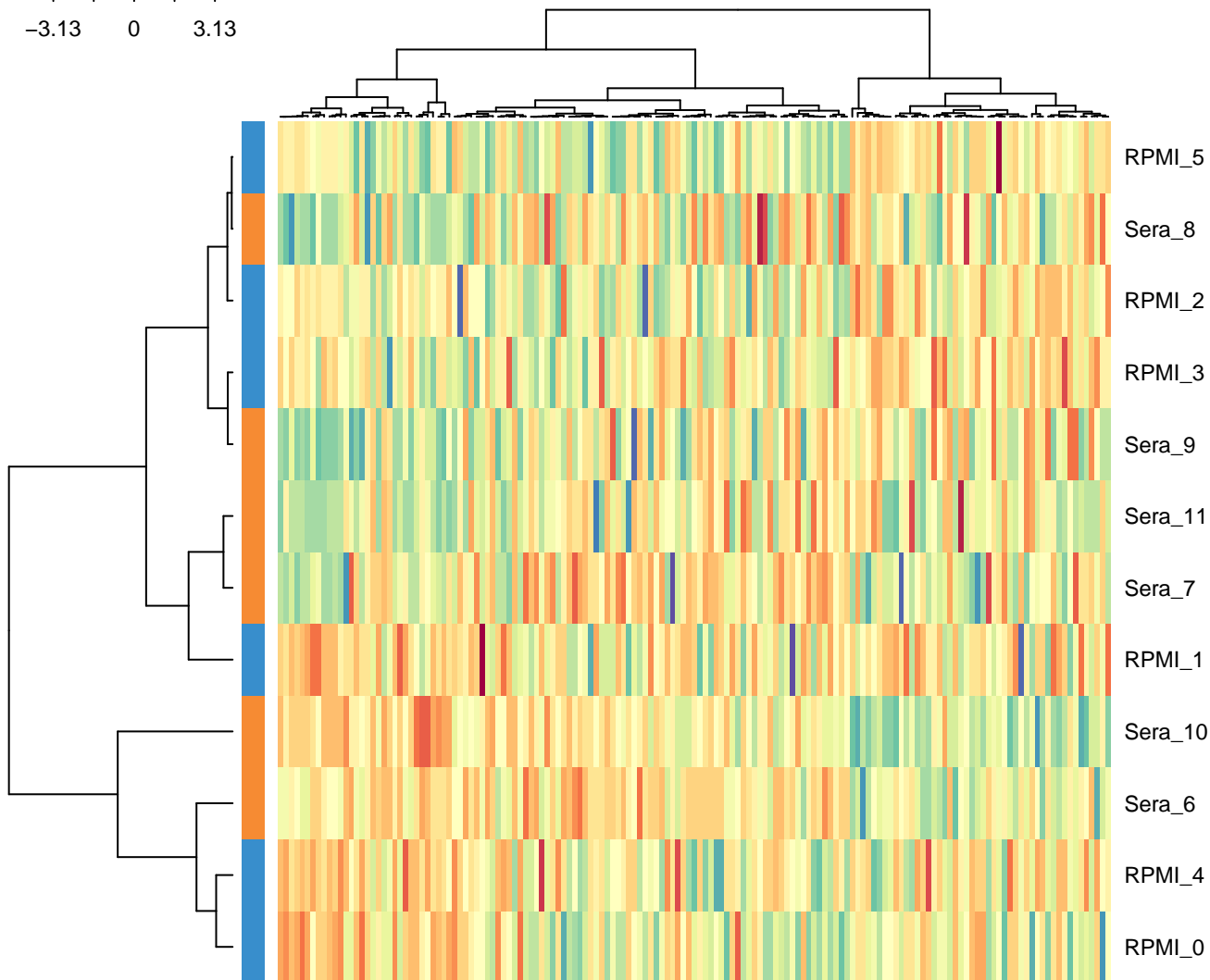


## PLSDA Component 2

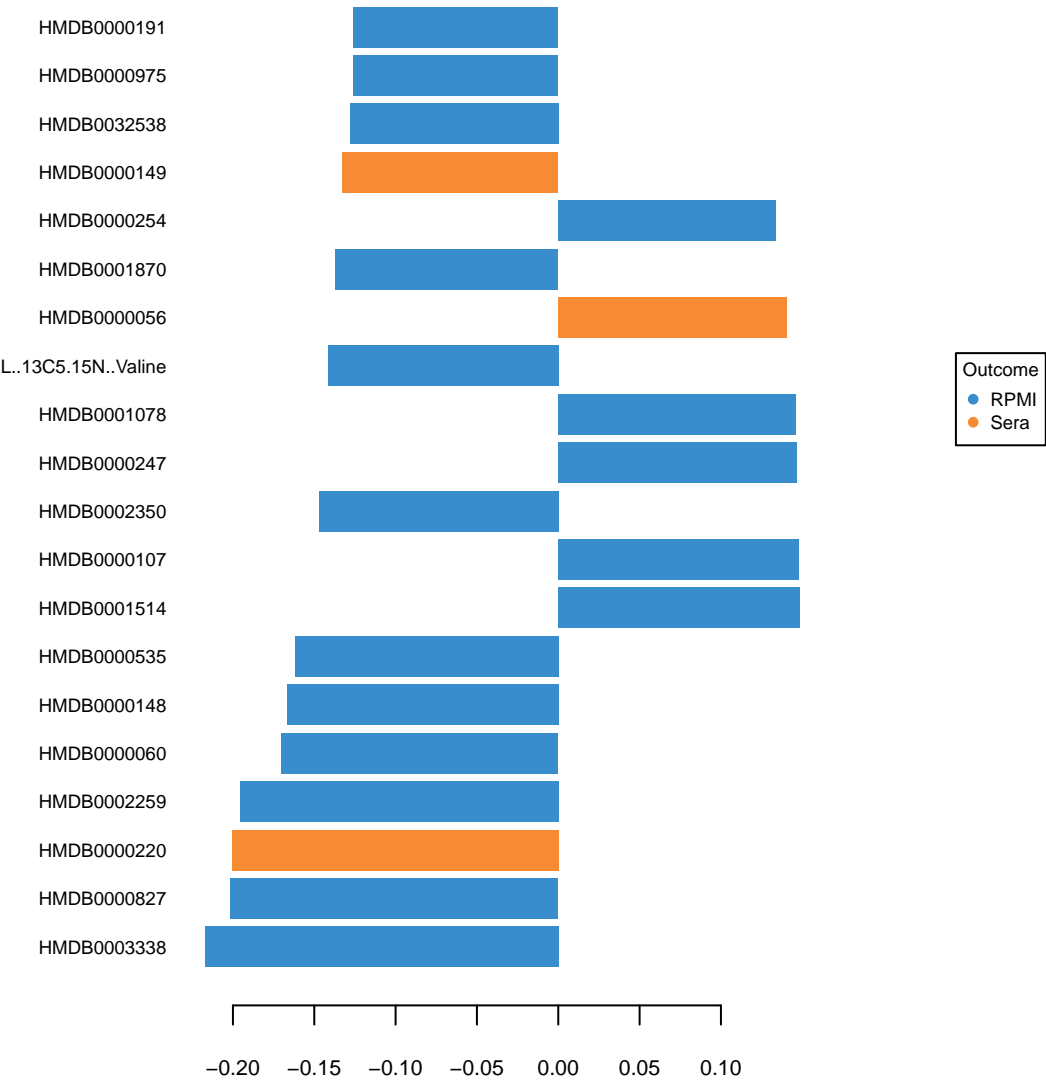
Status

■ RPMI

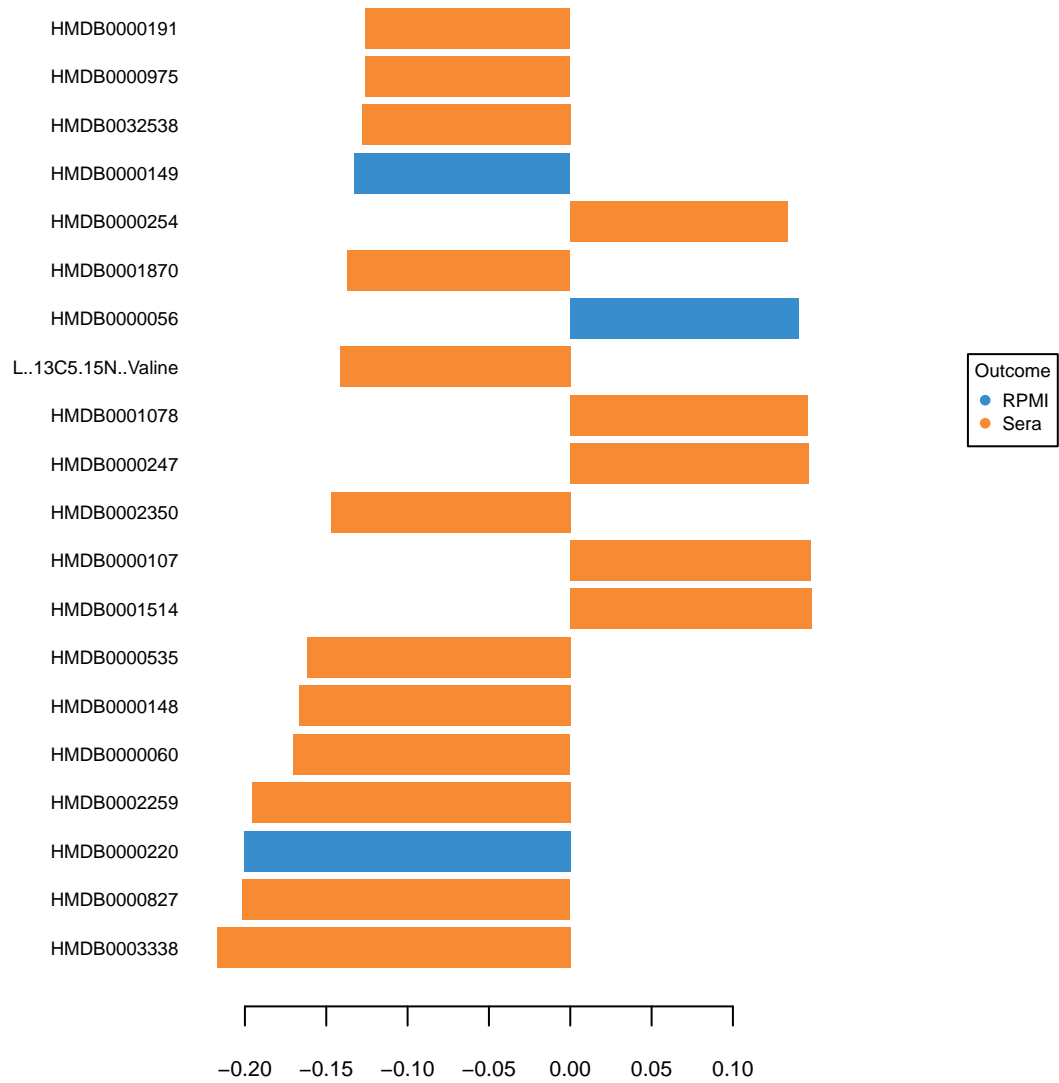
■ Sera



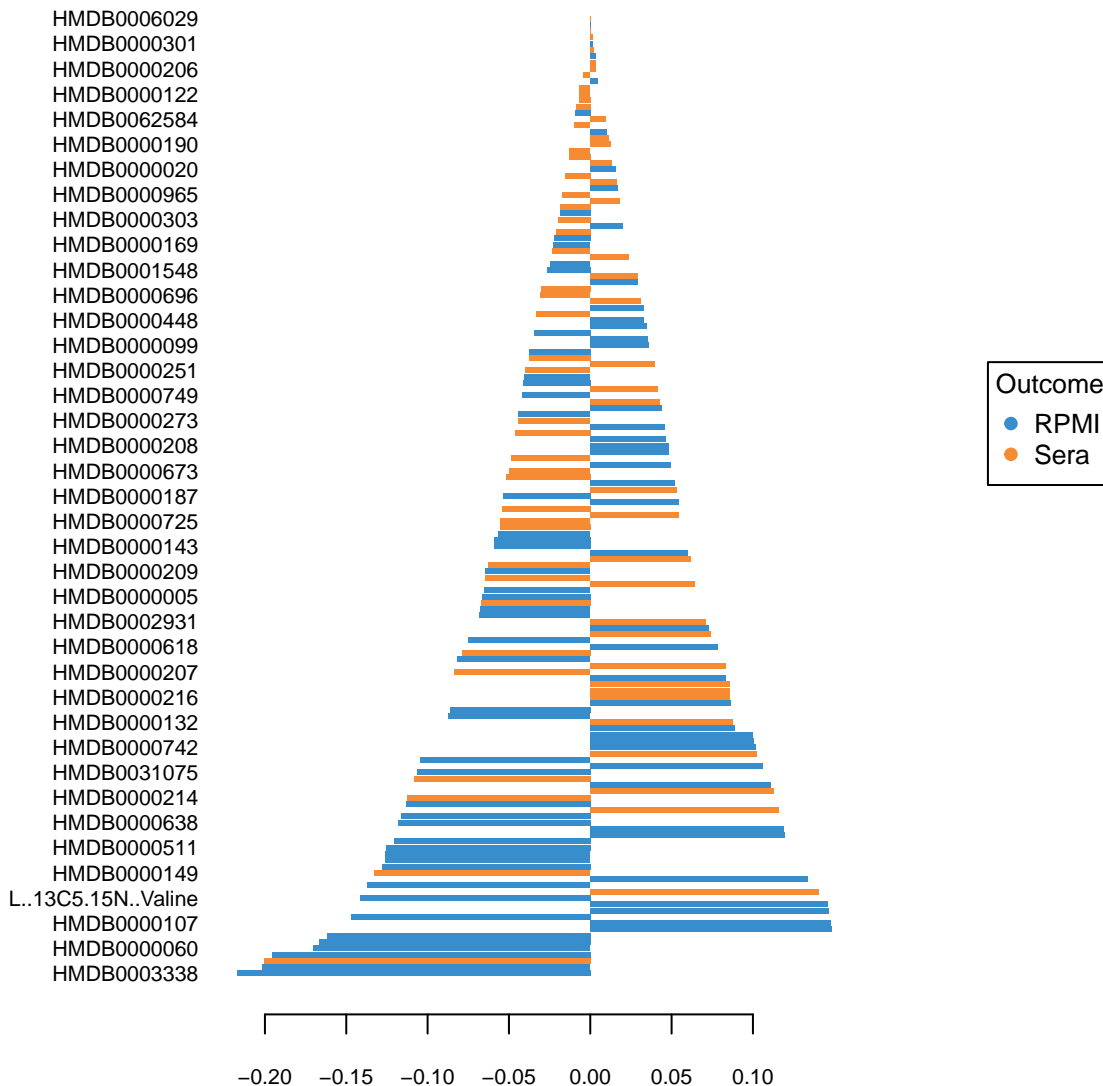
# Metabolomics 2 PLSDA max load



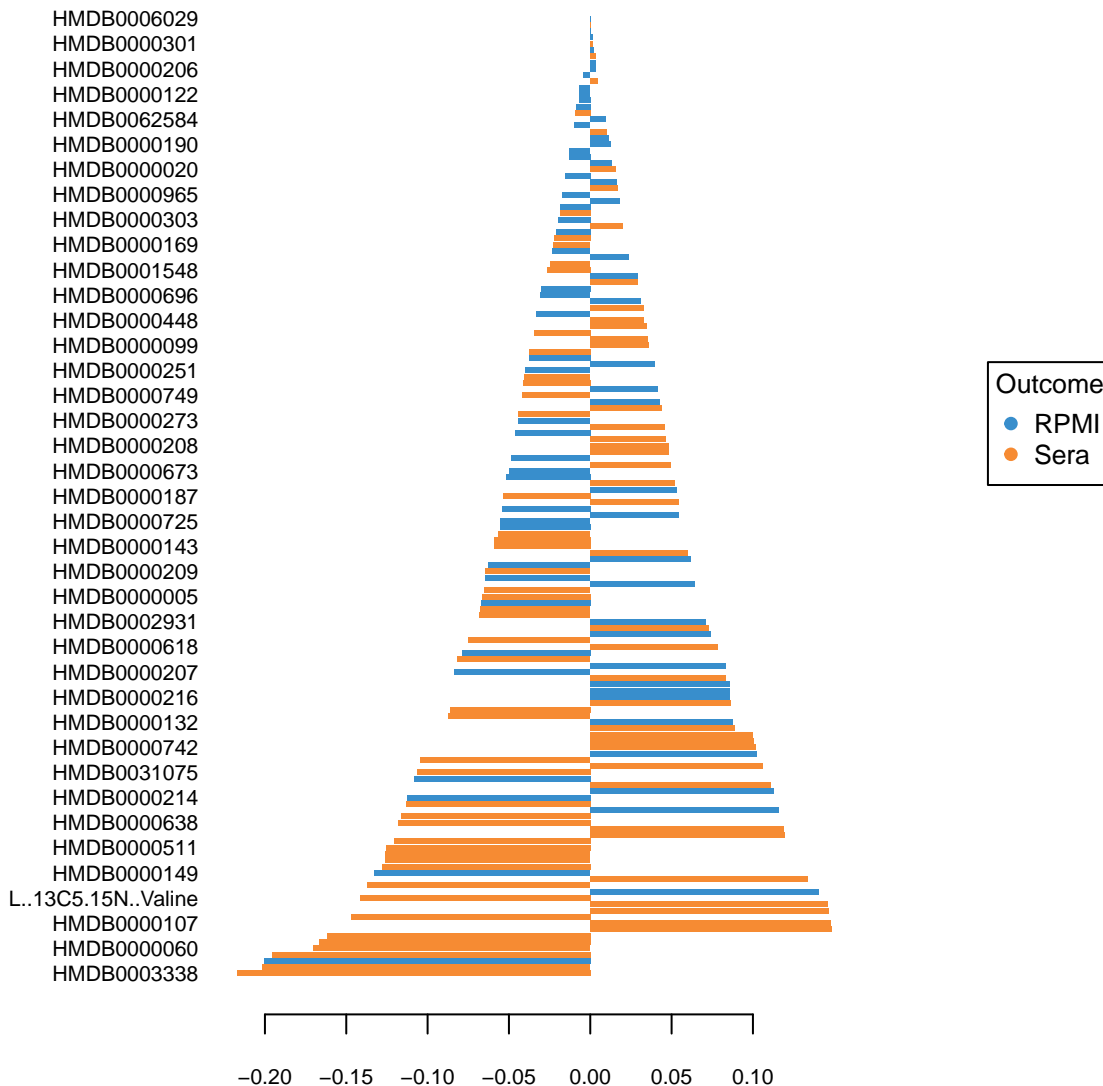
# Metabolomics 2 PLSDA min load



# Contribution on comp 2

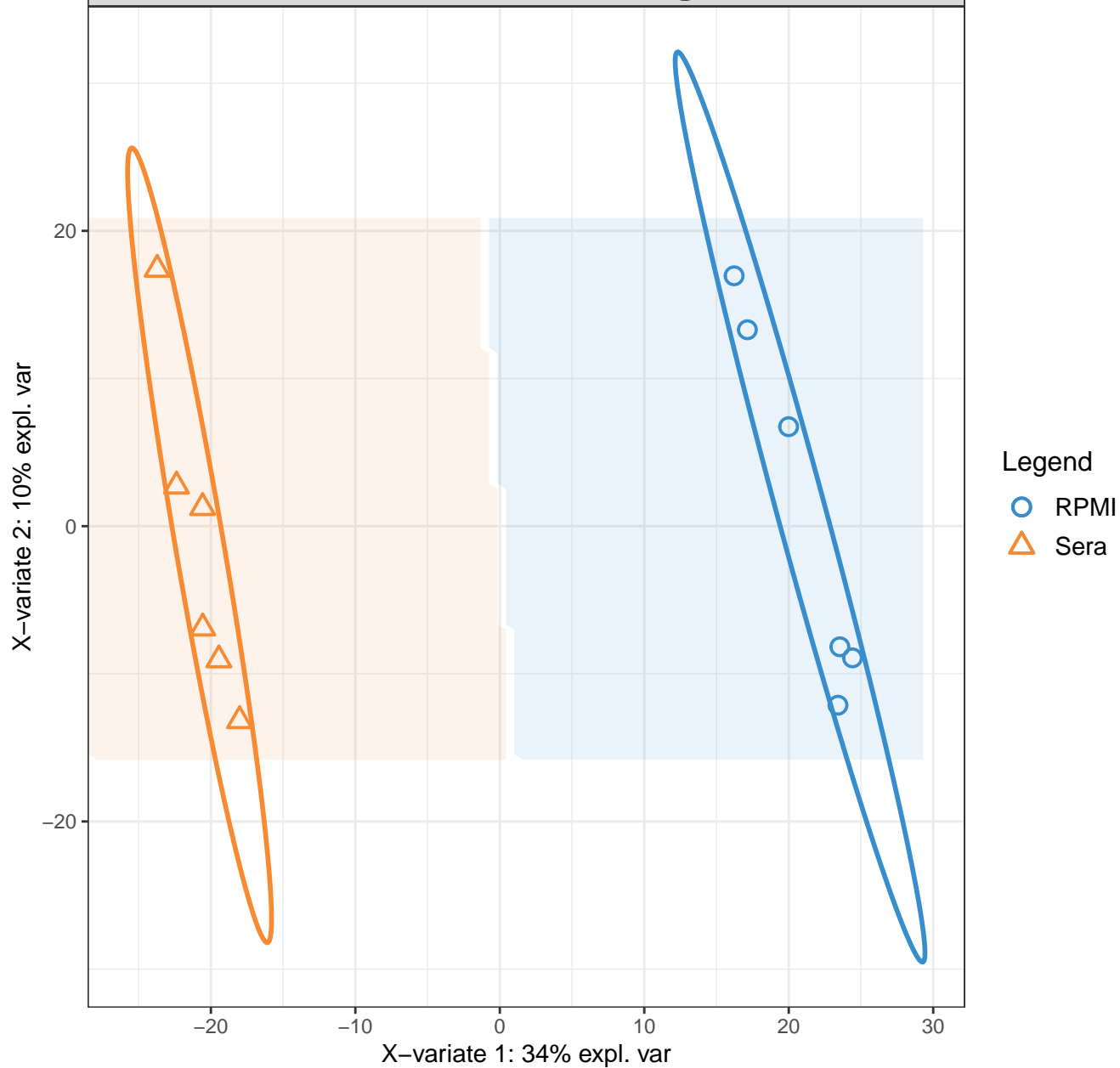


# Contribution on comp 2

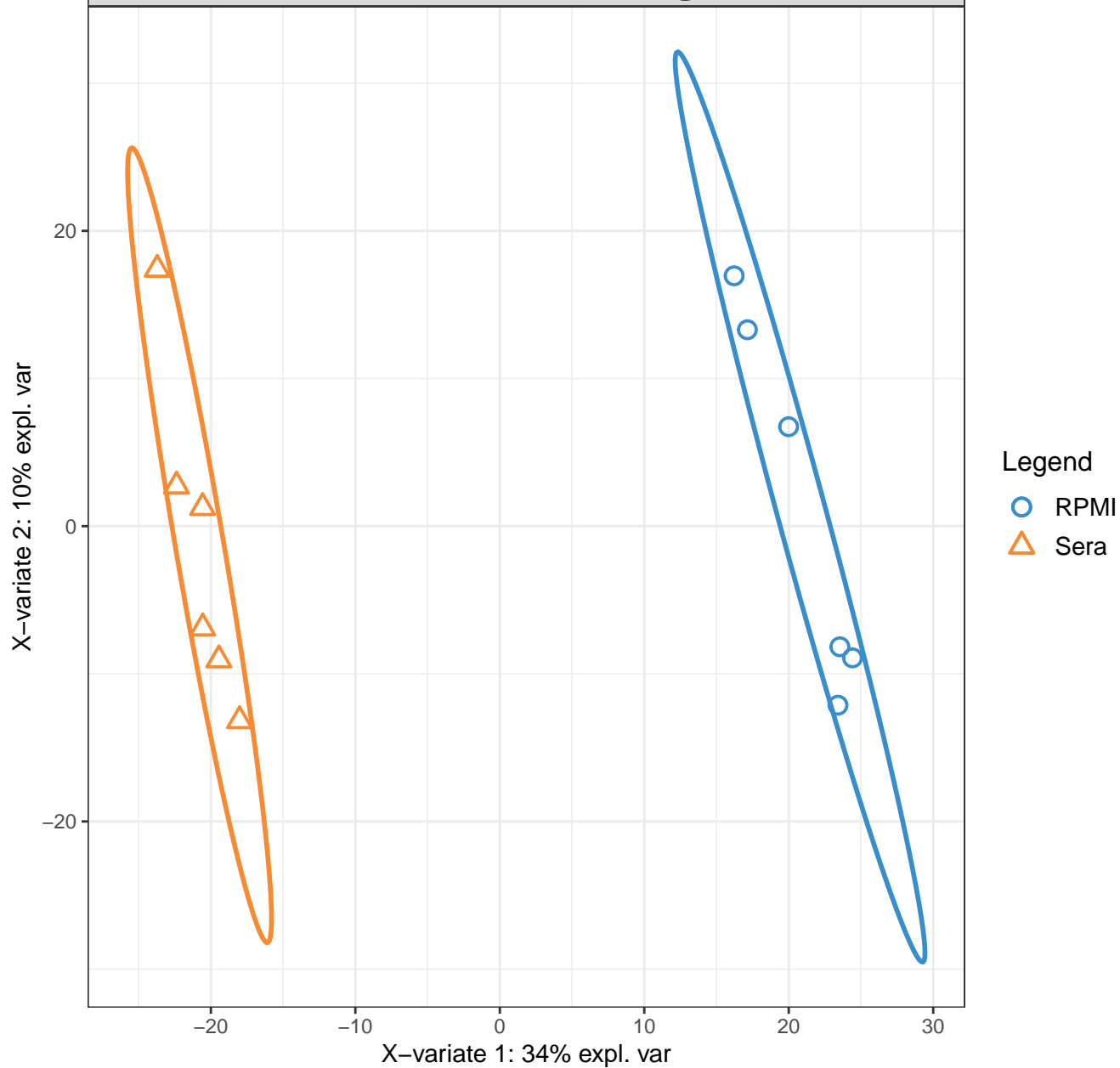




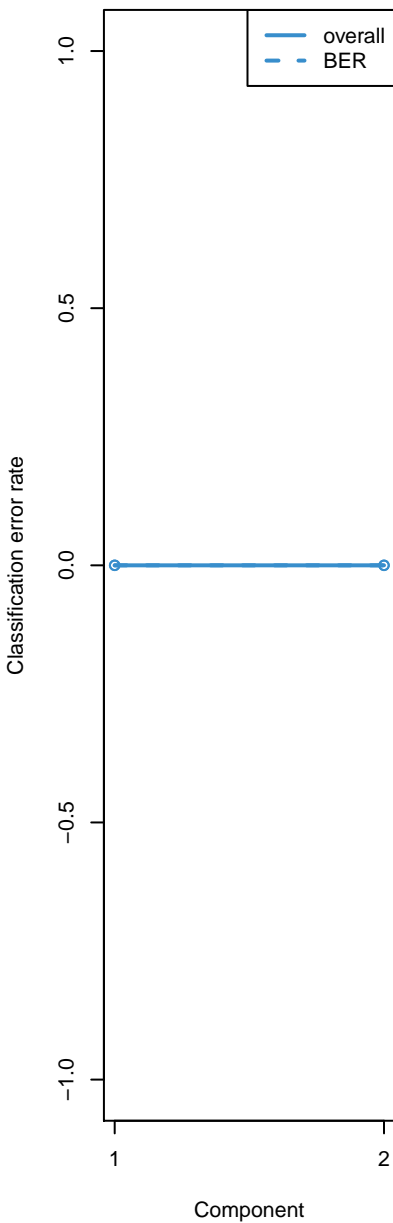
# Proteomics PLSDA single 1/2



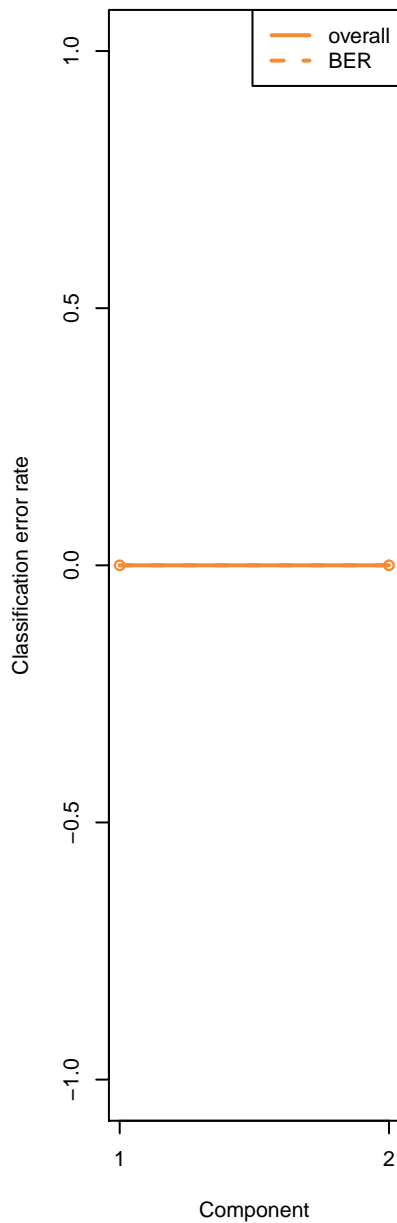
# Proteomics PLSDA single 1/2



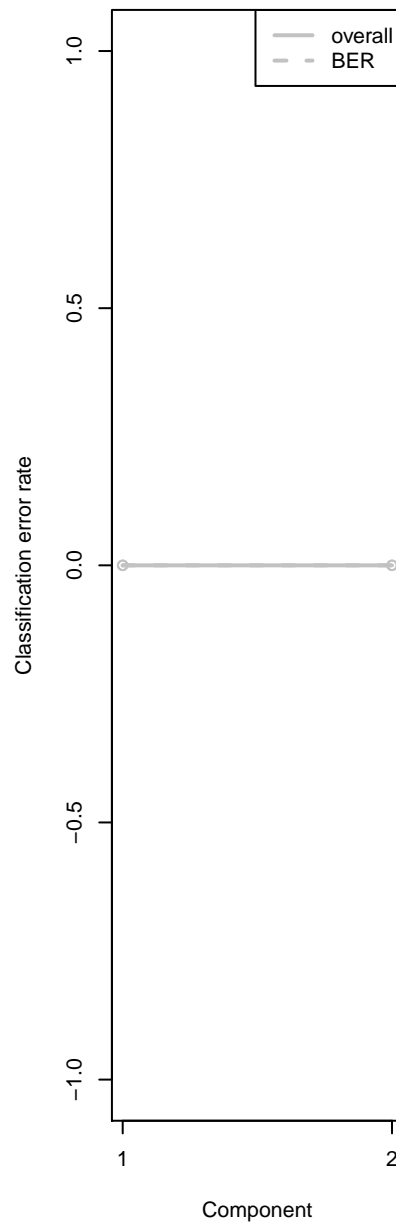
max.dist



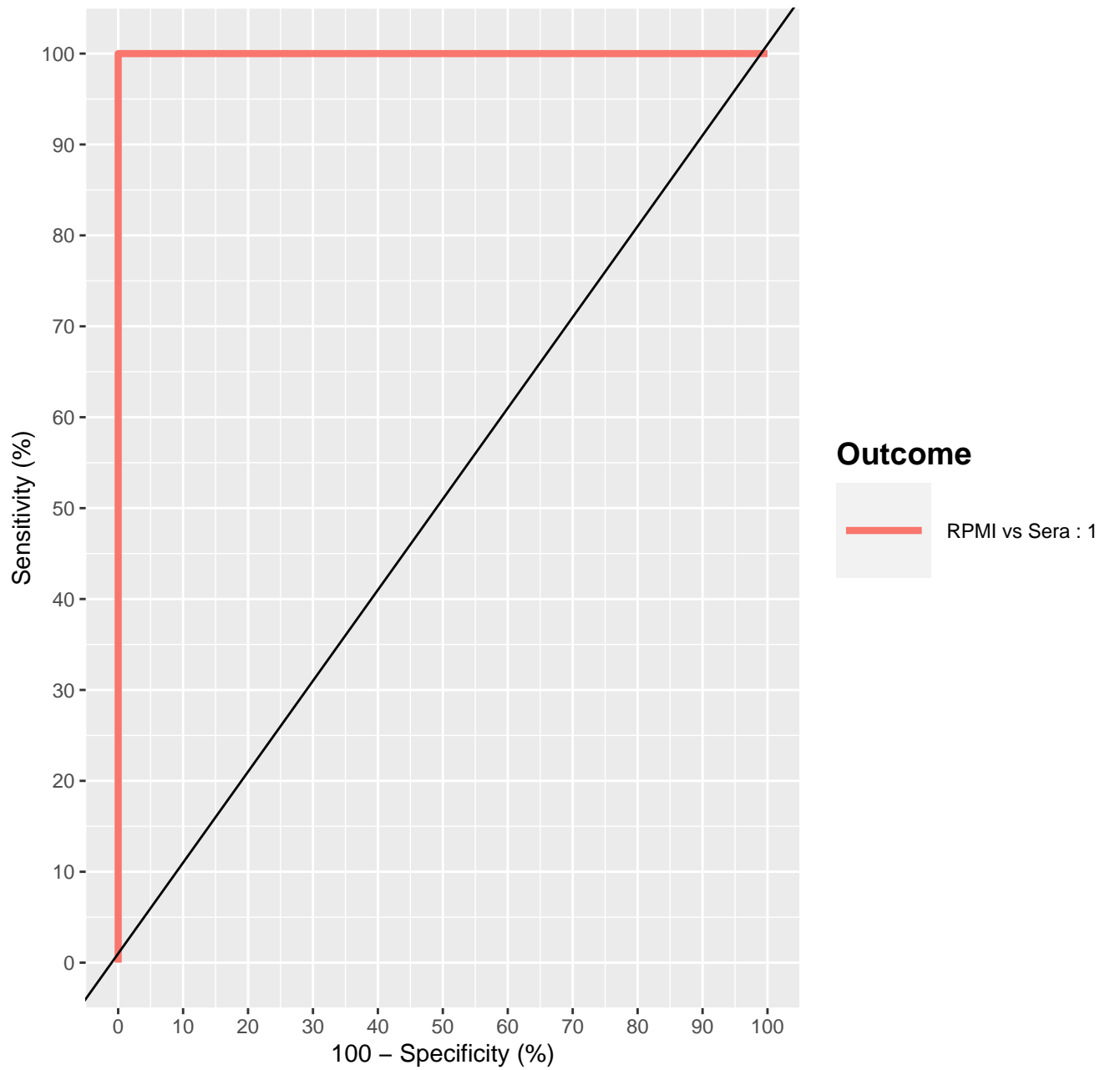
centroids.dist



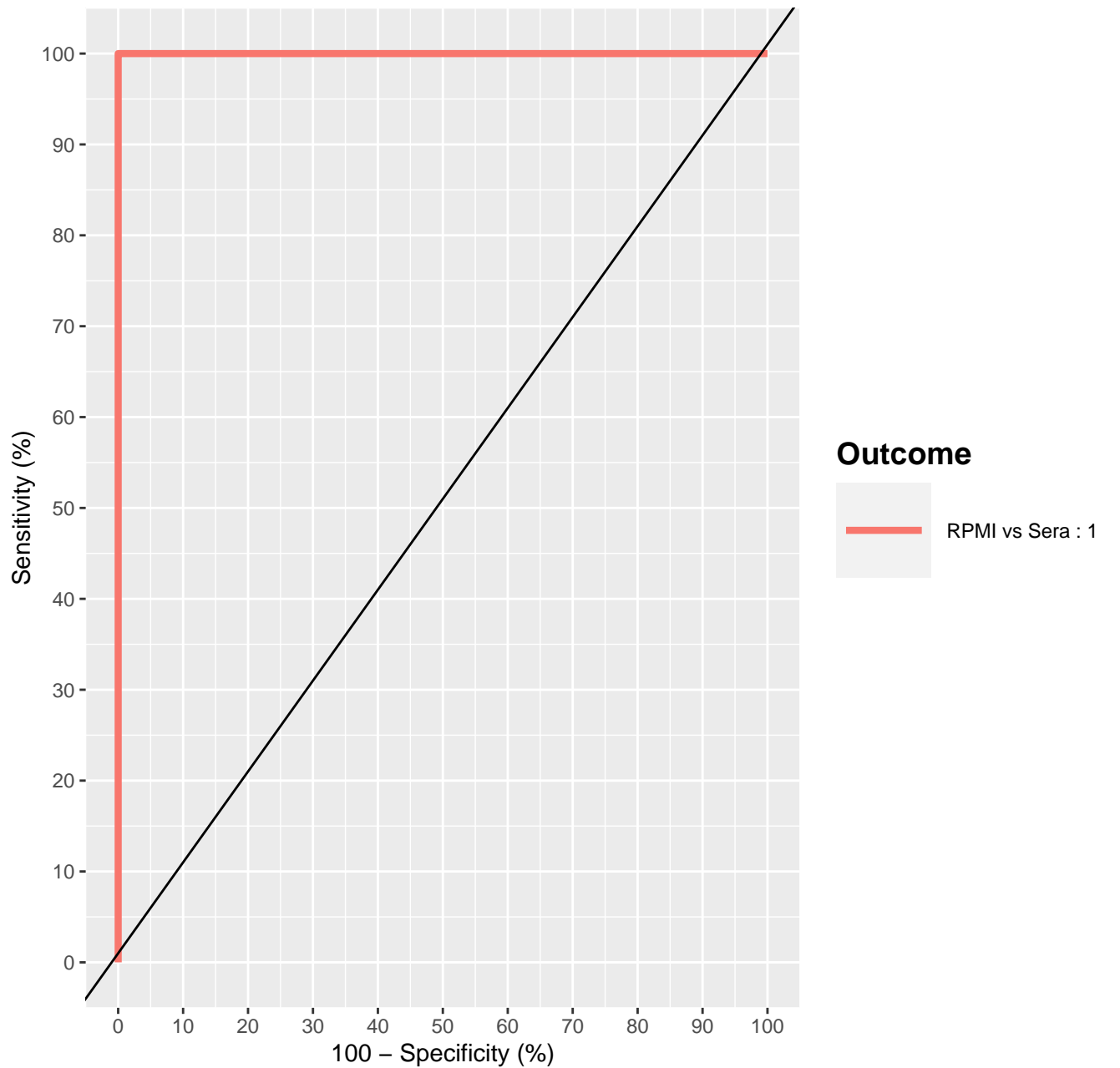
mahalanobis.dist



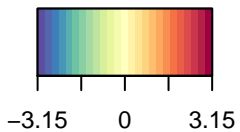
**ROC Curve Comp 1**



## ROC Curve Comp 2



Color key

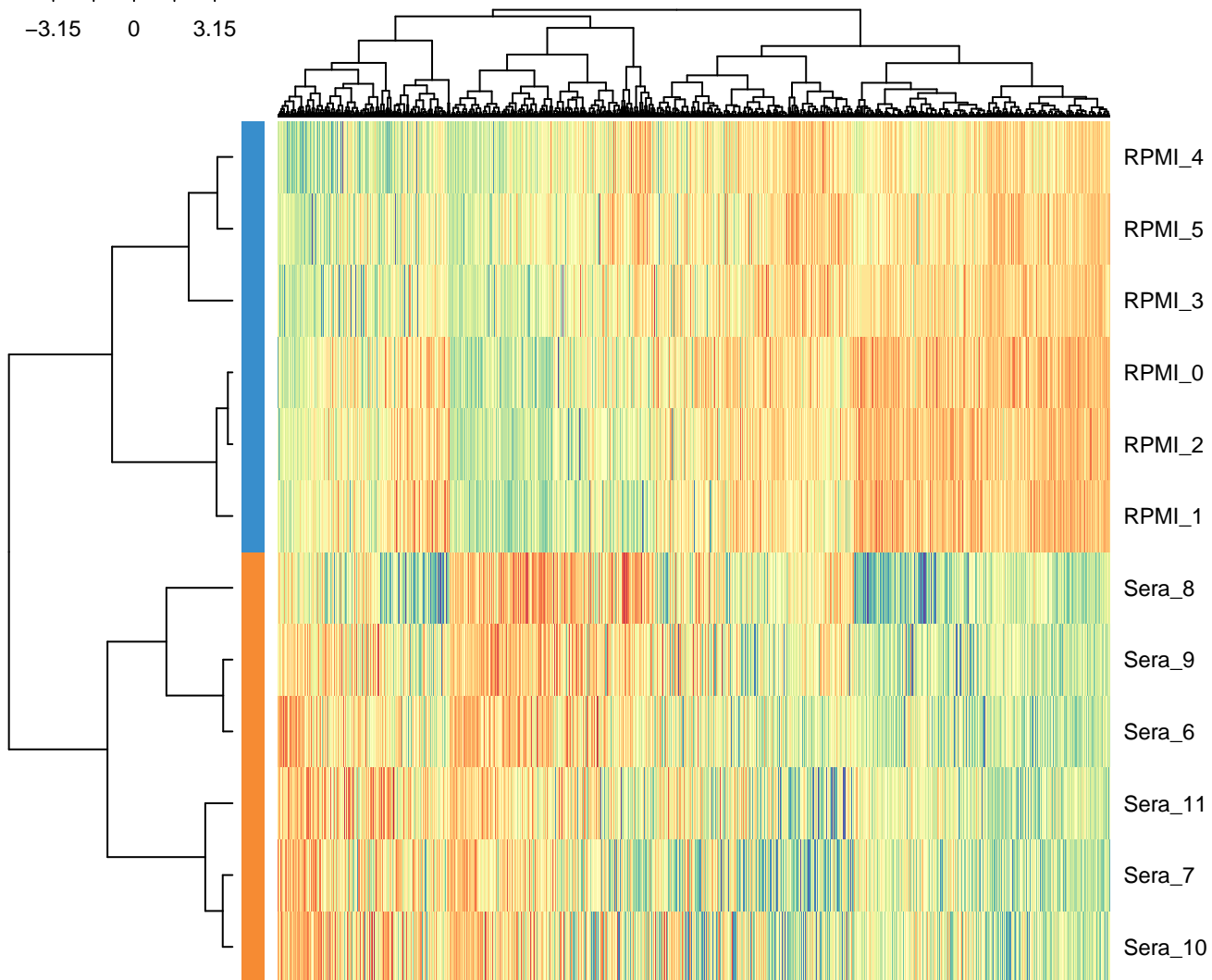


# PLSDA

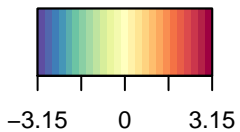
Status

RPMI

Sera



Color key

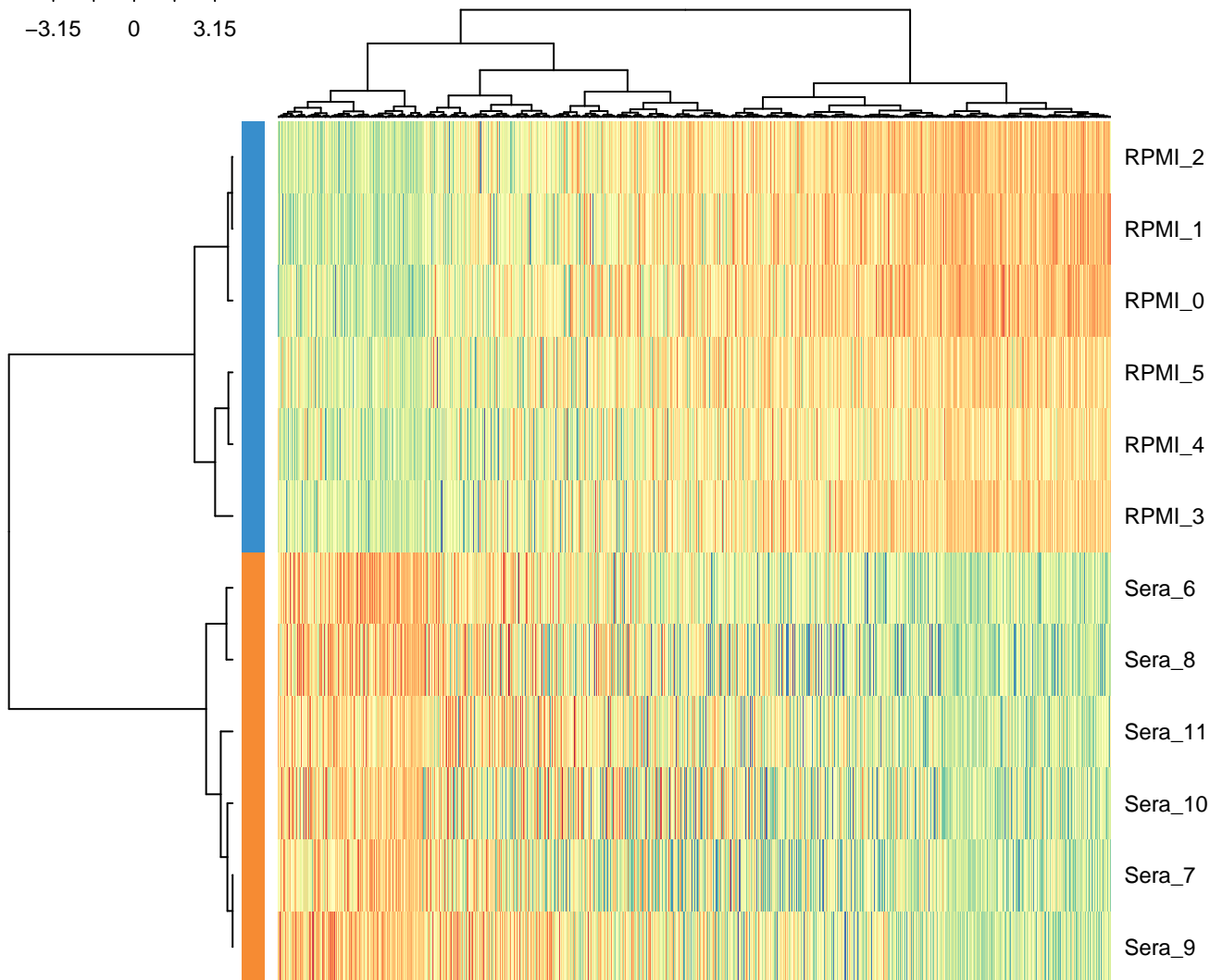


# PLSDA Component 1

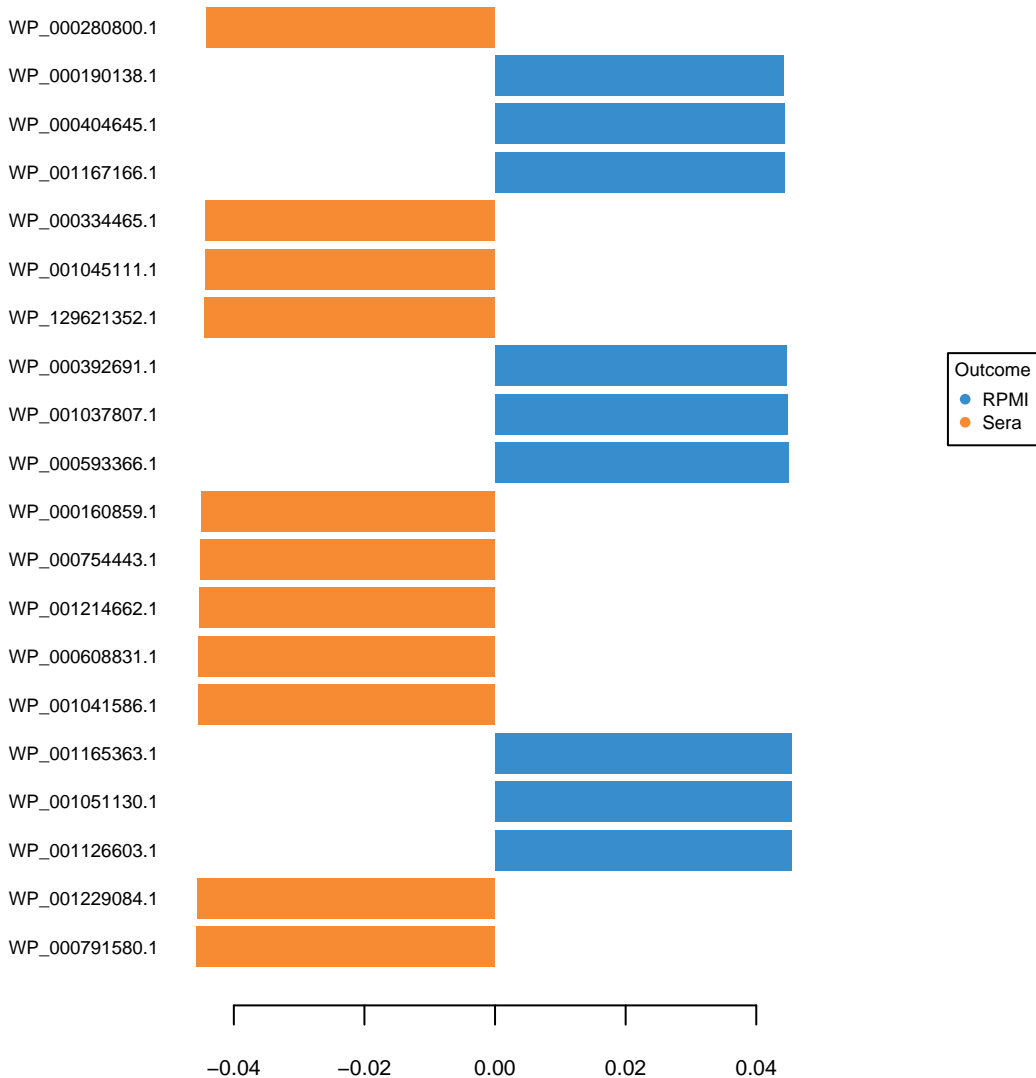
Status

RPMI

Sera

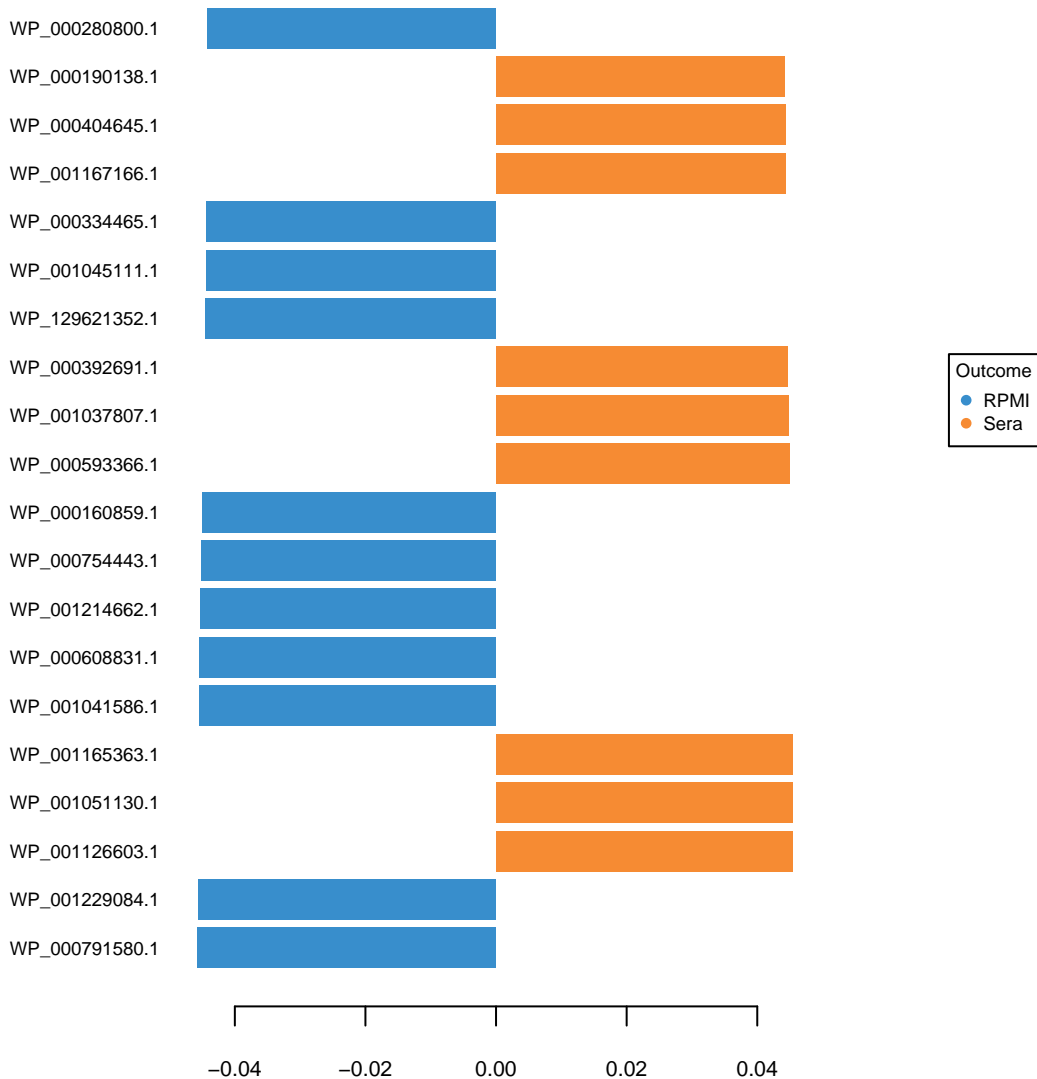


# Proteomics 1 PLSDA max loadings

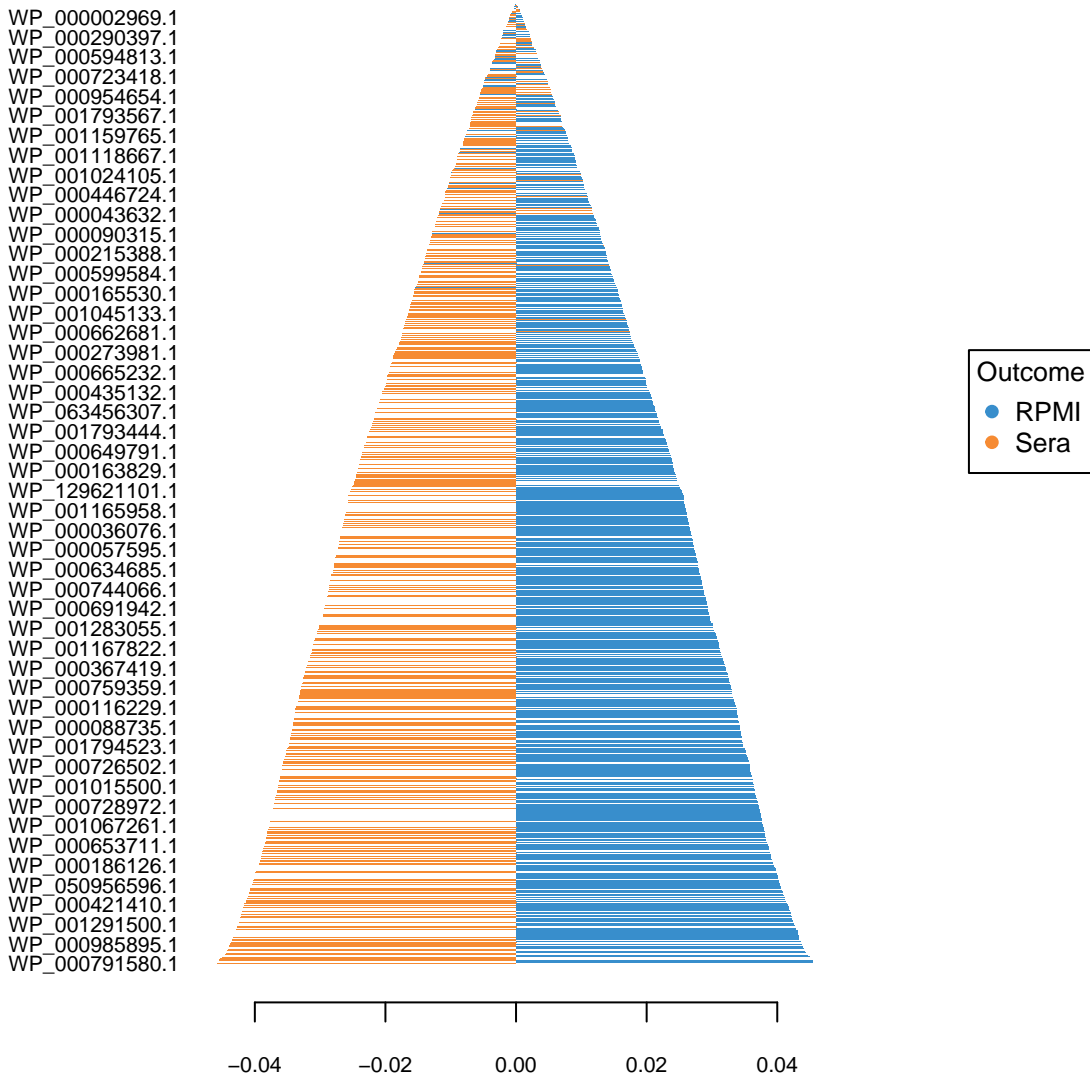




# Proteomics 1 PLSDA min load

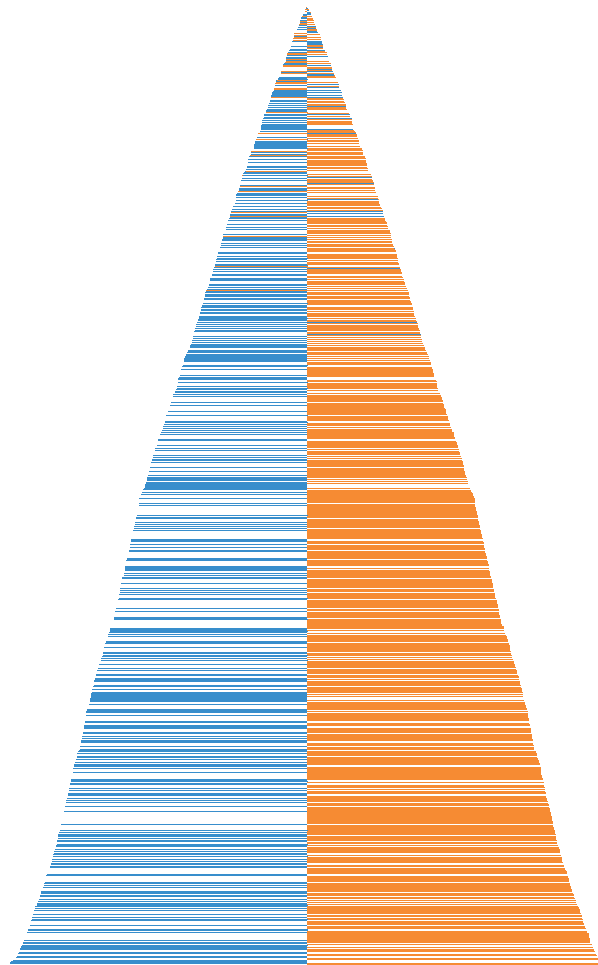


# Contribution on comp 1



# Contribution on comp 1

WP\_000002969.1  
WP\_000290397.1  
WP\_000594813.1  
WP\_000723418.1  
WP\_000954654.1  
WP\_001793567.1  
WP\_001159765.1  
WP\_001118667.1  
WP\_001024105.1  
WP\_000446724.1  
WP\_000043632.1  
WP\_000090315.1  
WP\_000215388.1  
WP\_000599584.1  
WP\_000165530.1  
WP\_001045133.1  
WP\_000662681.1  
WP\_000273981.1  
WP\_000665232.1  
WP\_000435132.1  
WP\_063456307.1  
WP\_001793444.1  
WP\_000649791.1  
WP\_000163829.1  
WP\_129621101.1  
WP\_001165958.1  
WP\_000036076.1  
WP\_000057595.1  
WP\_000634685.1  
WP\_000744066.1  
WP\_000691942.1  
WP\_001283055.1  
WP\_001167822.1  
WP\_000367419.1  
WP\_000759359.1  
WP\_000116229.1  
WP\_000088735.1  
WP\_001794523.1  
WP\_000726502.1  
WP\_001015500.1  
WP\_000728972.1  
WP\_001067261.1  
WP\_000653711.1  
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WP\_001291500.1  
WP\_000985895.1  
WP\_000791580.1

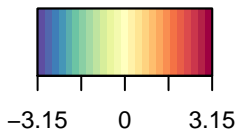


Outcome

- RPMI
- Sera

-0.04      -0.02      0.00      0.02      0.04

Color key

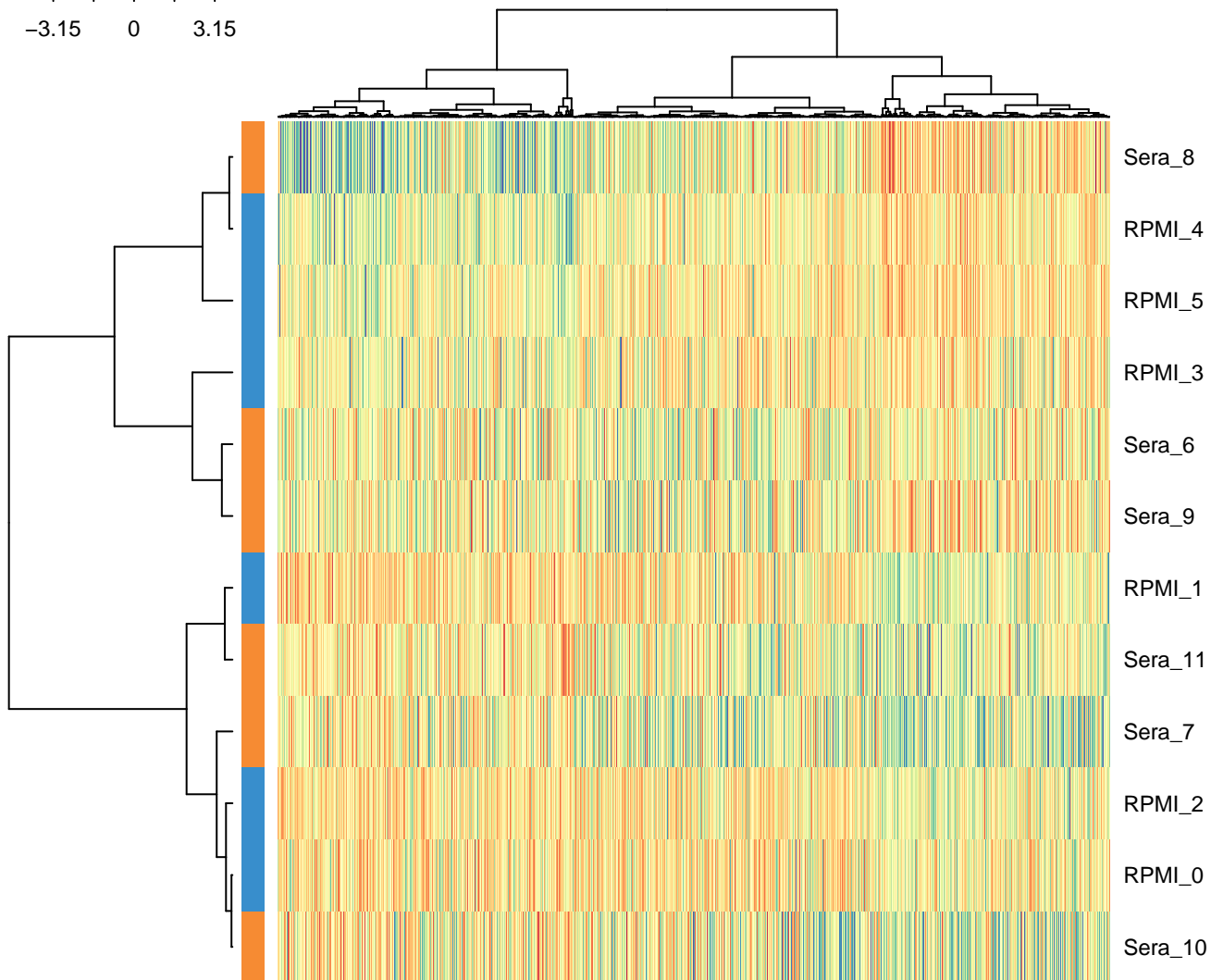


## PLSDA Component 2

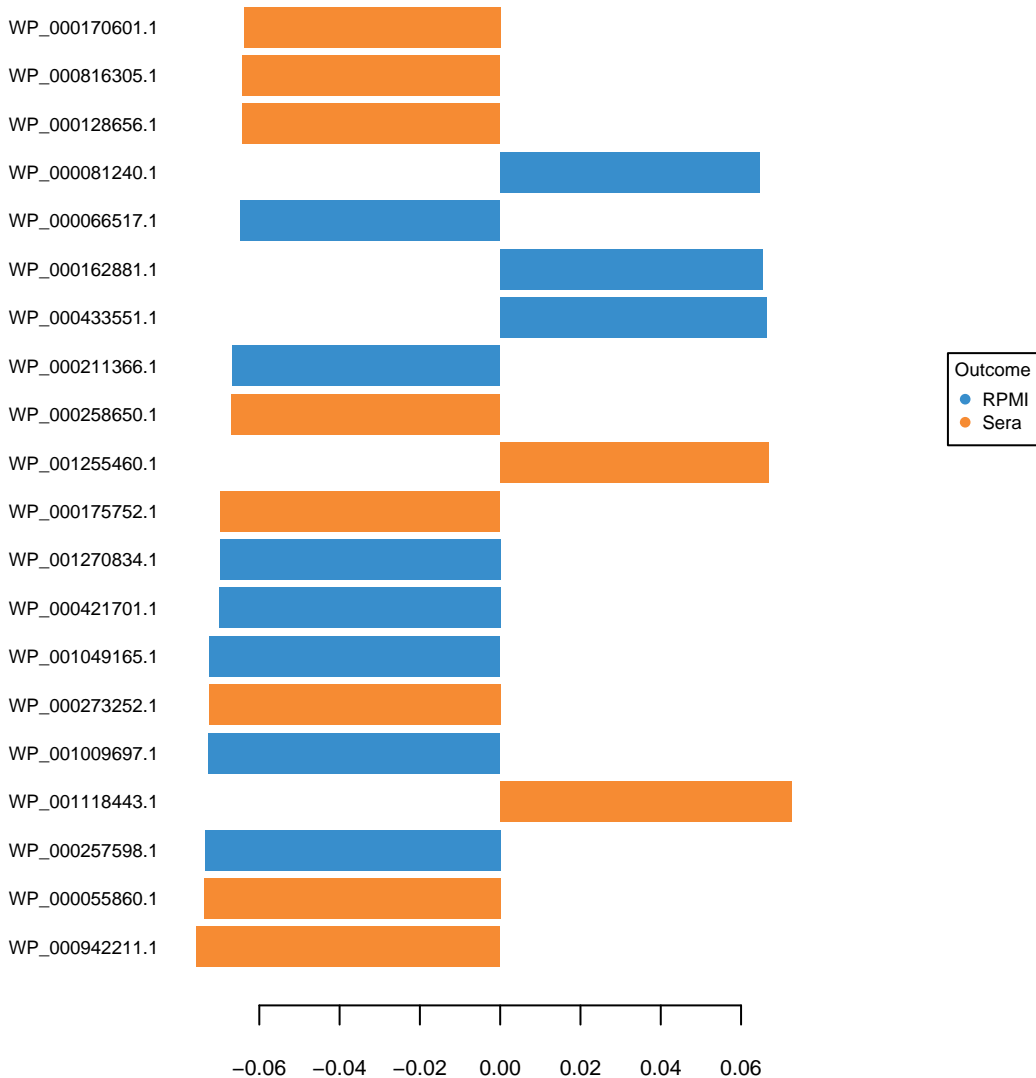
Status

RPMI

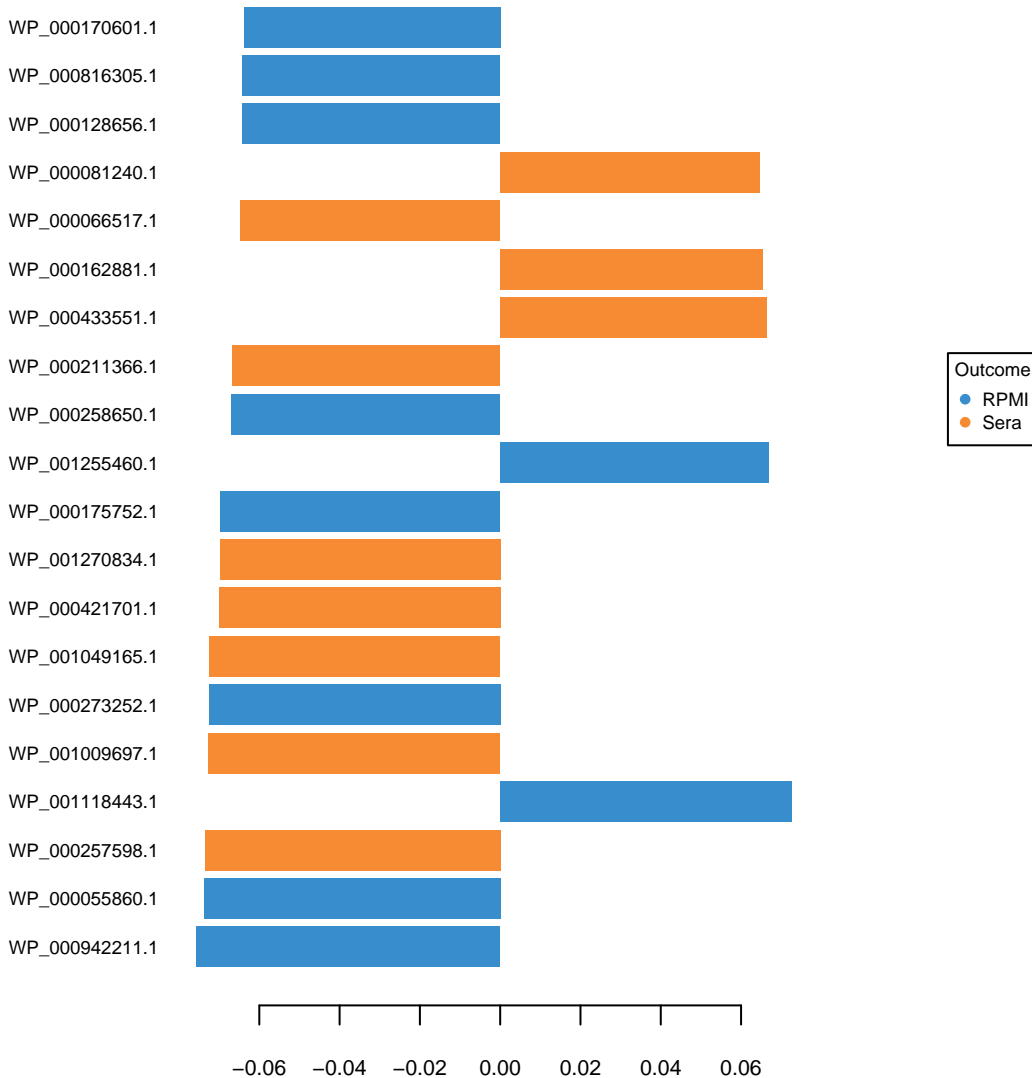
Sera



# Proteomics 2 PLSDA max loadings



# Proteomics 2 PLSDA min load



# Contribution on comp 2

WP\_000868999.1  
WP\_129621289.1  
WP\_000064078.1  
WP\_000503820.1  
WP\_000181832.1  
WP\_000108667.1  
WP\_001005768.1  
WP\_000985895.1  
WP\_000367419.1  
WP\_001291500.1  
WP\_000425353.1  
WP\_001049150.1  
WP\_000608440.1  
WP\_001024830.1  
WP\_000769416.1  
WP\_000076405.1  
WP\_000342192.1  
WP\_000999200.1  
WP\_129621225.1  
WP\_001165363.1  
WP\_000864305.1  
WP\_000006551.1  
WP\_000064778.1  
WP\_000365354.1  
WP\_000831495.1  
WP\_000368227.1  
WP\_000290301.1  
WP\_000871607.1  
WP\_000733409.1  
WP\_000285450.1  
WP\_000660041.1  
WP\_000911041.1  
WP\_000417016.1  
WP\_000224612.1  
WP\_000737686.1  
WP\_000011542.1  
WP\_000990133.1  
WP\_000230173.1  
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WP\_001288199.1  
WP\_000284431.1  
WP\_000785090.1  
WP\_000547794.1  
WP\_001228169.1  
WP\_000095327.1  
WP\_129621180.1  
WP\_129621249.1  
WP\_000446724.1  
WP\_000942211.1

Outcome

- RPMI
- Sera

-0.06 -0.04 -0.02 0.00 0.02 0.04 0.06

# Contribution on comp 2

WP\_000868999.1  
WP\_129621289.1  
WP\_000064078.1  
WP\_000503820.1  
WP\_000181832.1  
WP\_000108667.1  
WP\_001005768.1  
WP\_000985895.1  
WP\_000367419.1  
WP\_001291500.1  
WP\_000425353.1  
WP\_001049150.1  
WP\_000608440.1  
WP\_001024830.1  
WP\_000769416.1  
WP\_000076405.1  
WP\_000342192.1  
WP\_000999200.1  
WP\_129621225.1  
WP\_001165363.1  
WP\_000864305.1  
WP\_000006551.1  
WP\_000064778.1  
WP\_000365354.1  
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WP\_000230173.1  
WP\_000897044.1  
WP\_001288199.1  
WP\_000284431.1  
WP\_000785090.1  
WP\_000547794.1  
WP\_001228169.1  
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WP\_000446724.1  
WP\_000942211.1

Outcome

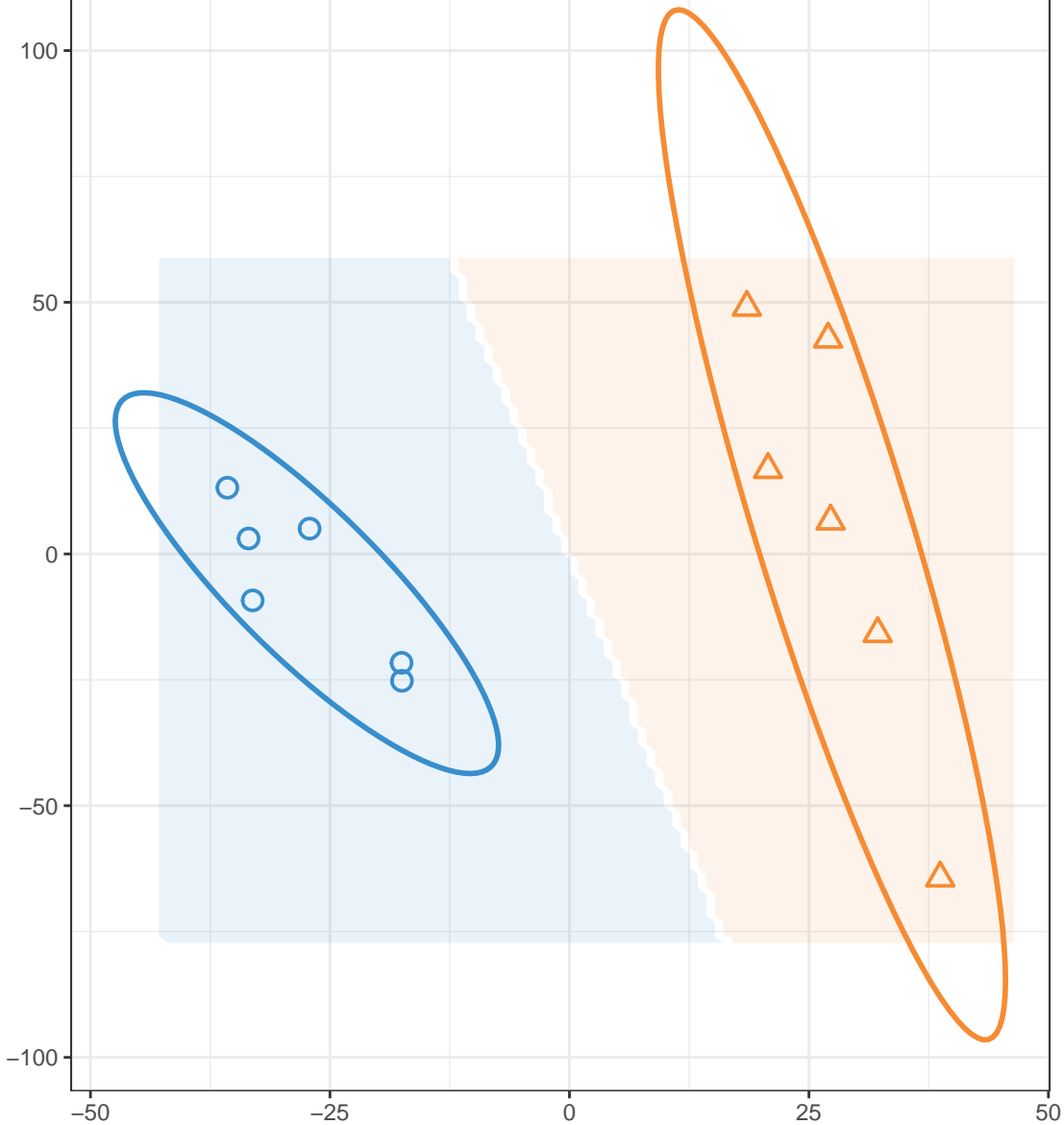
- RPMI
- Sera

-0.06 -0.04 -0.02 0.00 0.02 0.04 0.06



# RNA\_Seq PLSDA single 1/2

X-variate 2: 36% expl. var

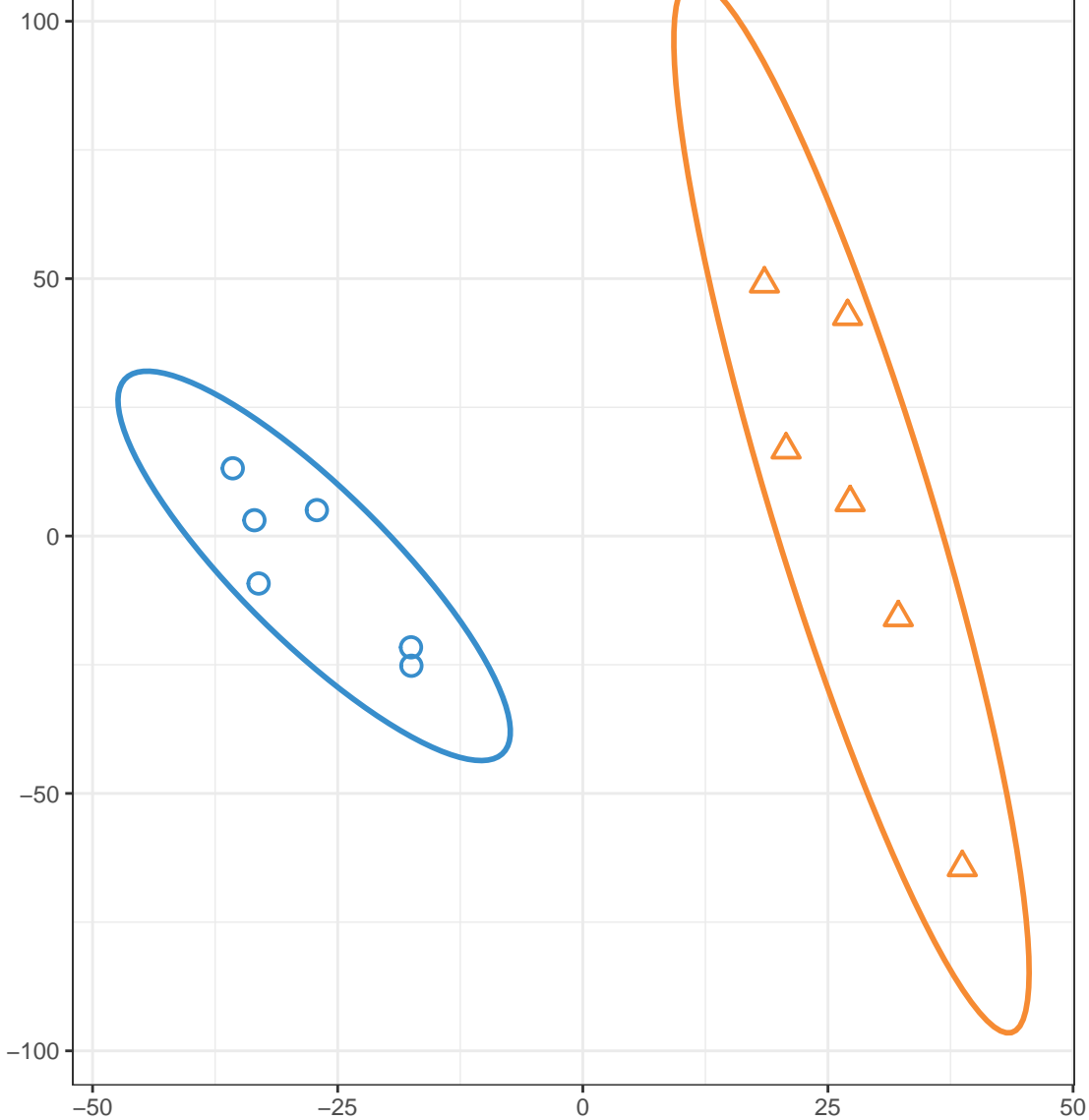


Legend

- RPMI
- △ Sera

# RNA\_Seq PLSDA single 1/2

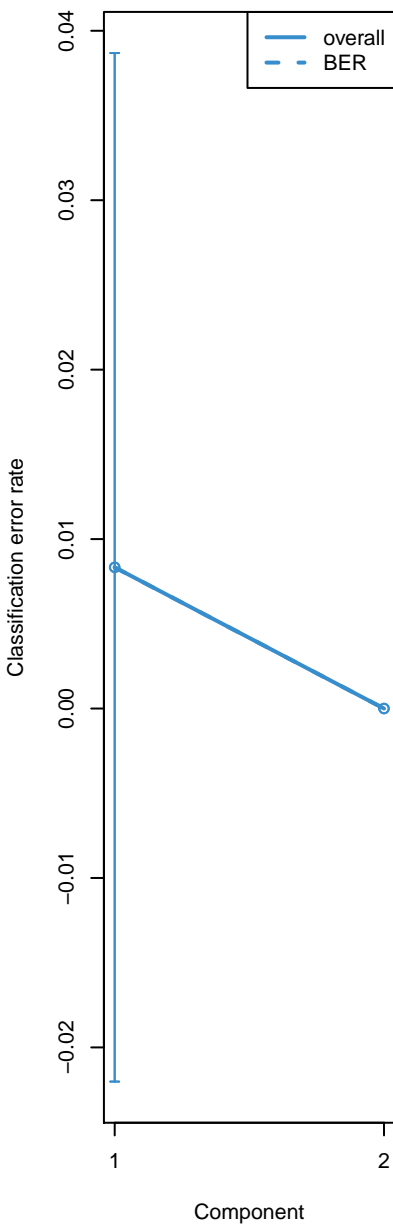
X-variate 2: 36% expl. var



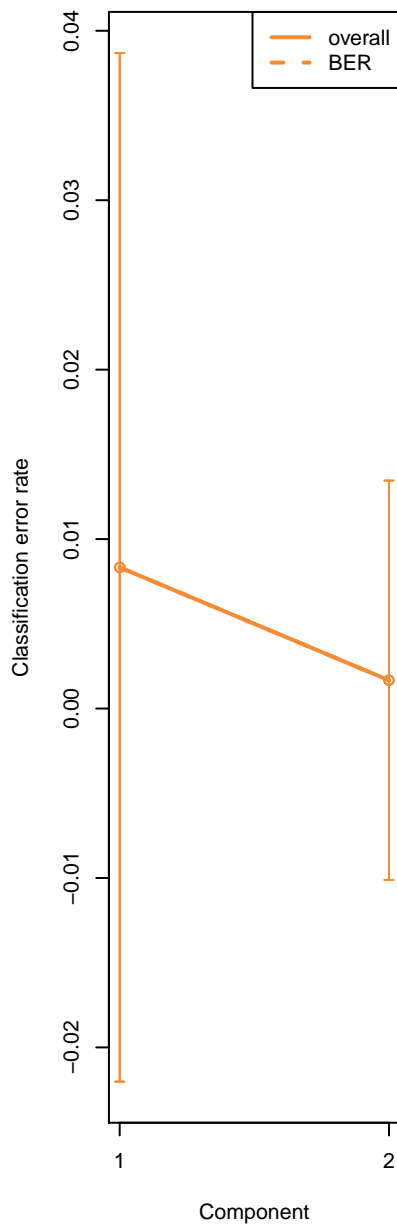
Legend

- RPMI
- △ Sera

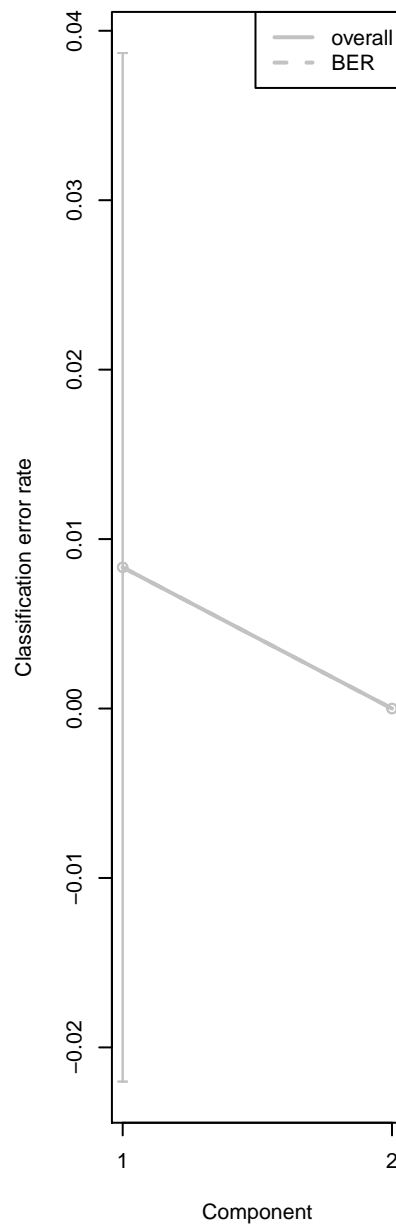
max.dist



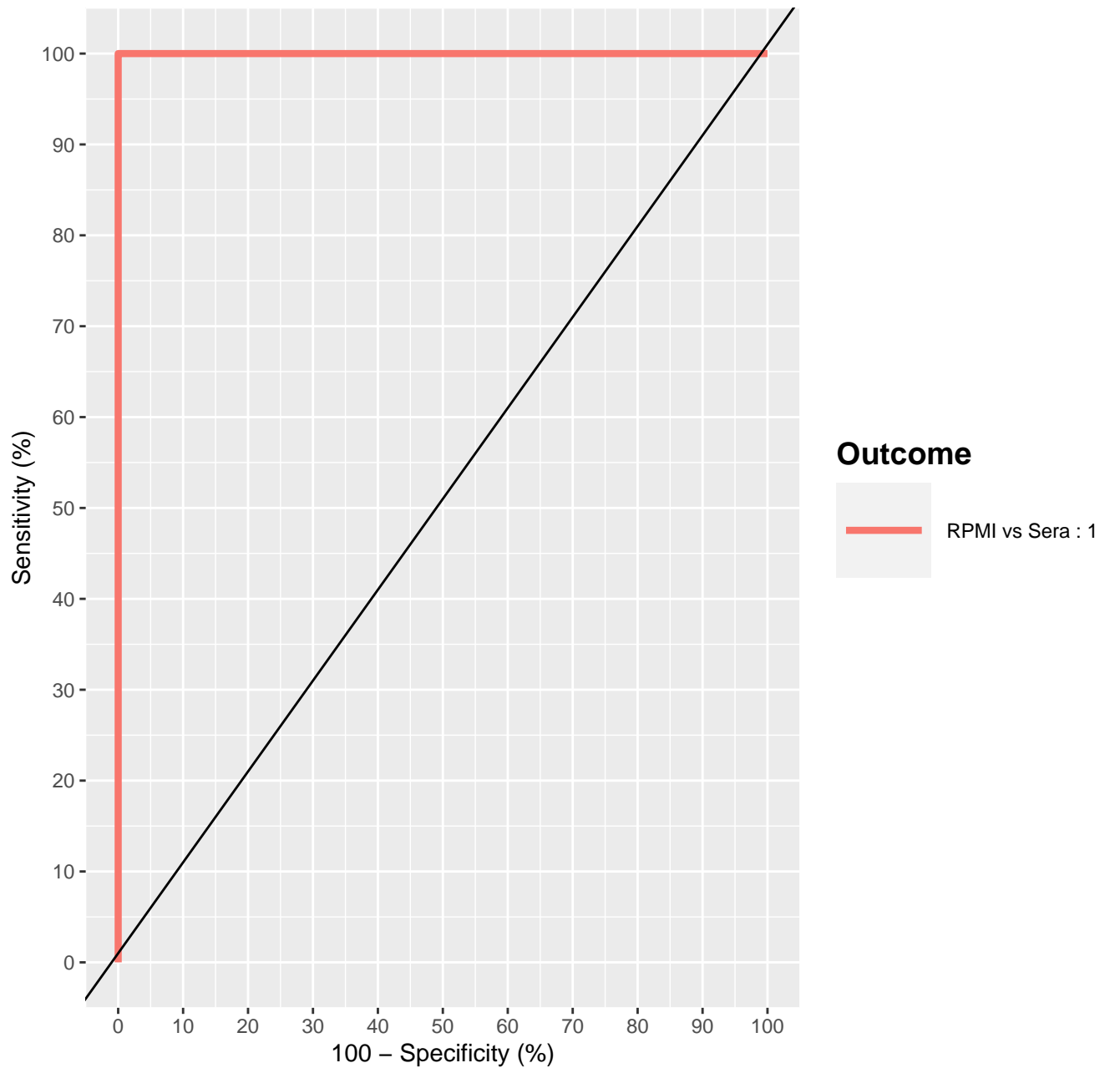
centroids.dist



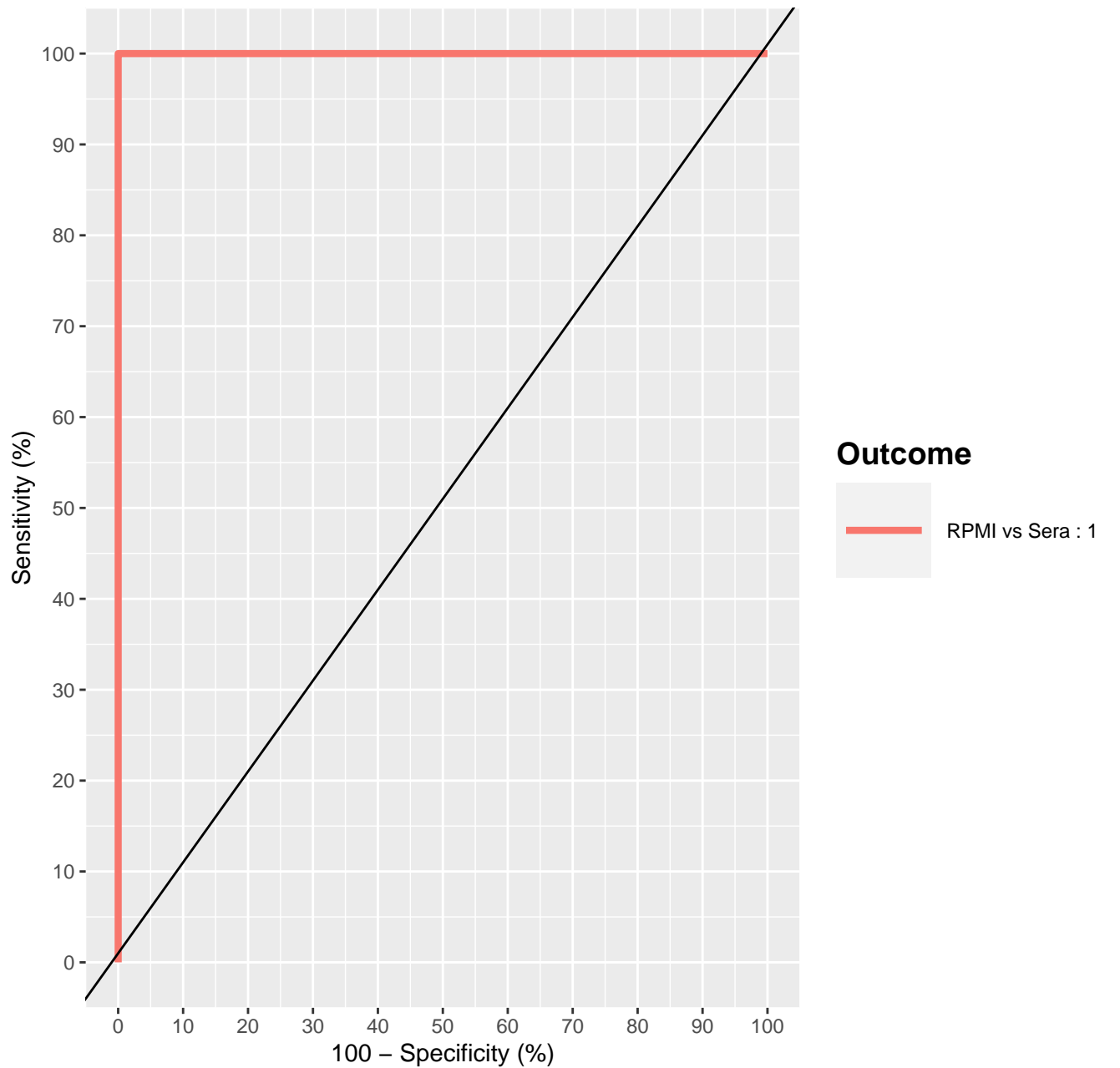
mahalanobis.dist



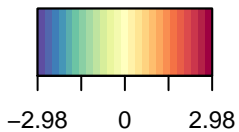
**ROC Curve Comp 1**



**ROC Curve Comp 2**



Color key

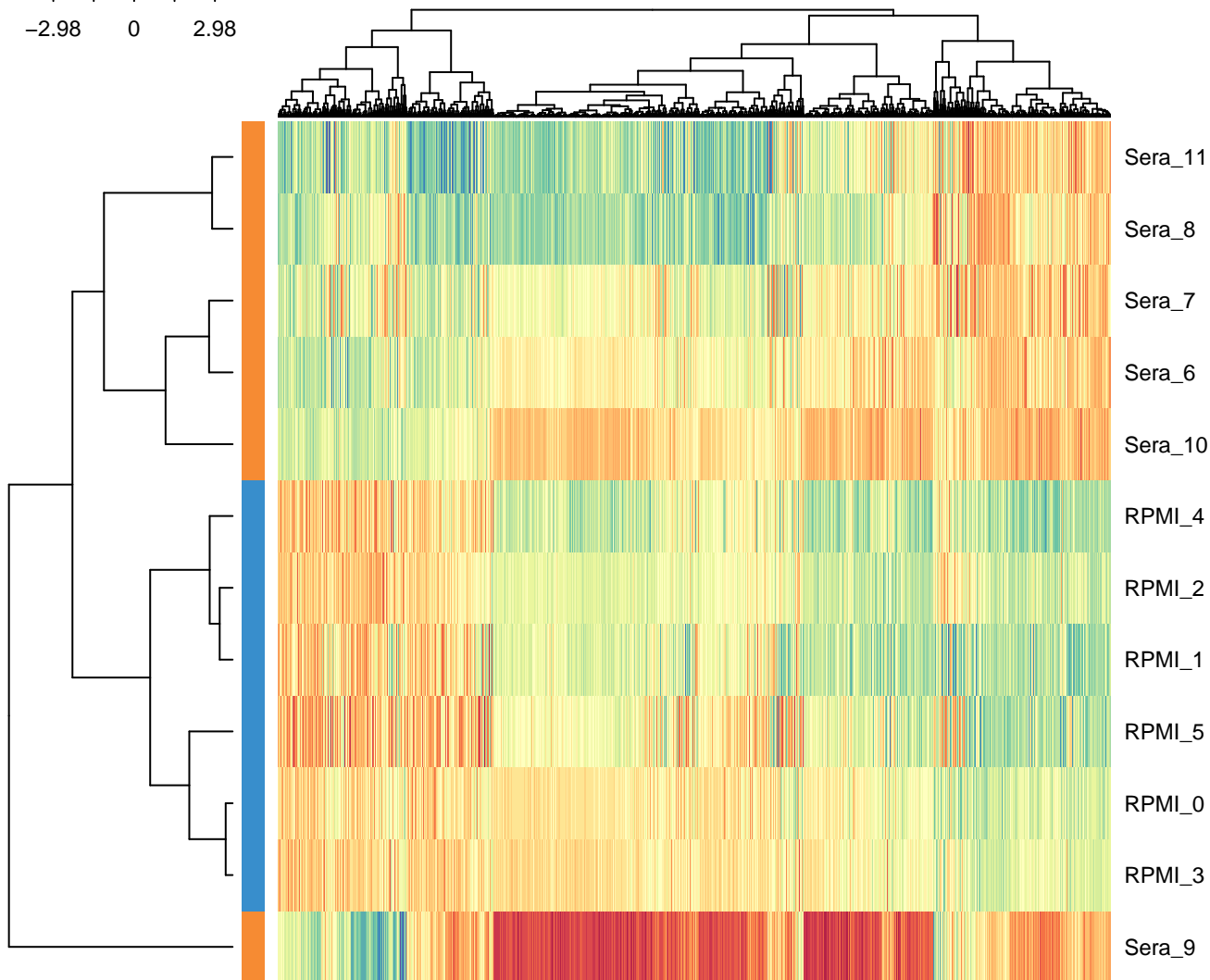


PLSDA

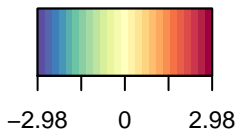
Status

RPMI

Sera



Color key

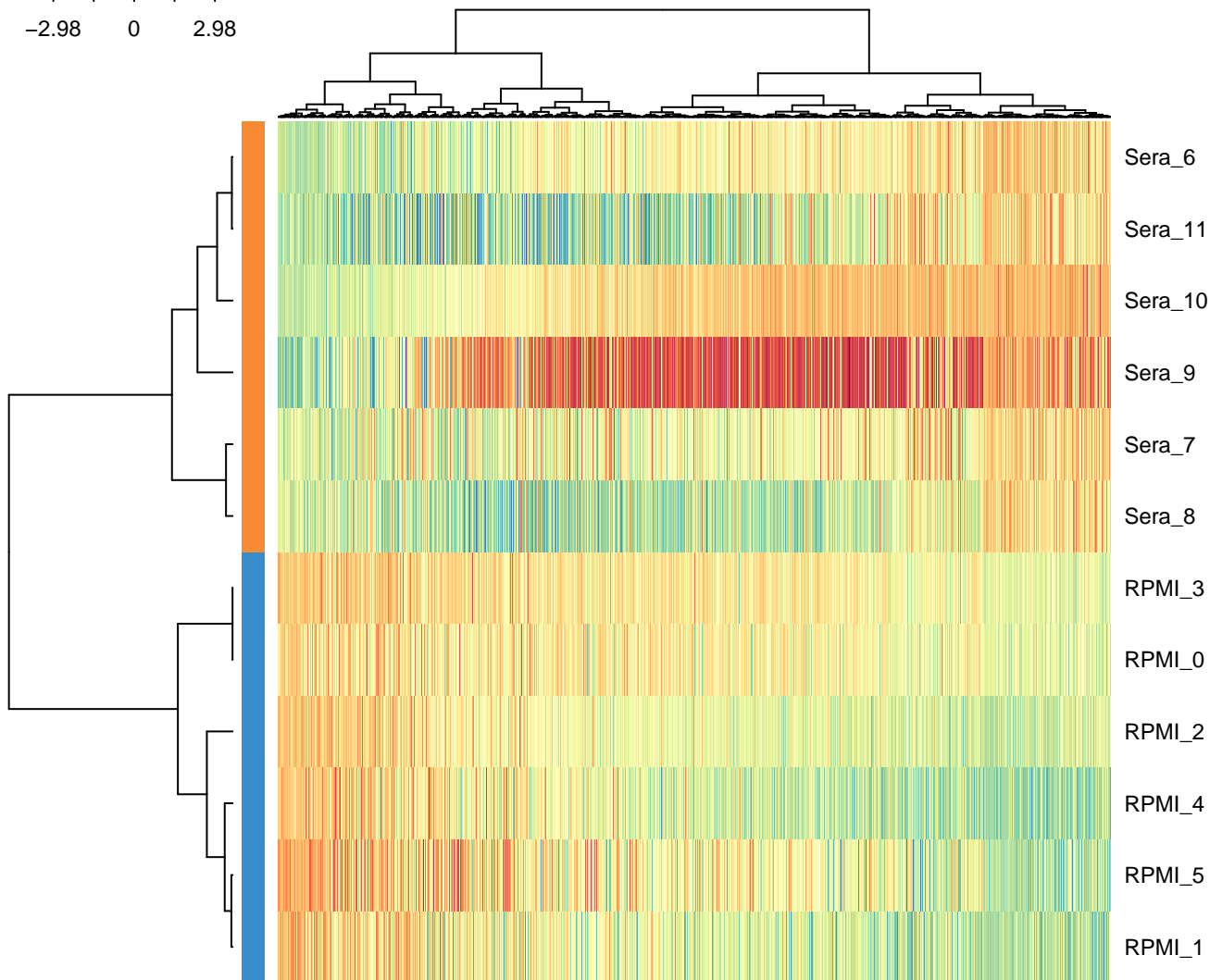


# PLSDA Component 1

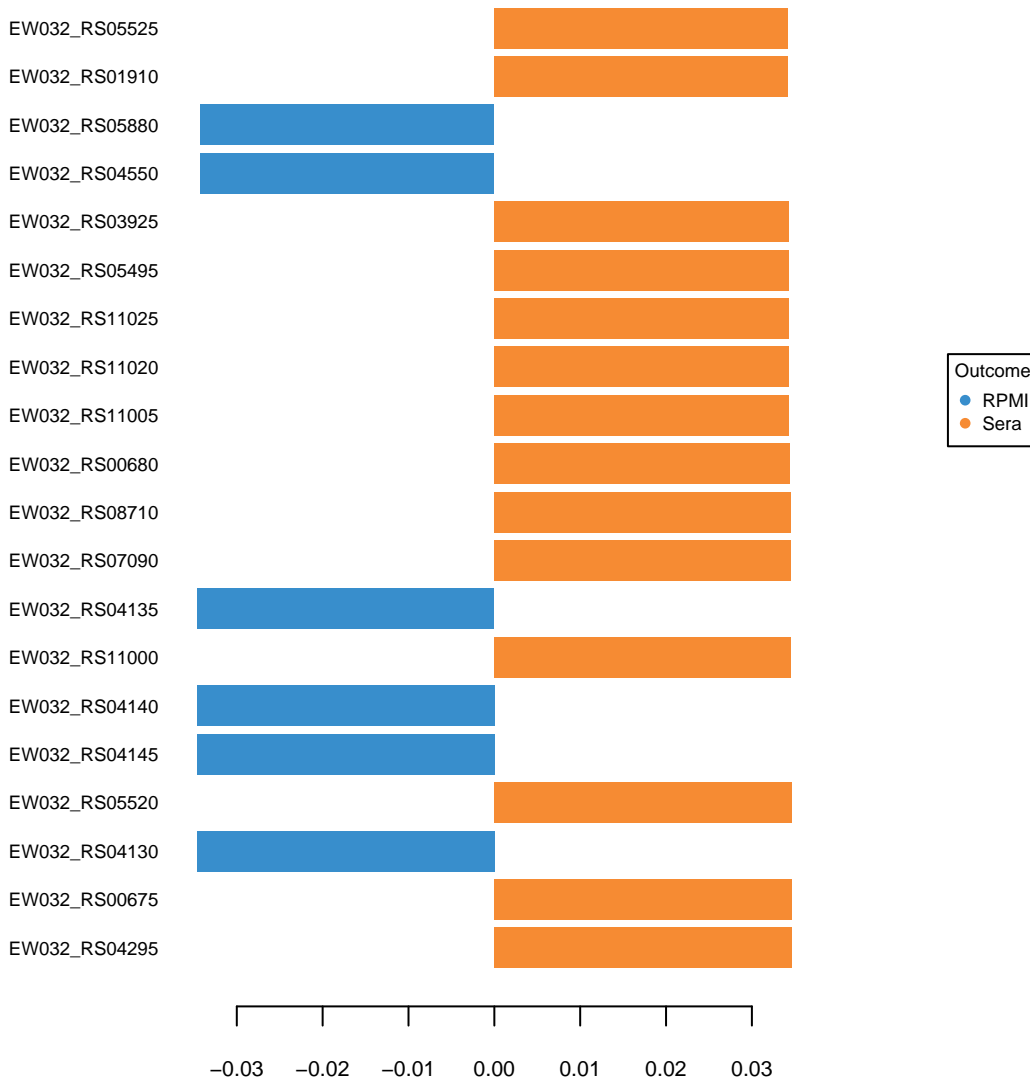
Status

RPMI

Sera

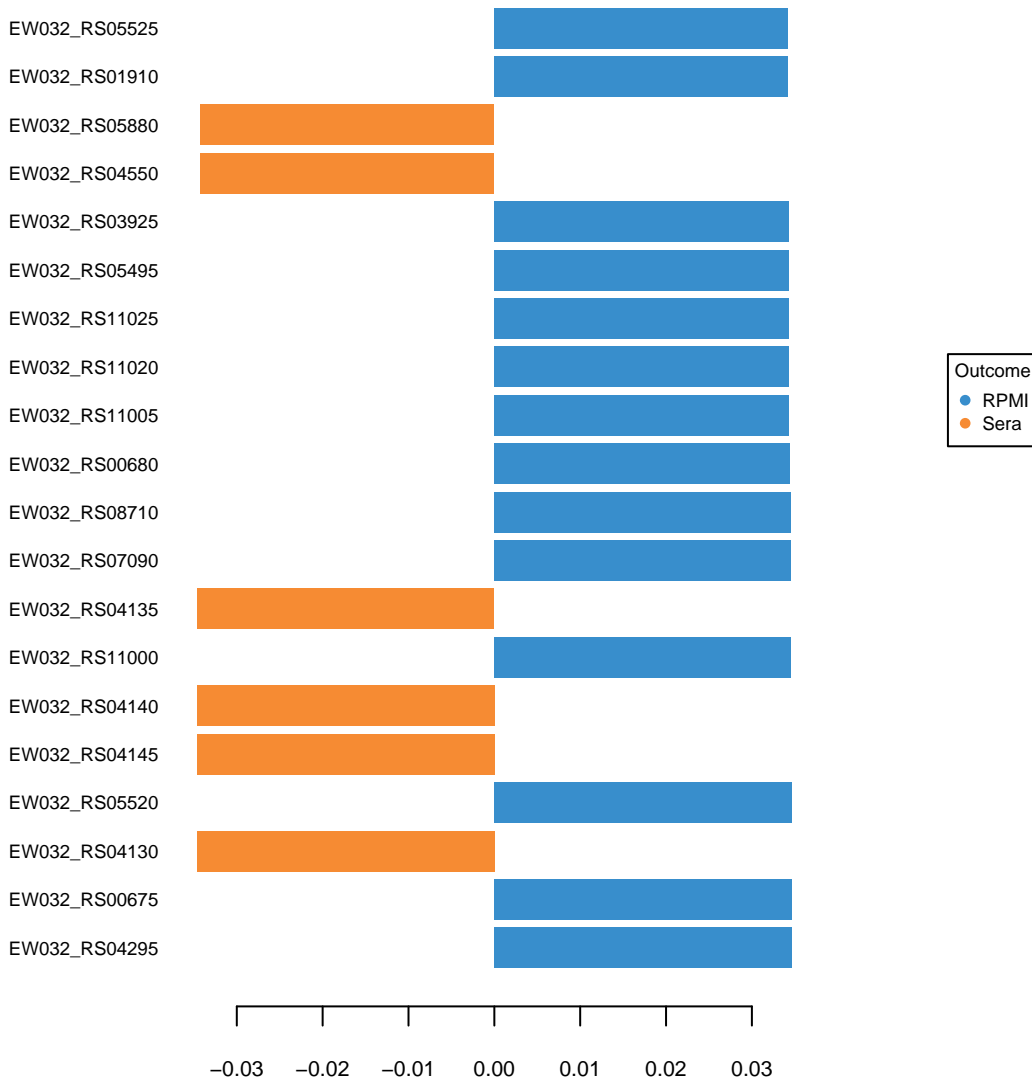


# RNA\_Seq 1 PLSDA max loadir

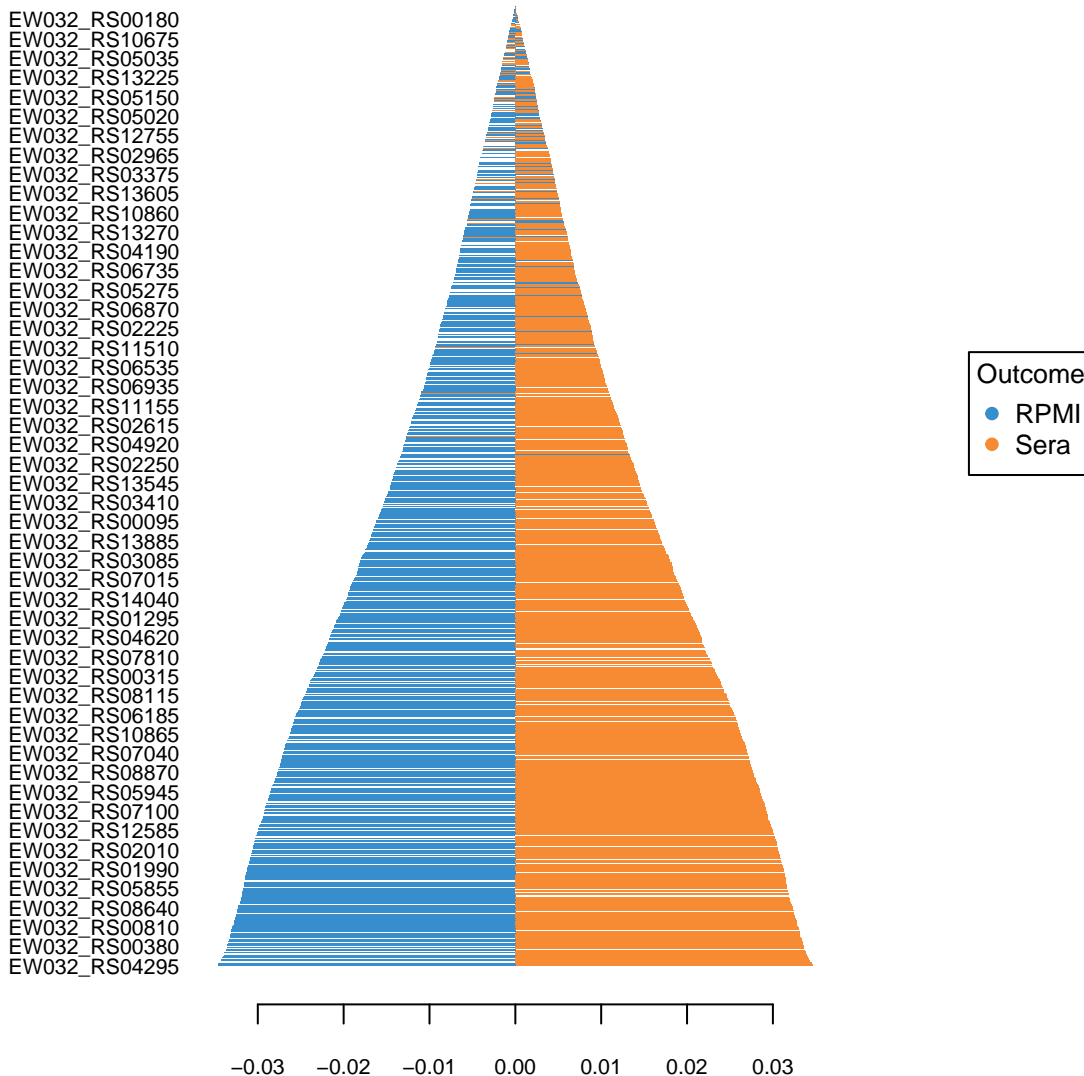




# RNA\_Seq 1 PLSDA min loading

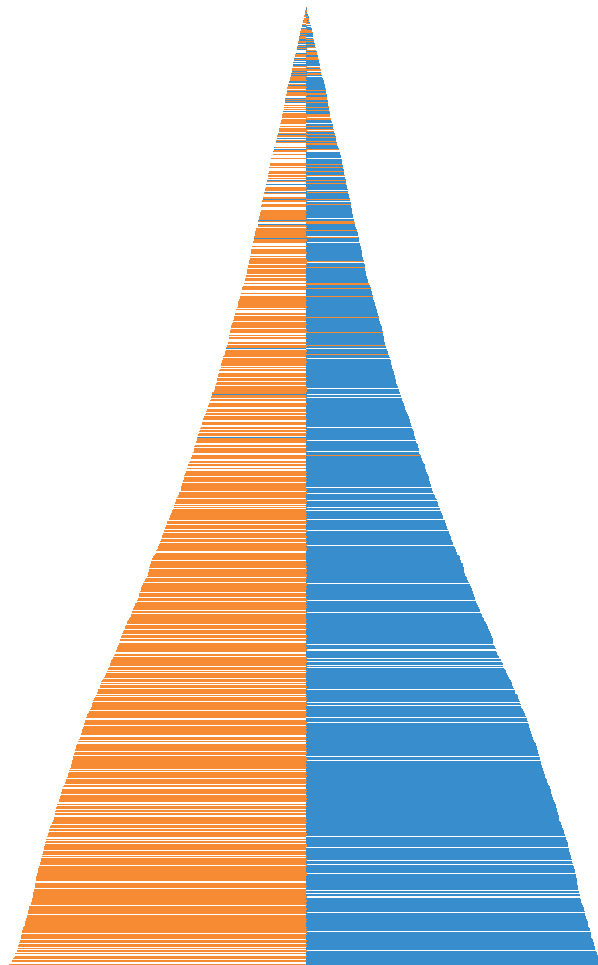


# Contribution on comp 1



# Contribution on comp 1

EW032\_RS00180  
EW032\_RS10675  
EW032\_RS05035  
EW032\_RS13225  
EW032\_RS05150  
EW032\_RS05020  
EW032\_RS12755  
EW032\_RS02965  
EW032\_RS03375  
EW032\_RS13605  
EW032\_RS10860  
EW032\_RS13270  
EW032\_RS04190  
EW032\_RS06735  
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EW032\_RS06935  
EW032\_RS11155  
EW032\_RS02615  
EW032\_RS04920  
EW032\_RS02250  
EW032\_RS13545  
EW032\_RS03410  
EW032\_RS00095  
EW032\_RS13885  
EW032\_RS03085  
EW032\_RS07015  
EW032\_RS14040  
EW032\_RS01295  
EW032\_RS04620  
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EW032\_RS00315  
EW032\_RS08115  
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EW032\_RS10865  
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EW032\_RS08870  
EW032\_RS05945  
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EW032\_RS12585  
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EW032\_RS00380  
EW032\_RS04295



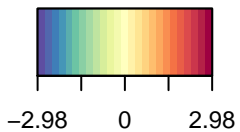
Outcome

- RPMI
- Sera

-0.03 -0.02 -0.01 0.00 0.01 0.02 0.03

# PLSDA Component 2

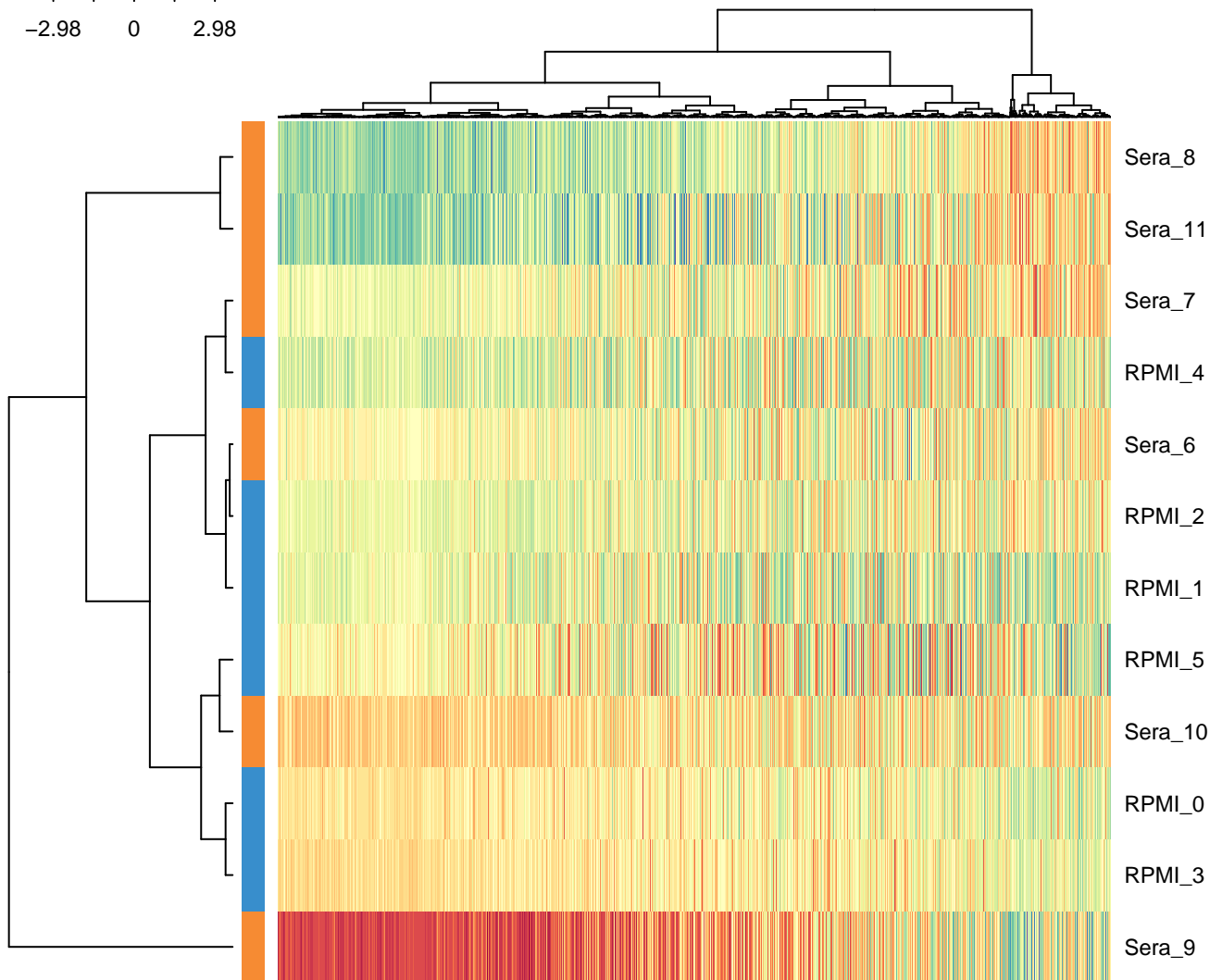
Color key



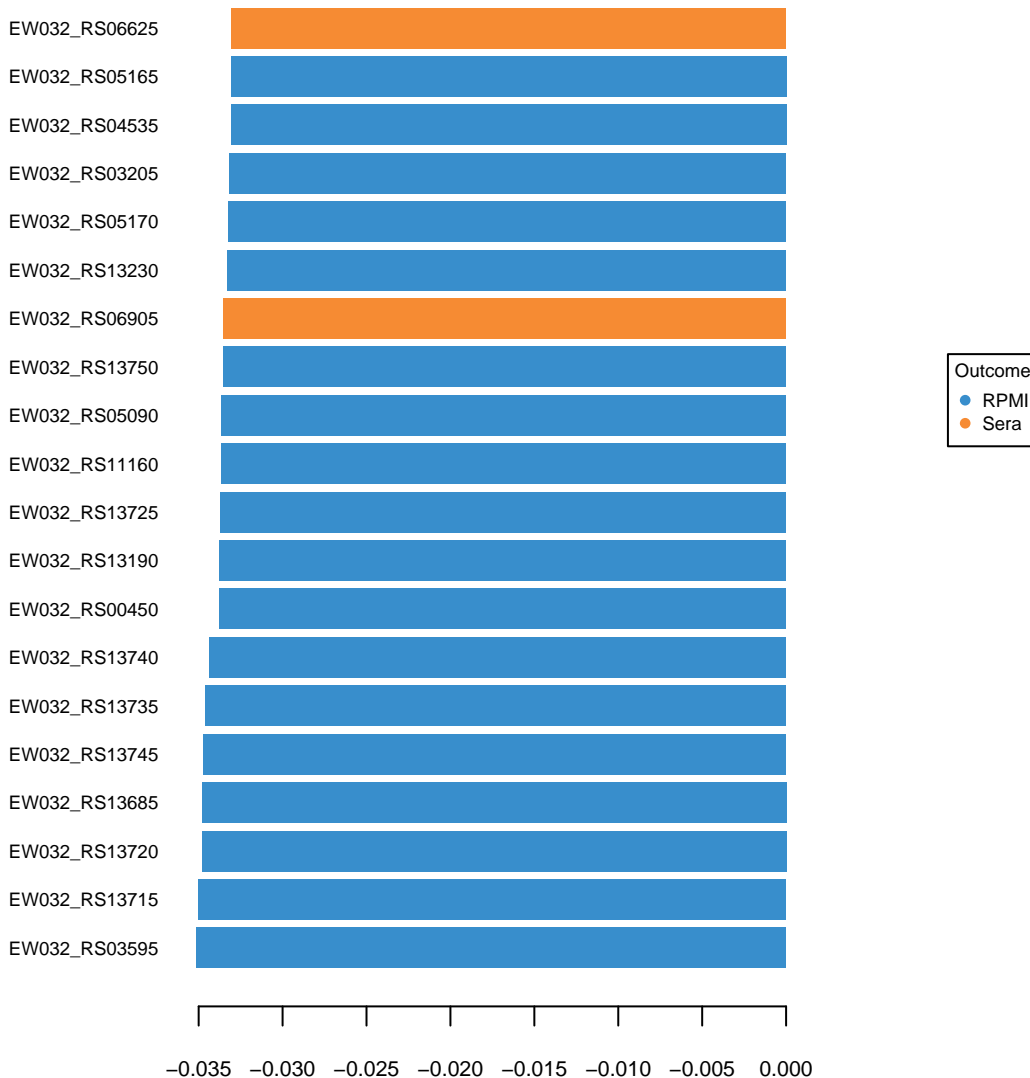
Status

RPMI

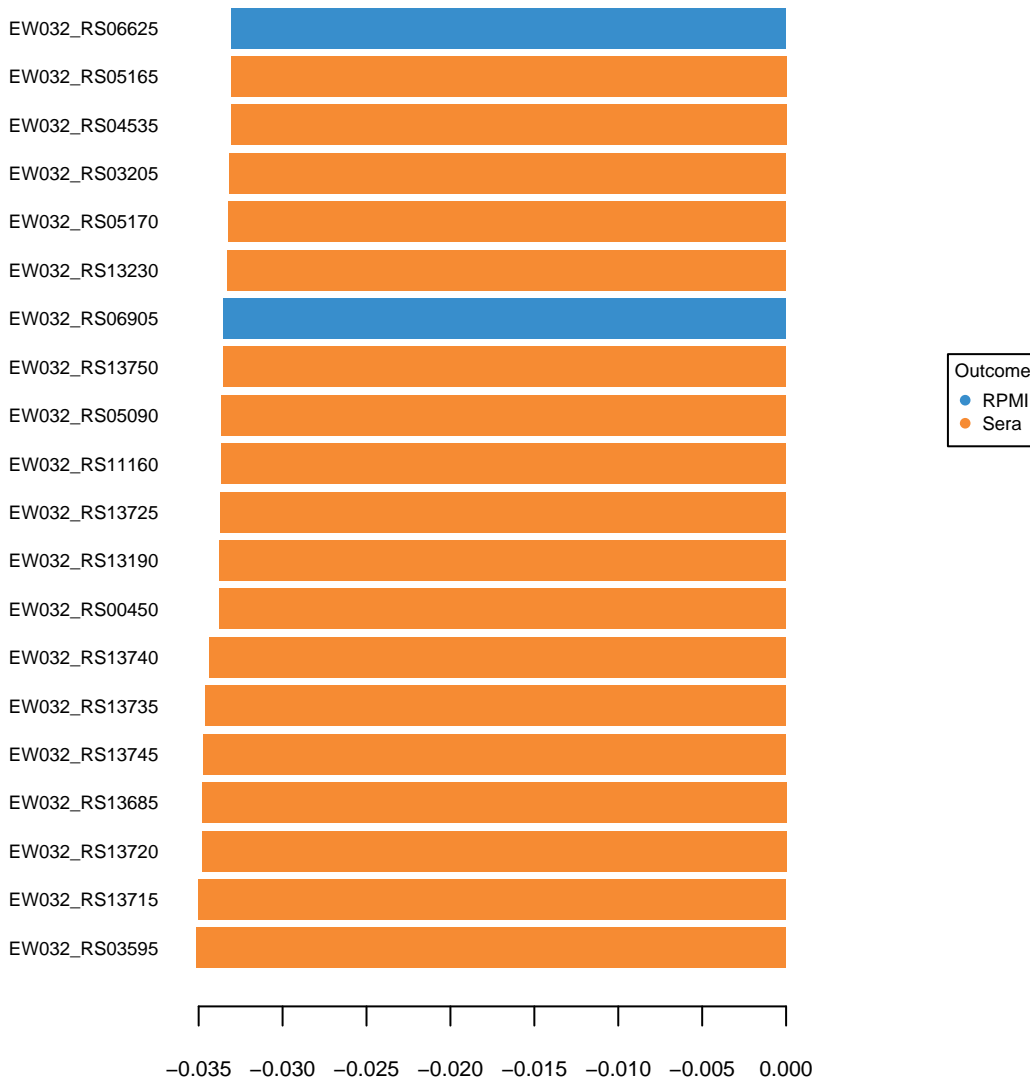
Sera



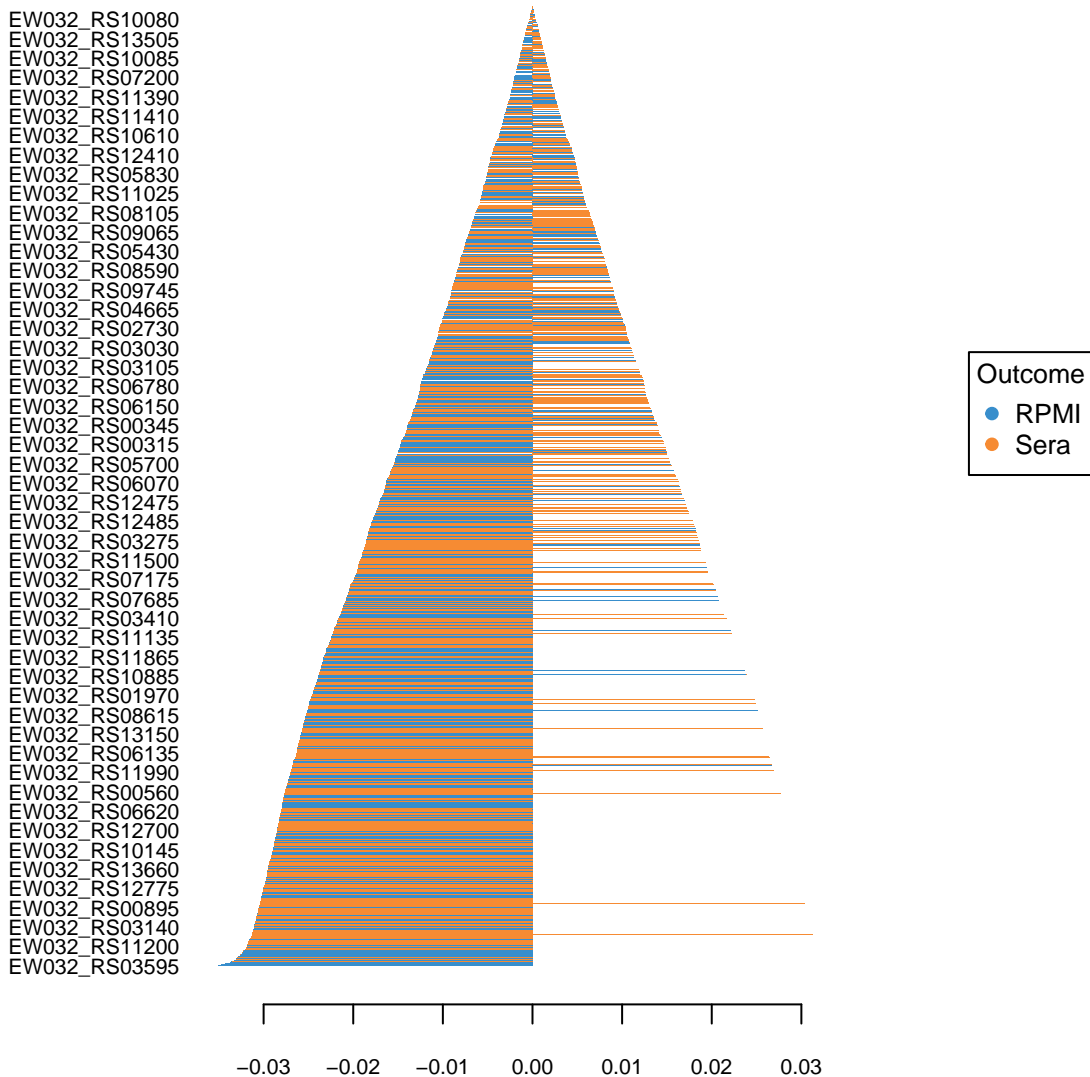
# RNA\_Seq 2 PLSDA max loadir



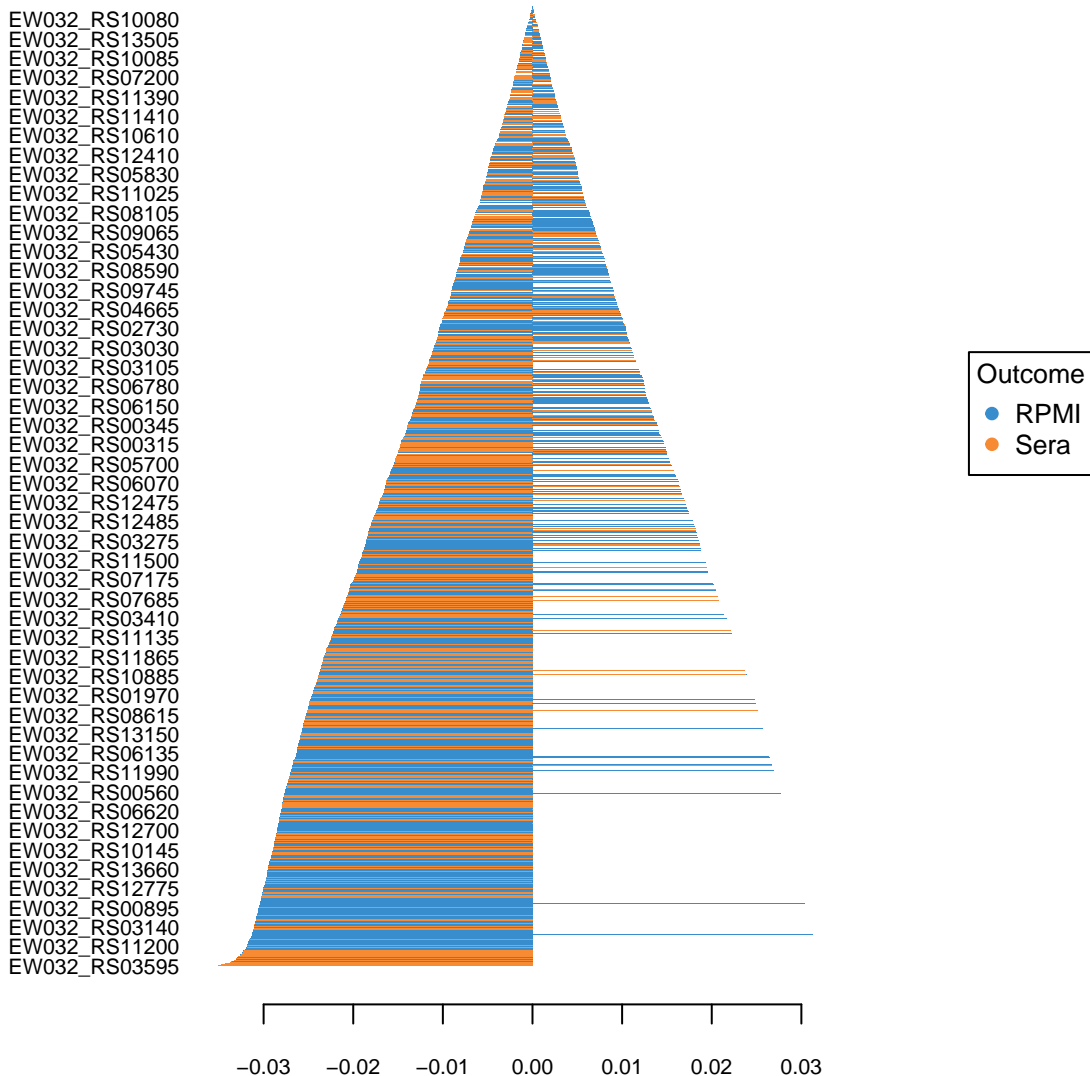
# RNA\_Seq 2 PLSDA min loadin



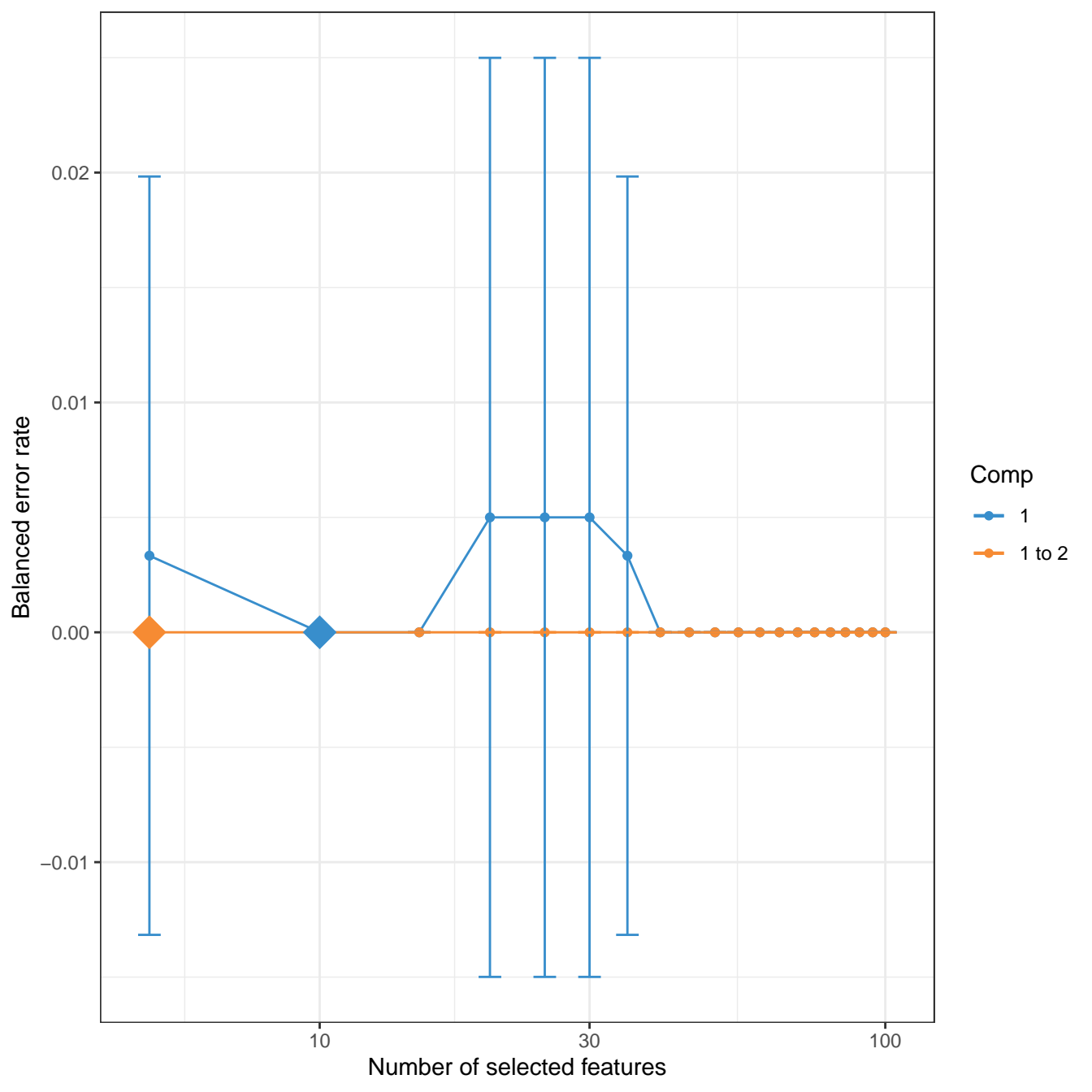
# Contribution on comp 2

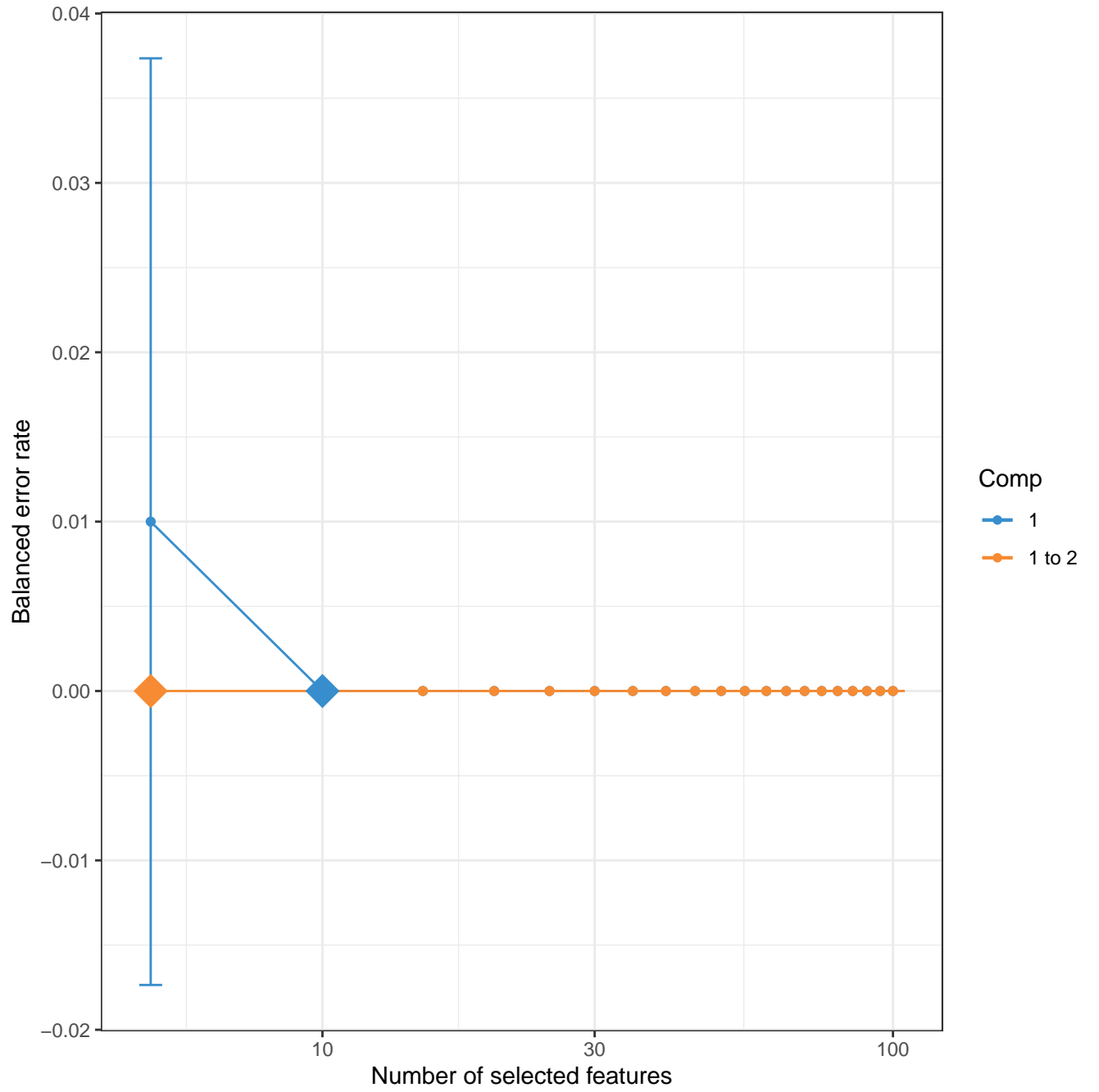


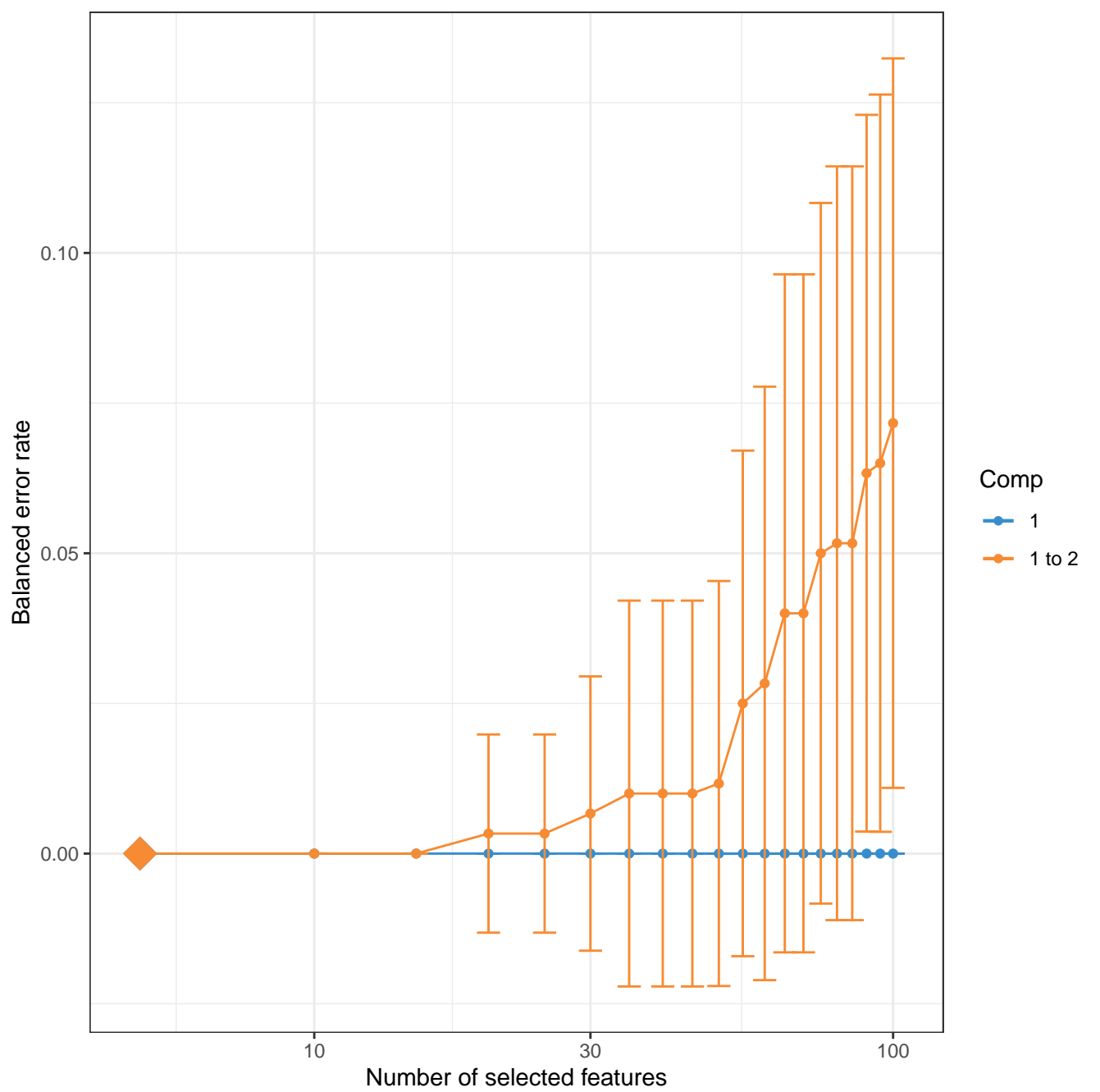
# Contribution on comp 2

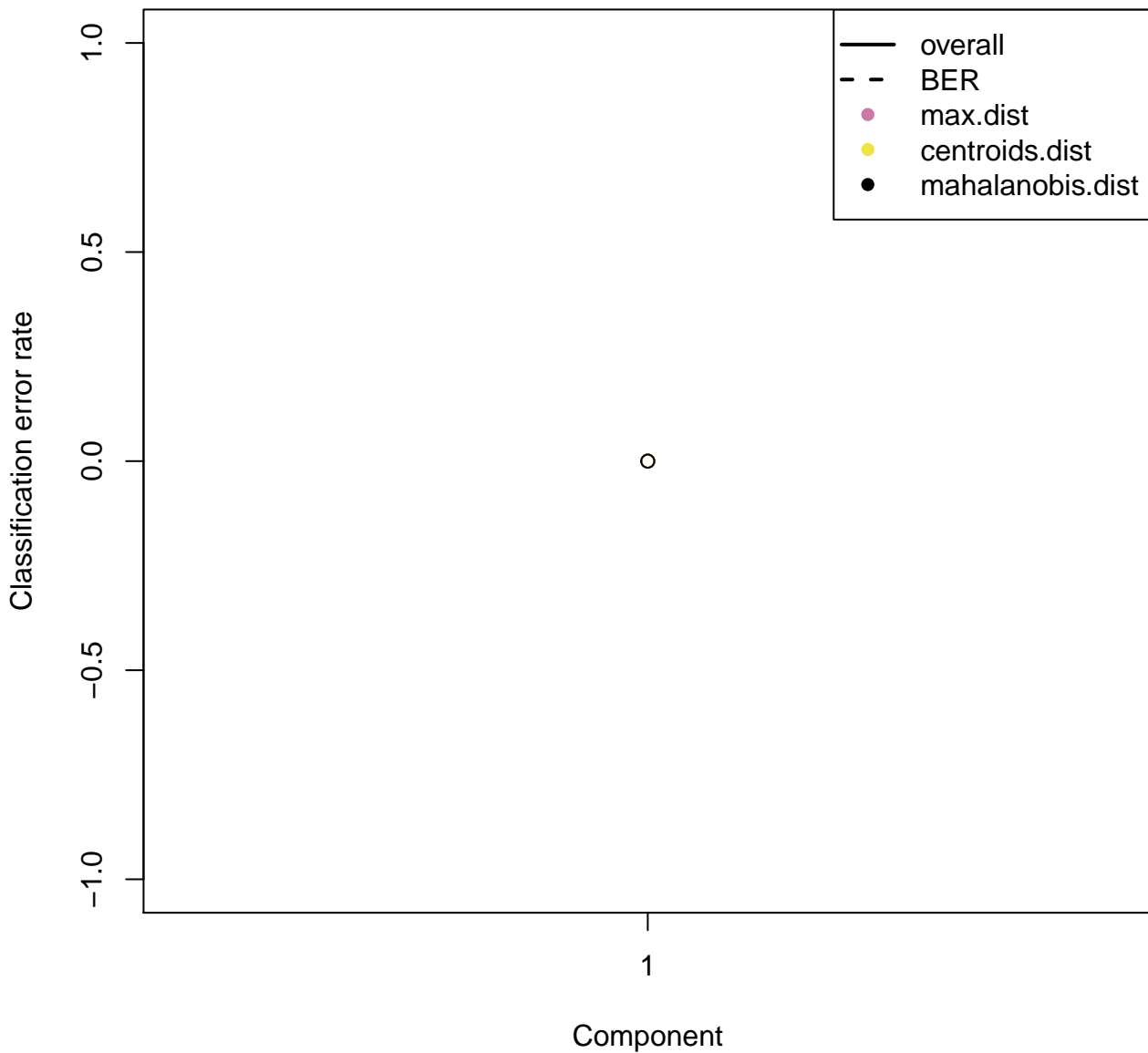




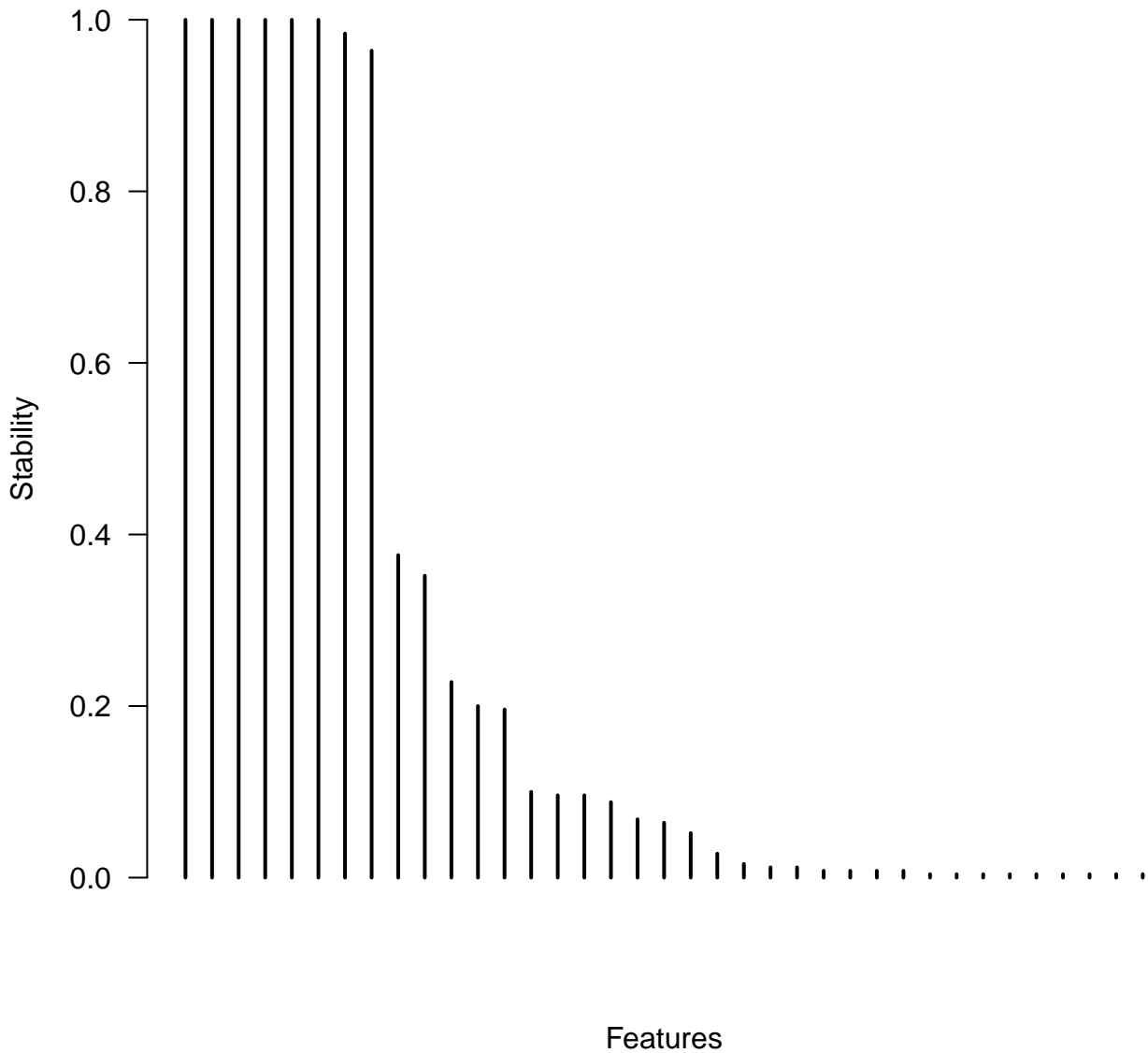




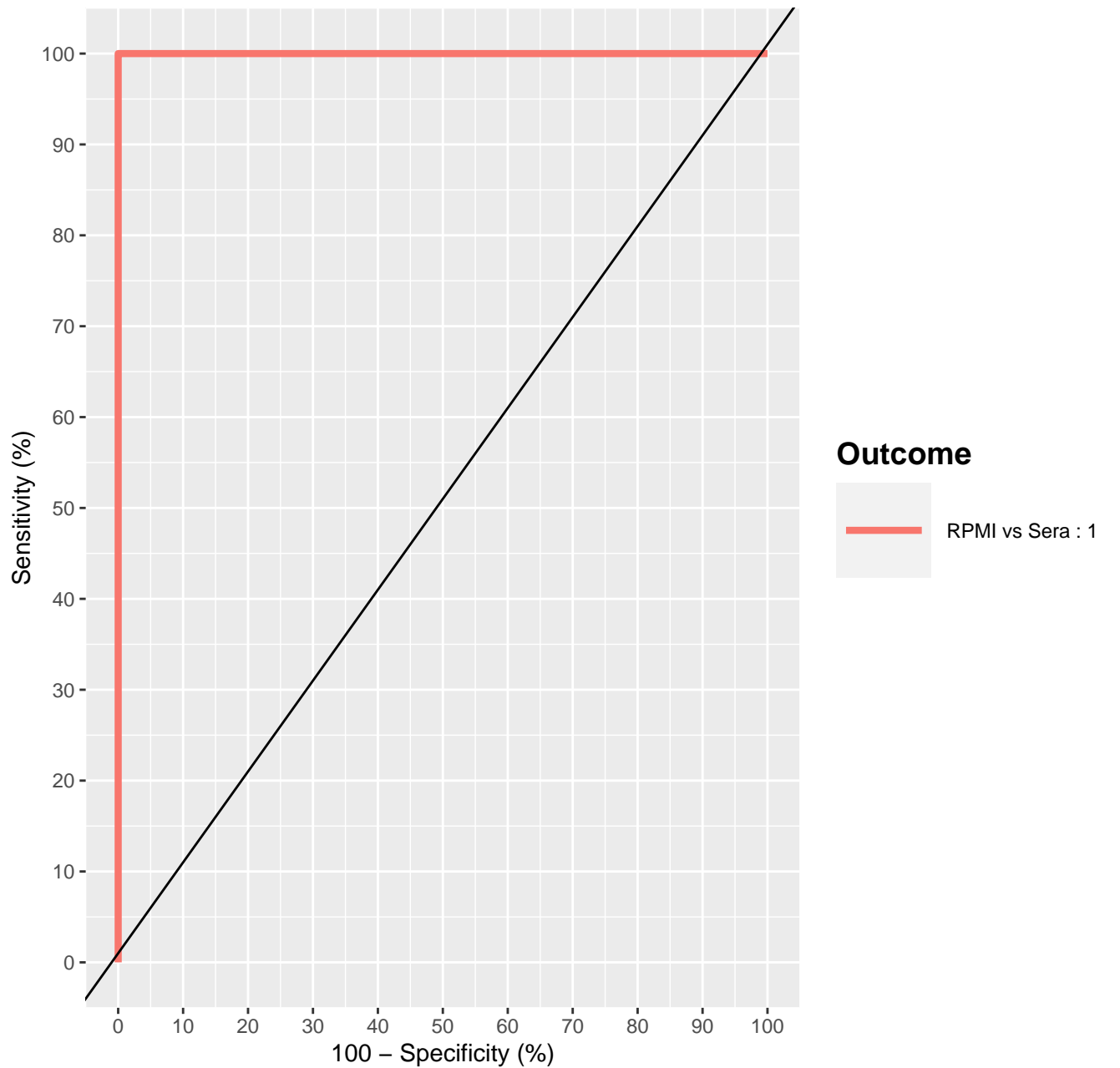




## Comp 1



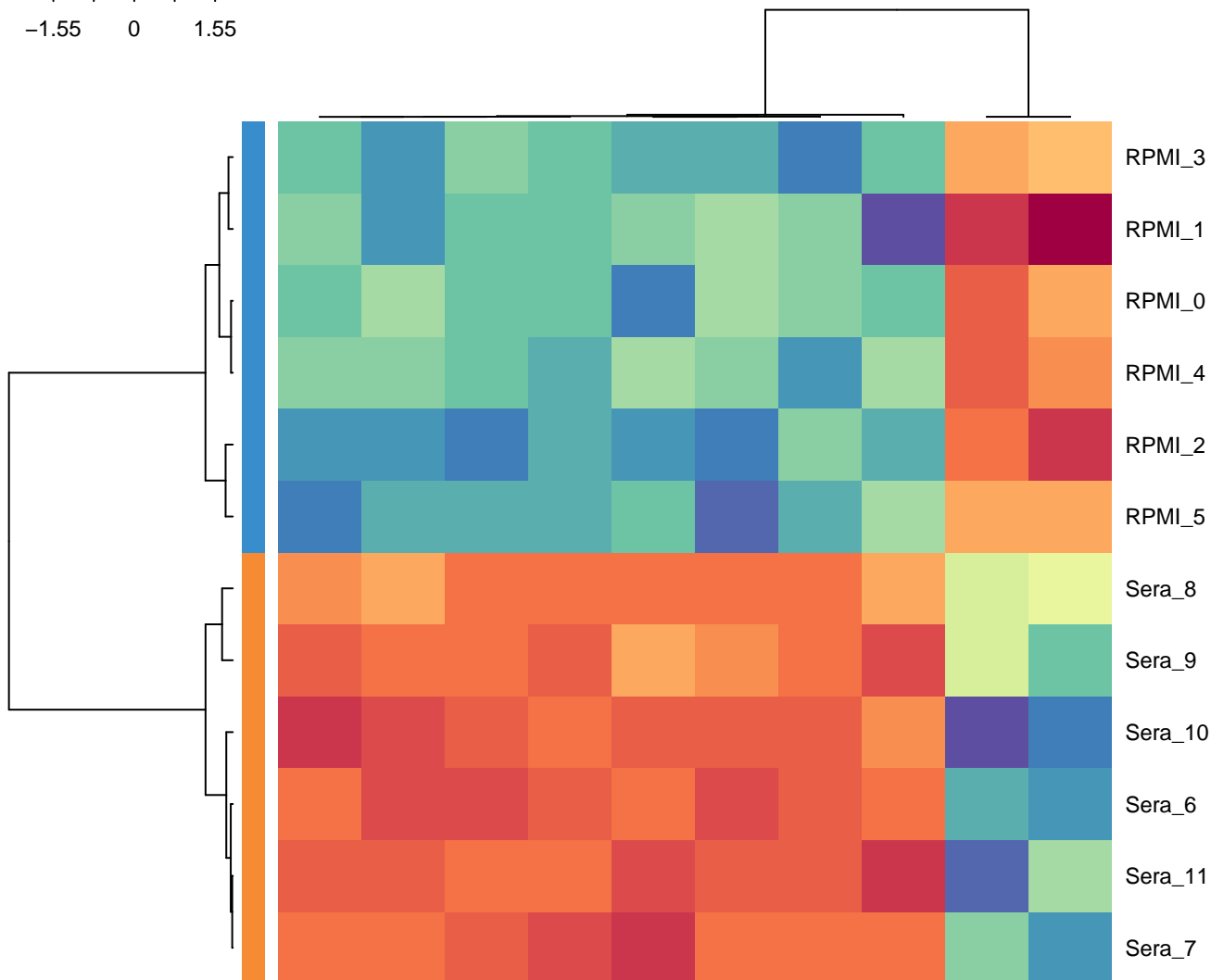
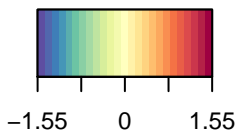
**ROC Curve Comp 1**



## sPLSDA

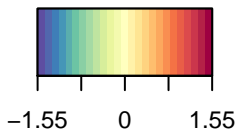
■ RPMI

■ Sera



# sPLSDA Component 1

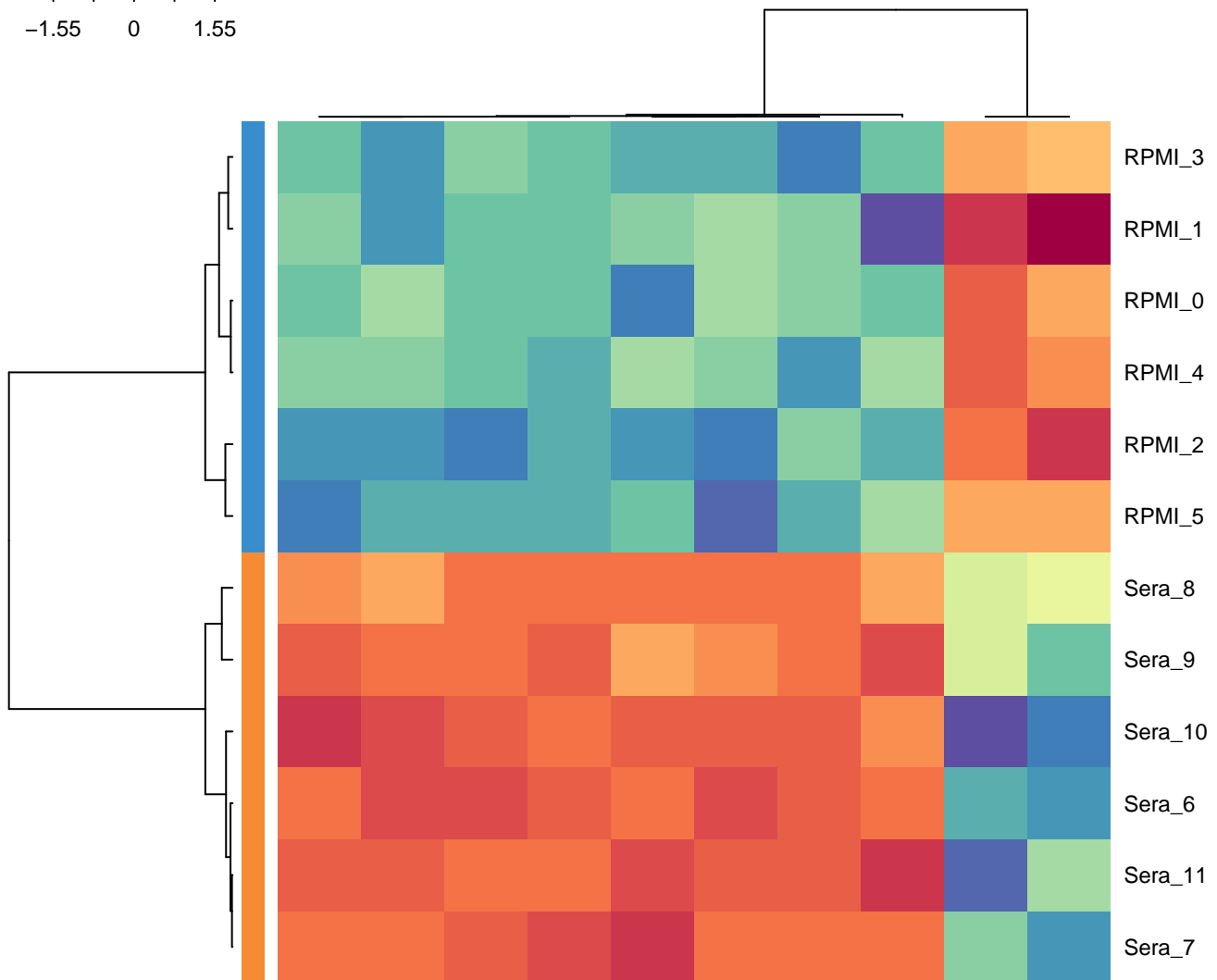
Color key



Status

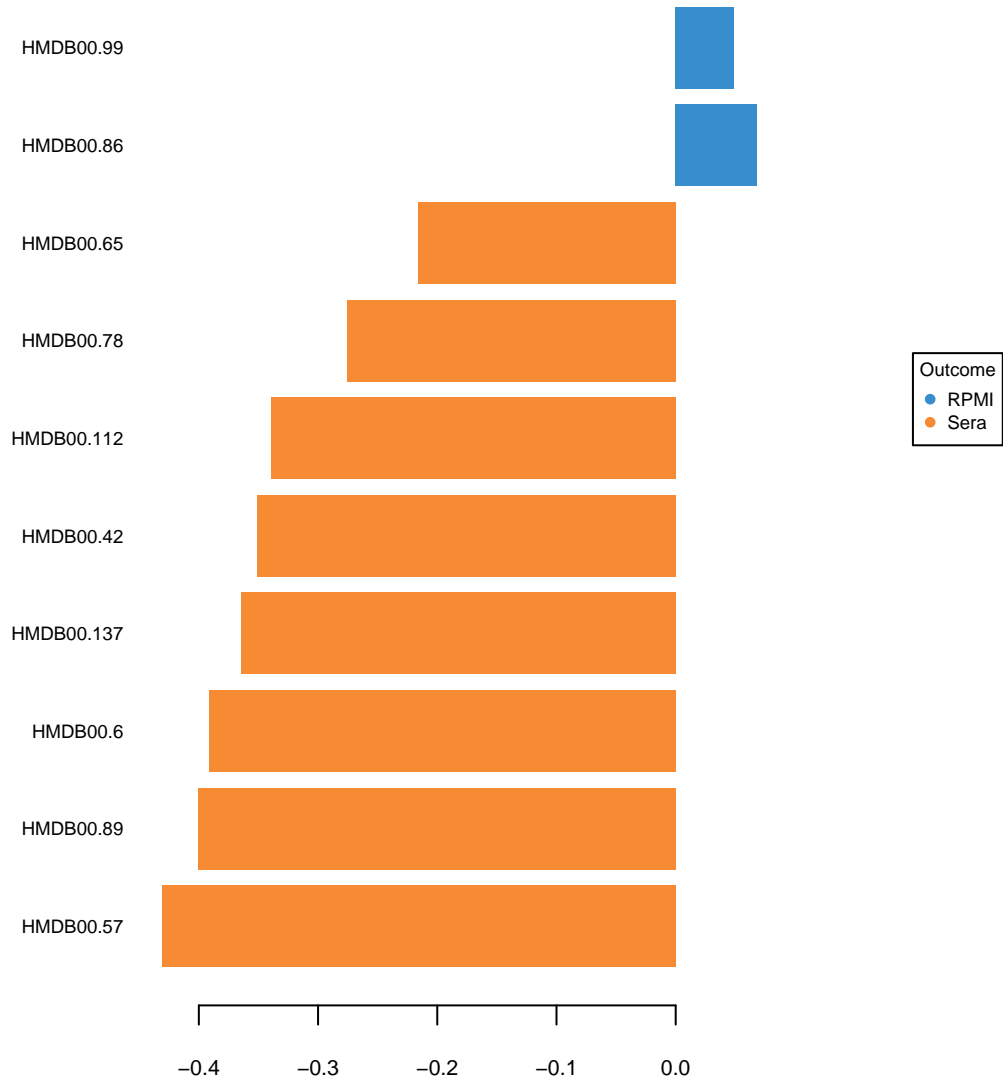
RPMI

Sera

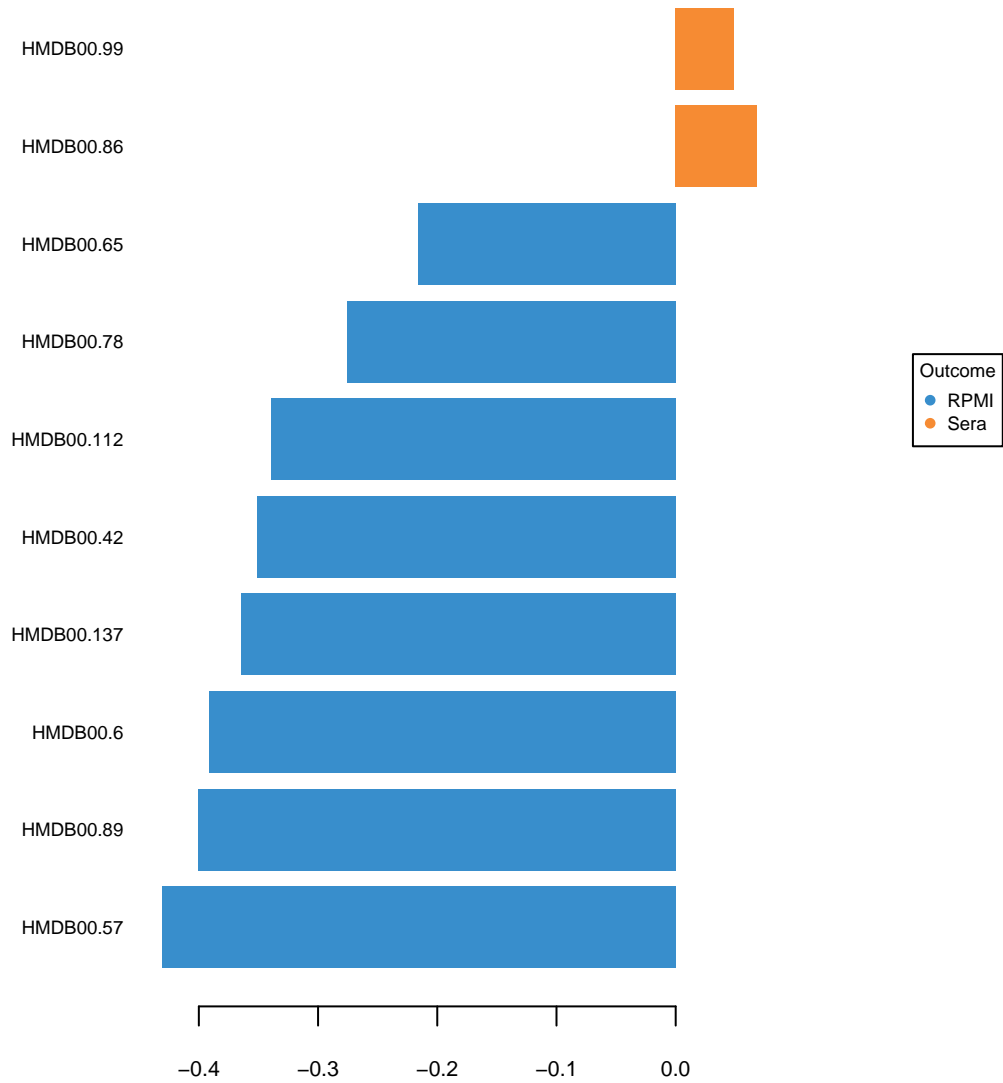




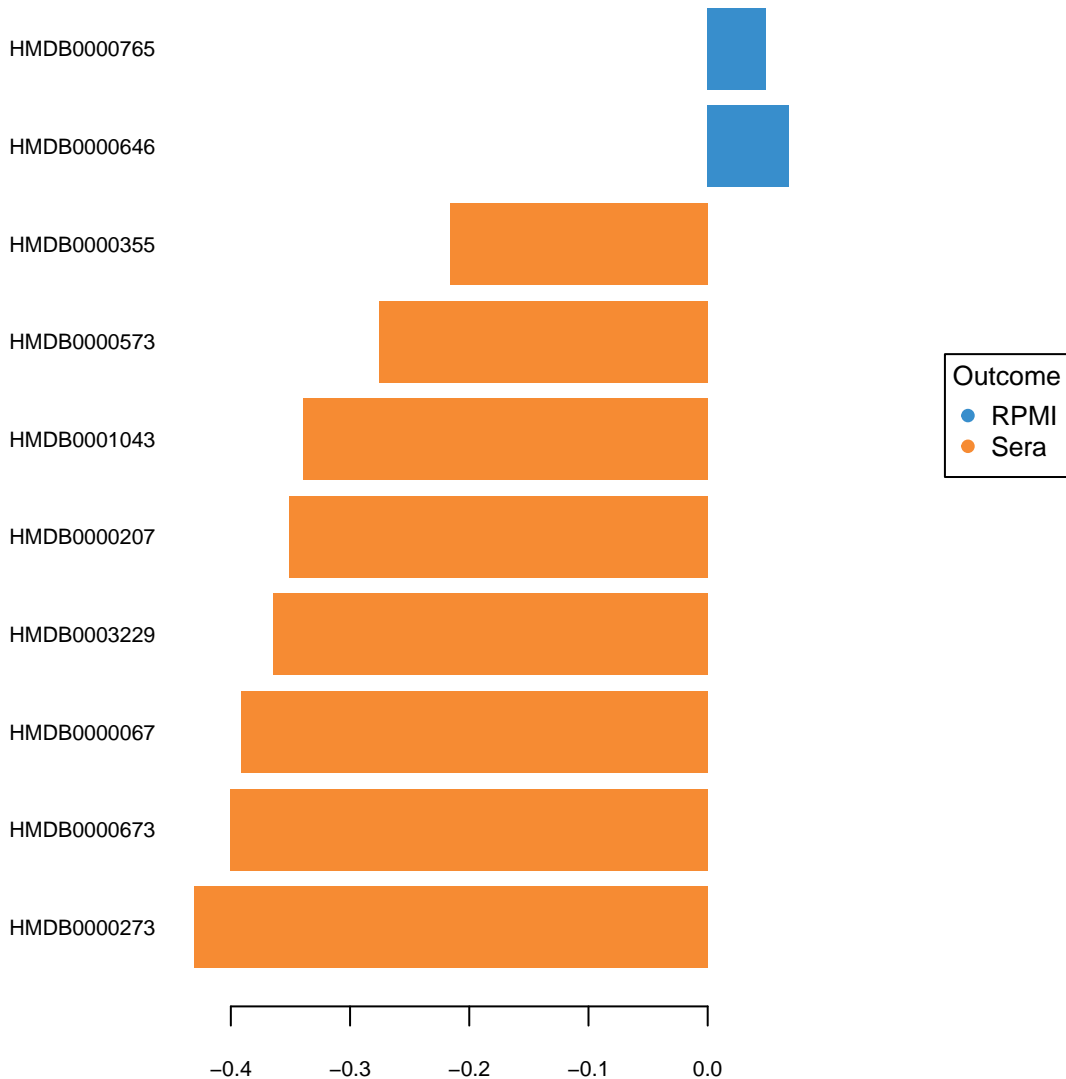
# Metabolomics 1 sPLSDA max loa



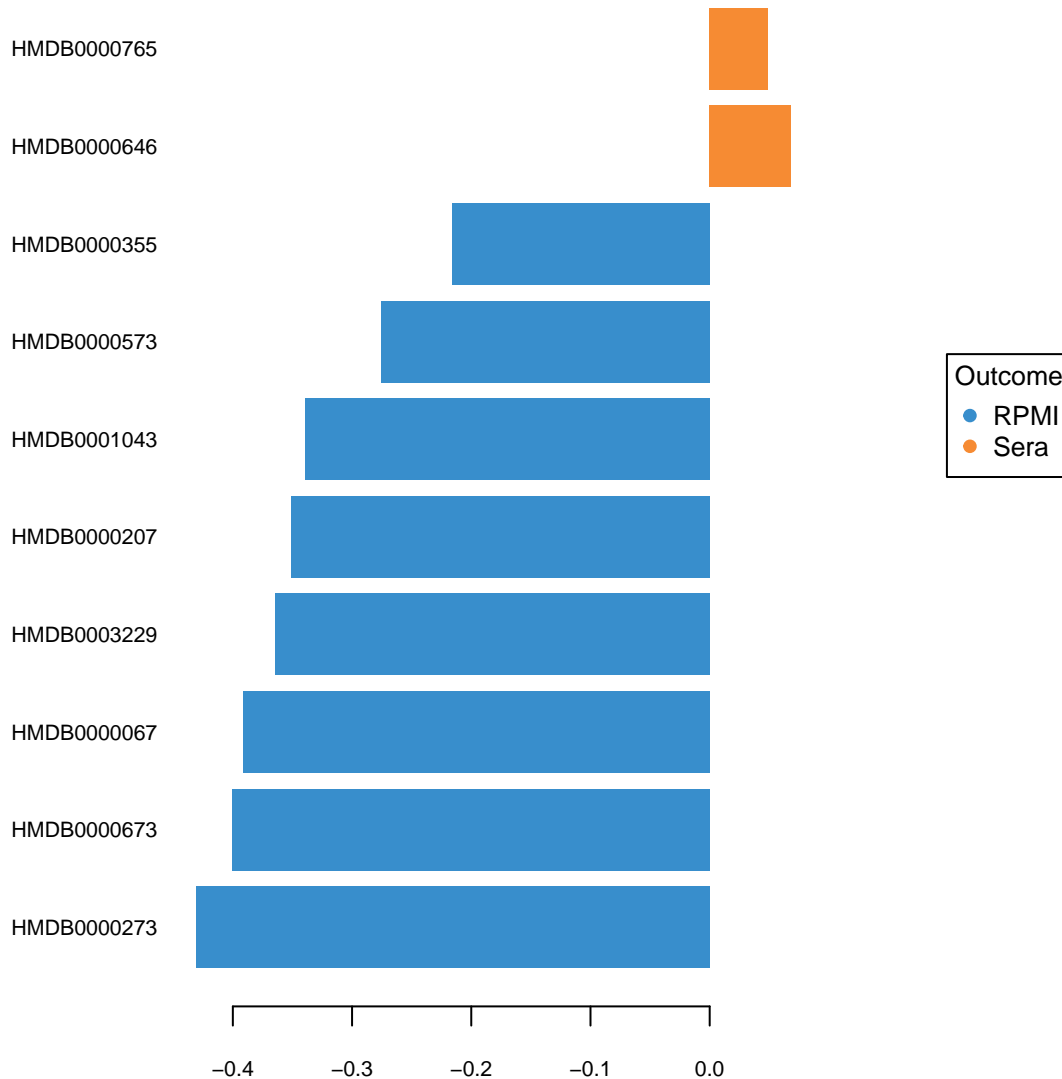
# Metabolomics 1 sPLSDA min loa

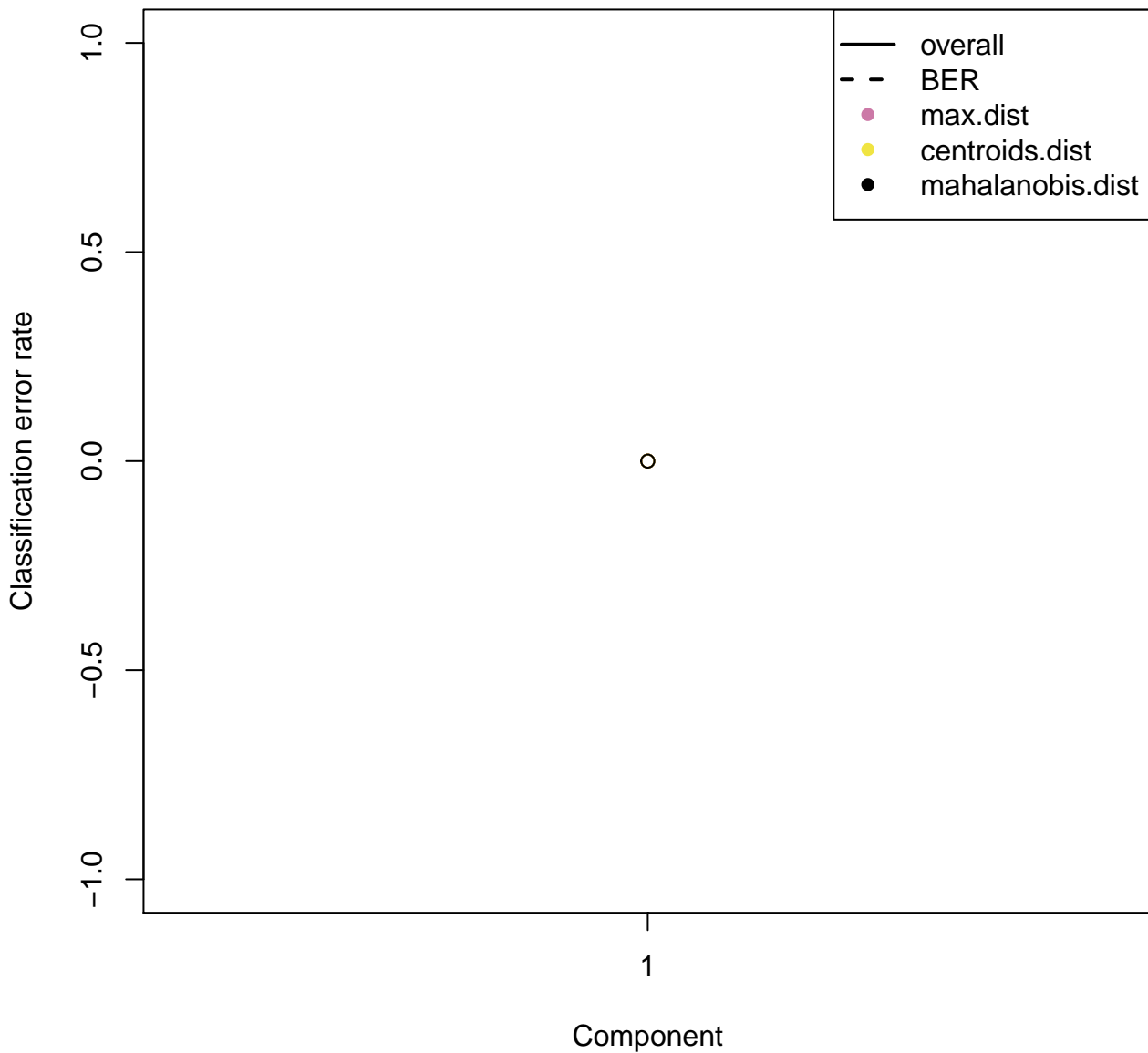


# Contribution on comp 1

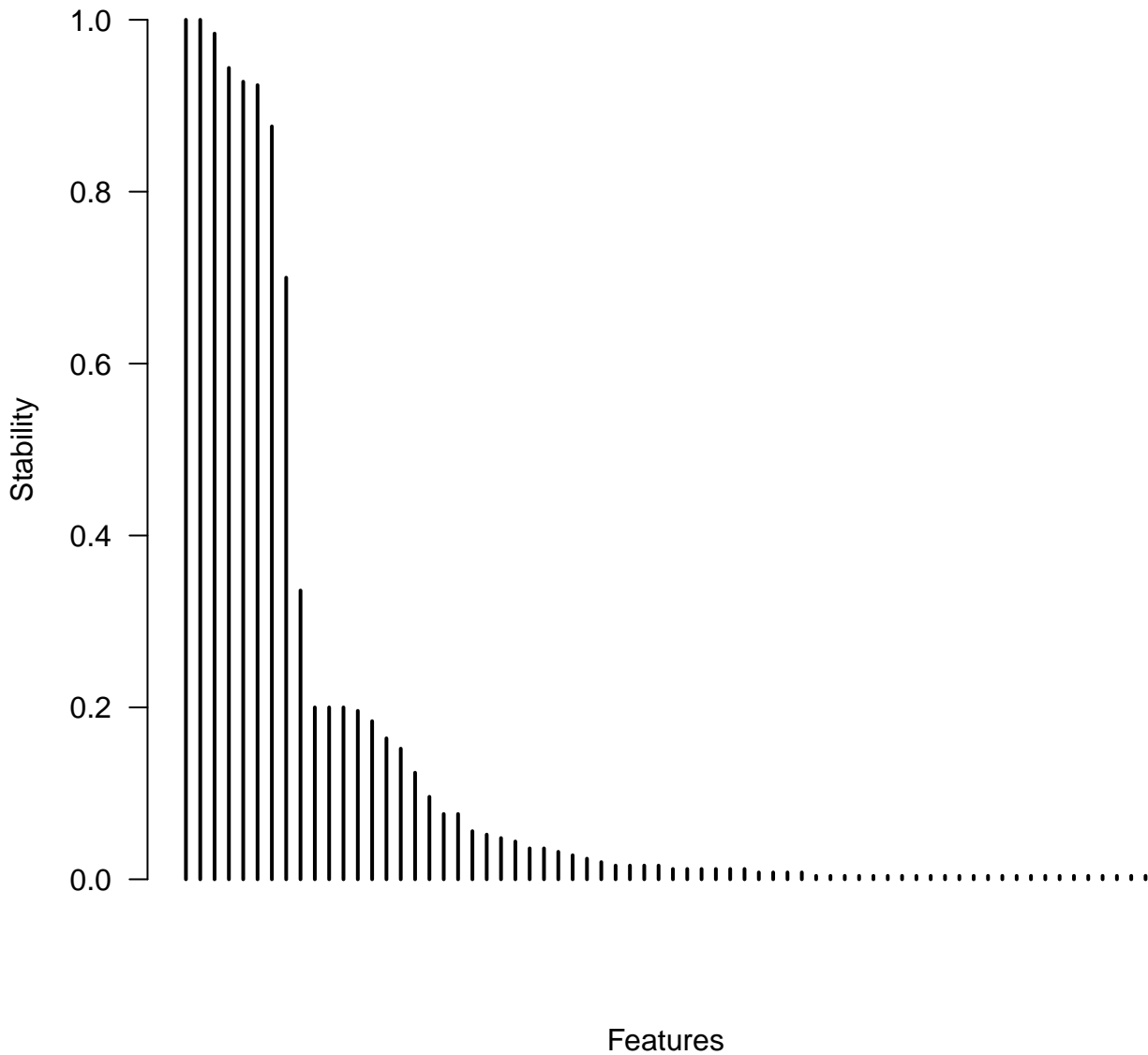


# Contribution on comp 1

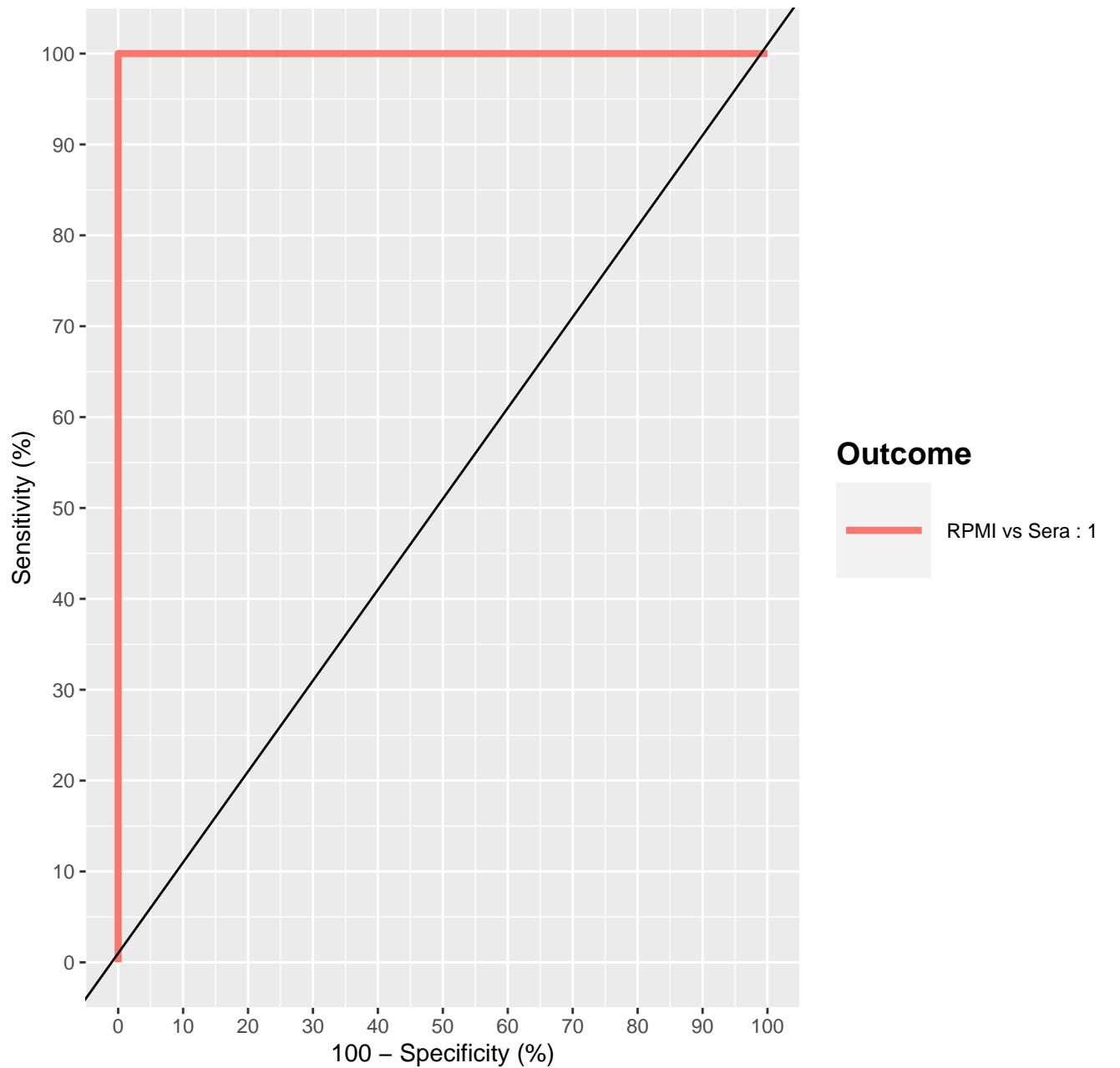




# Comp 1

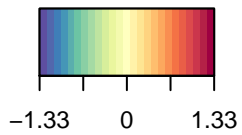


**ROC Curve Comp 1**



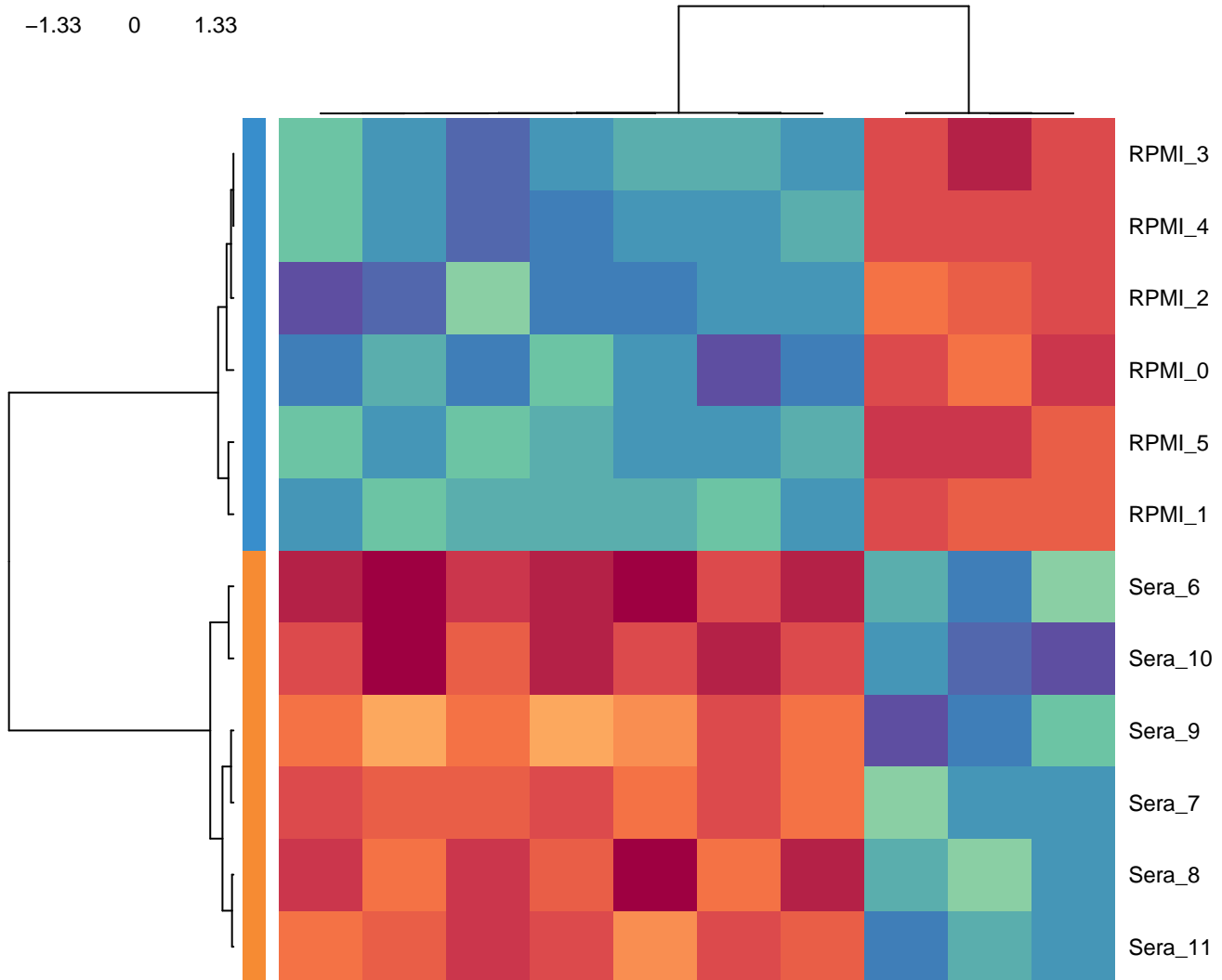
# sPLSDA

Color key



Status

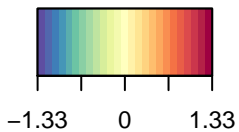
- RPMI
- Sera





# sPLSDA Component 1

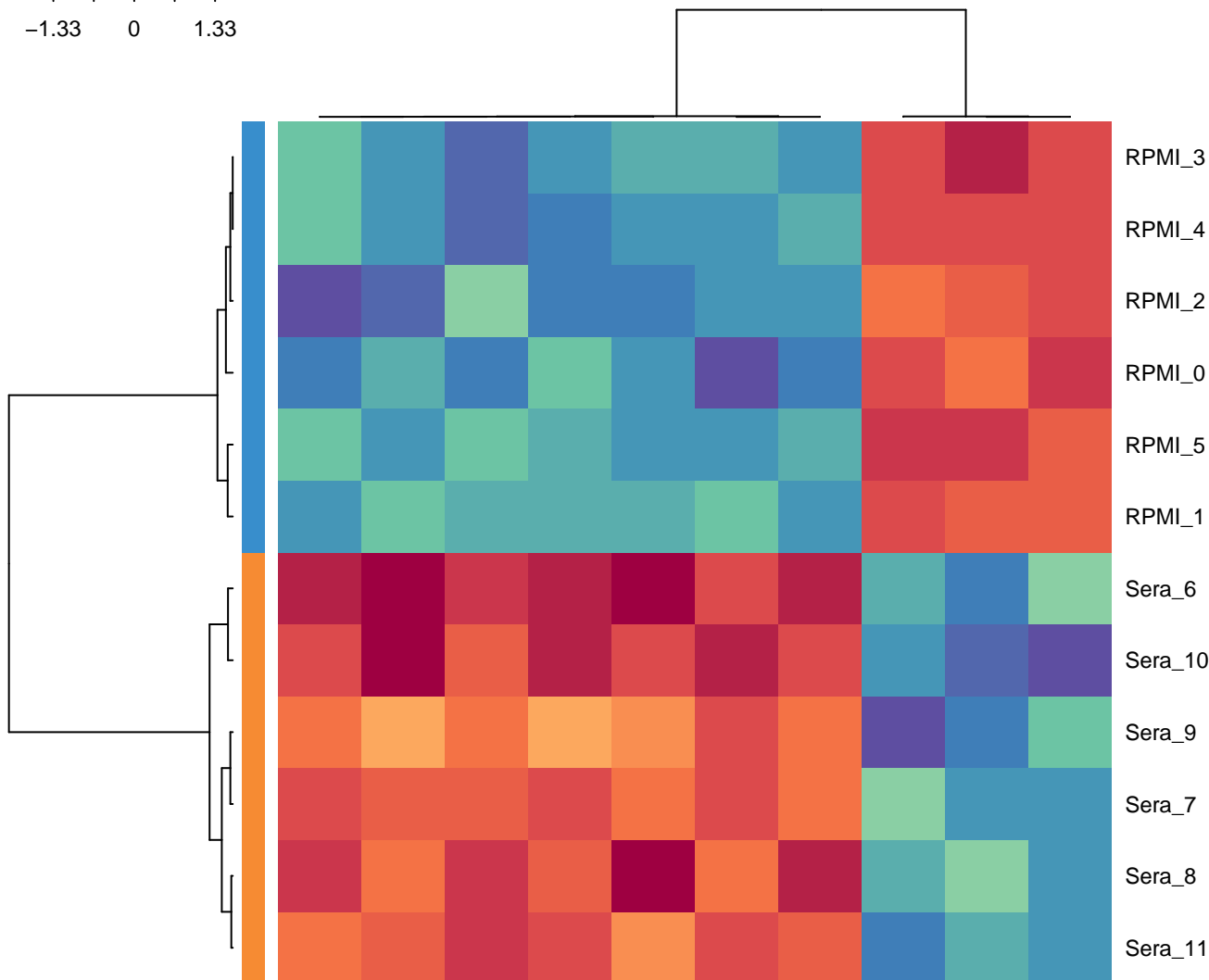
Color key



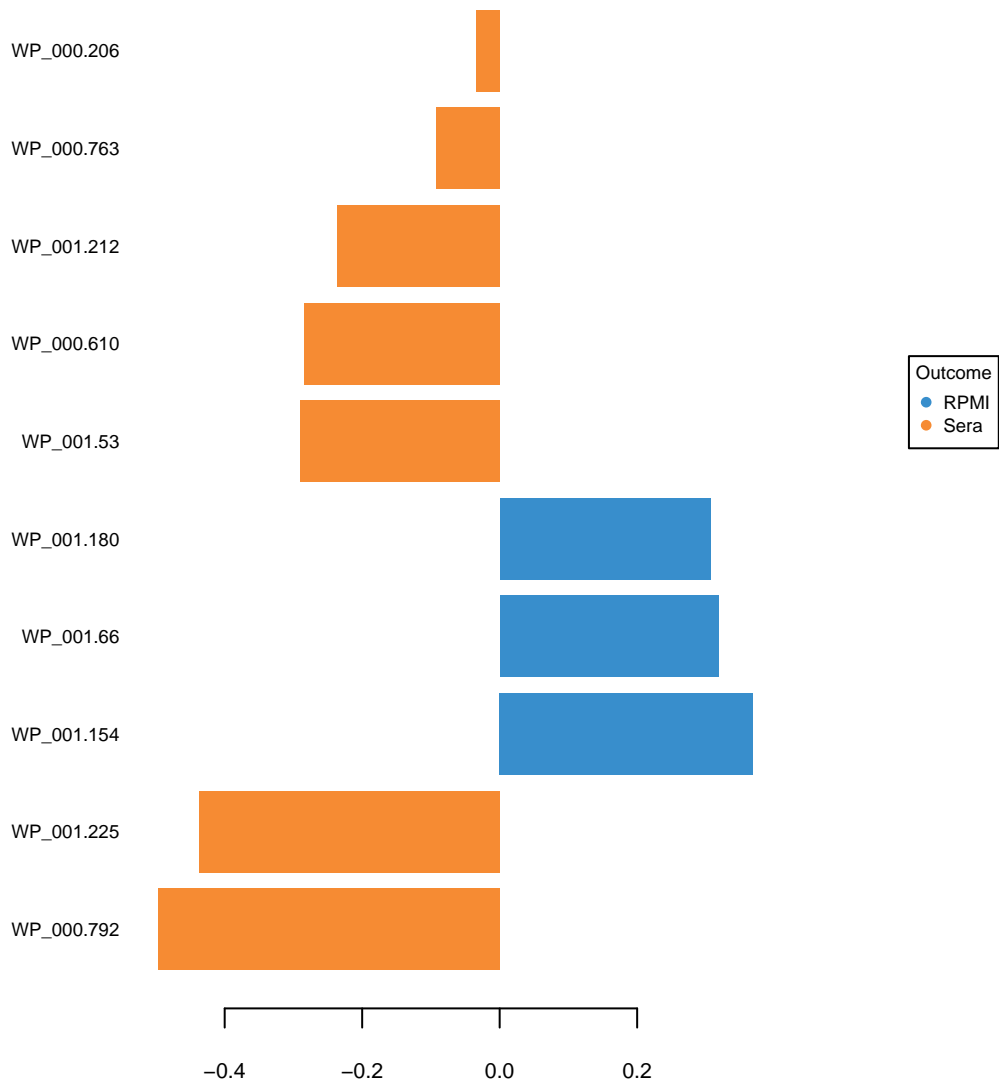
Status

RPMI

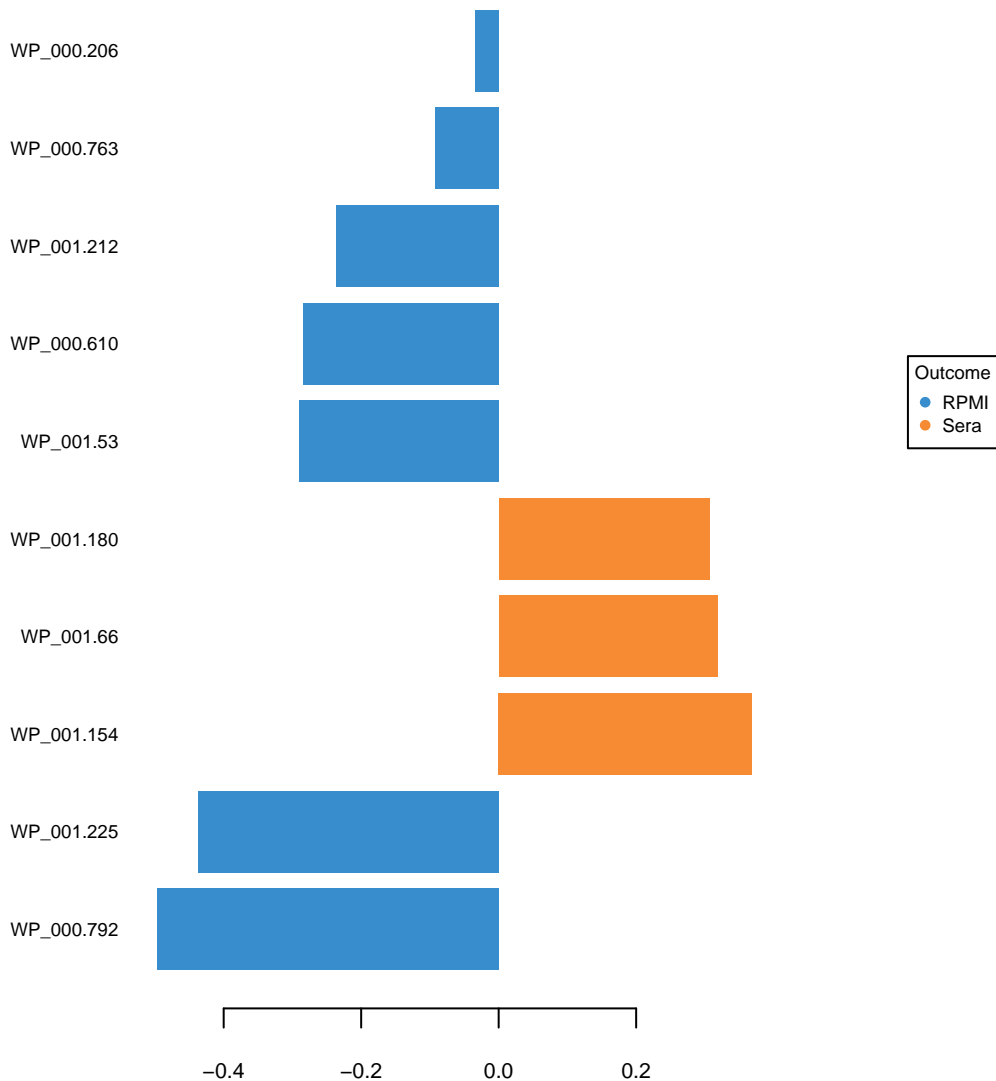
Sera



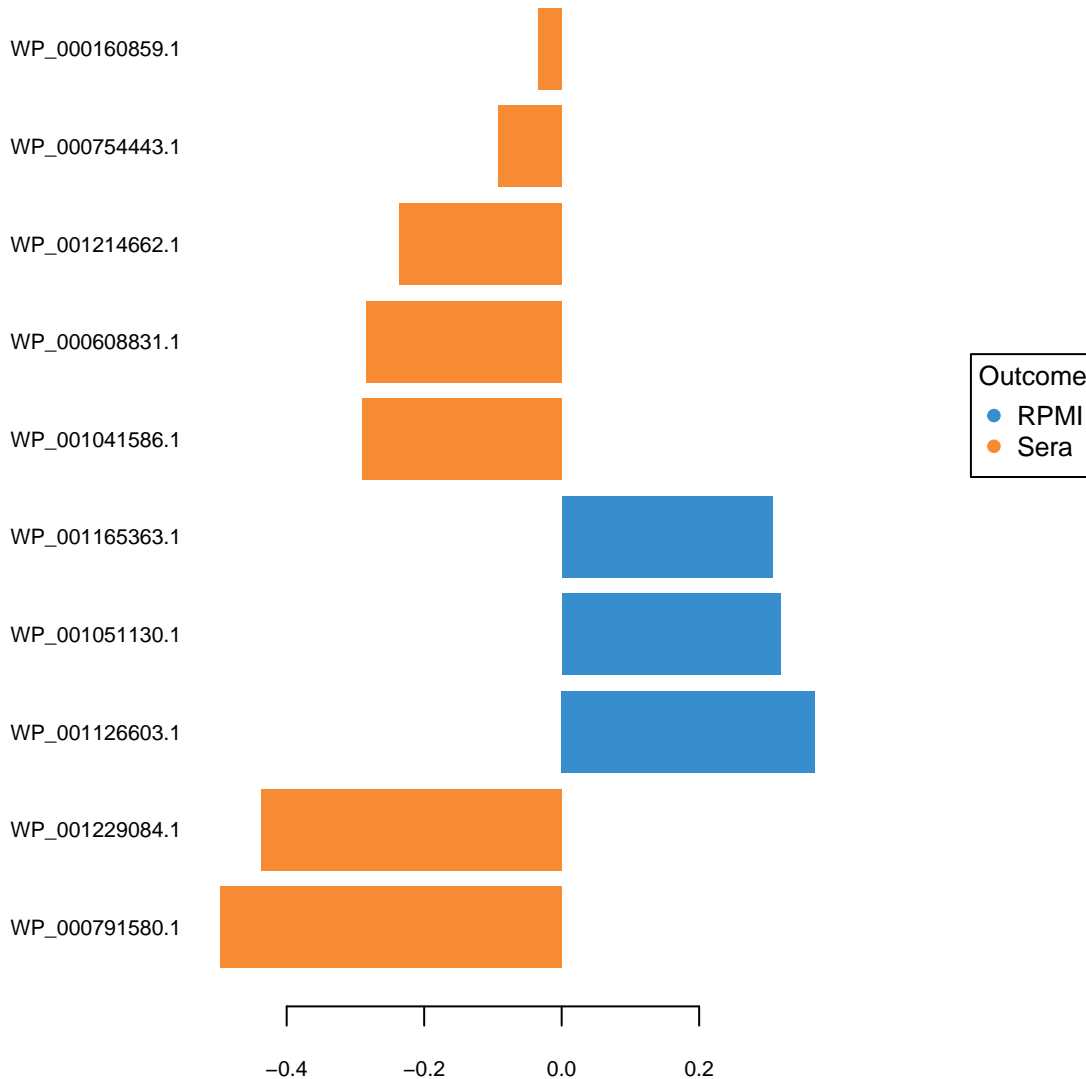
# Proteomics 1 sPLSDA max load



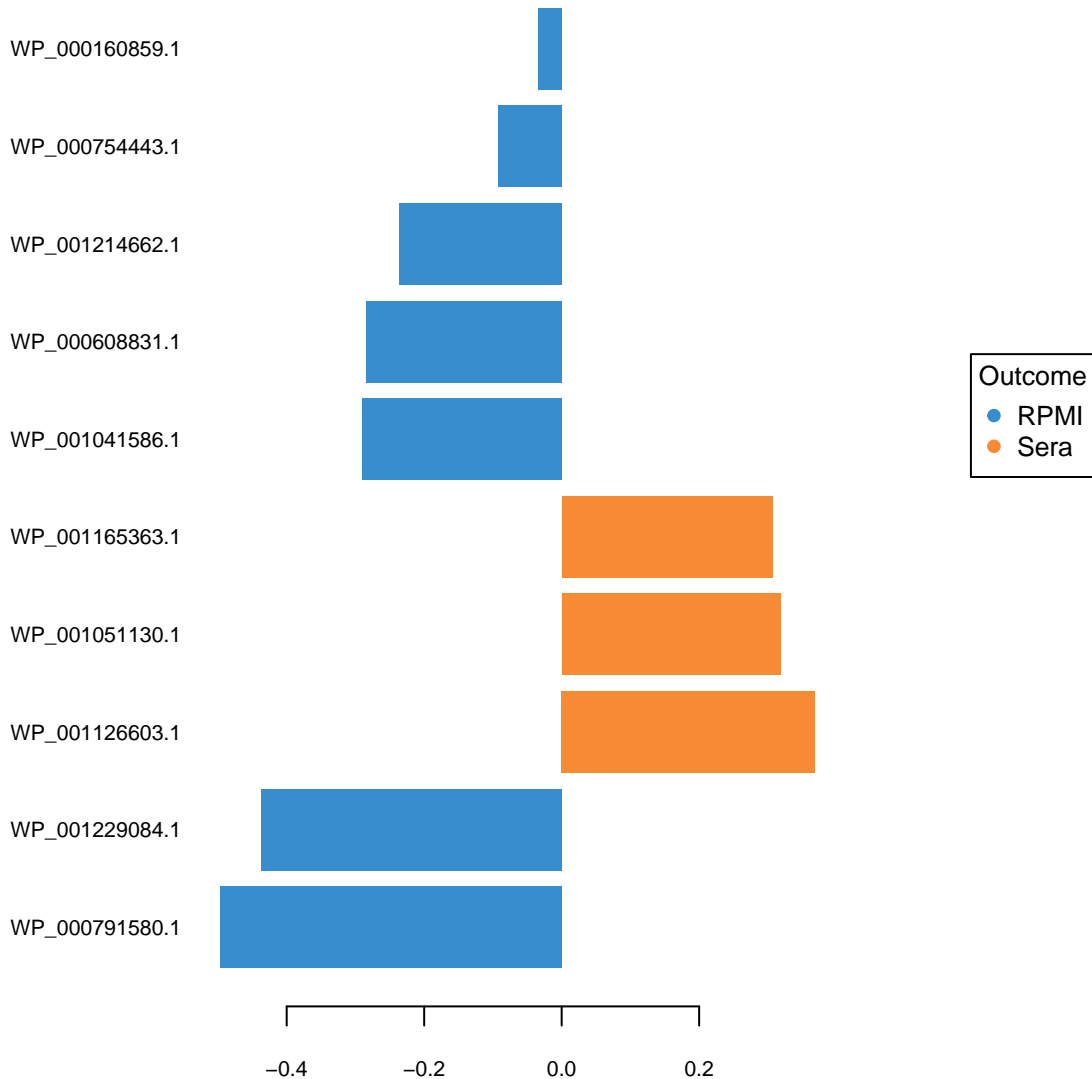
# Proteomics 1 sPLSDA min load

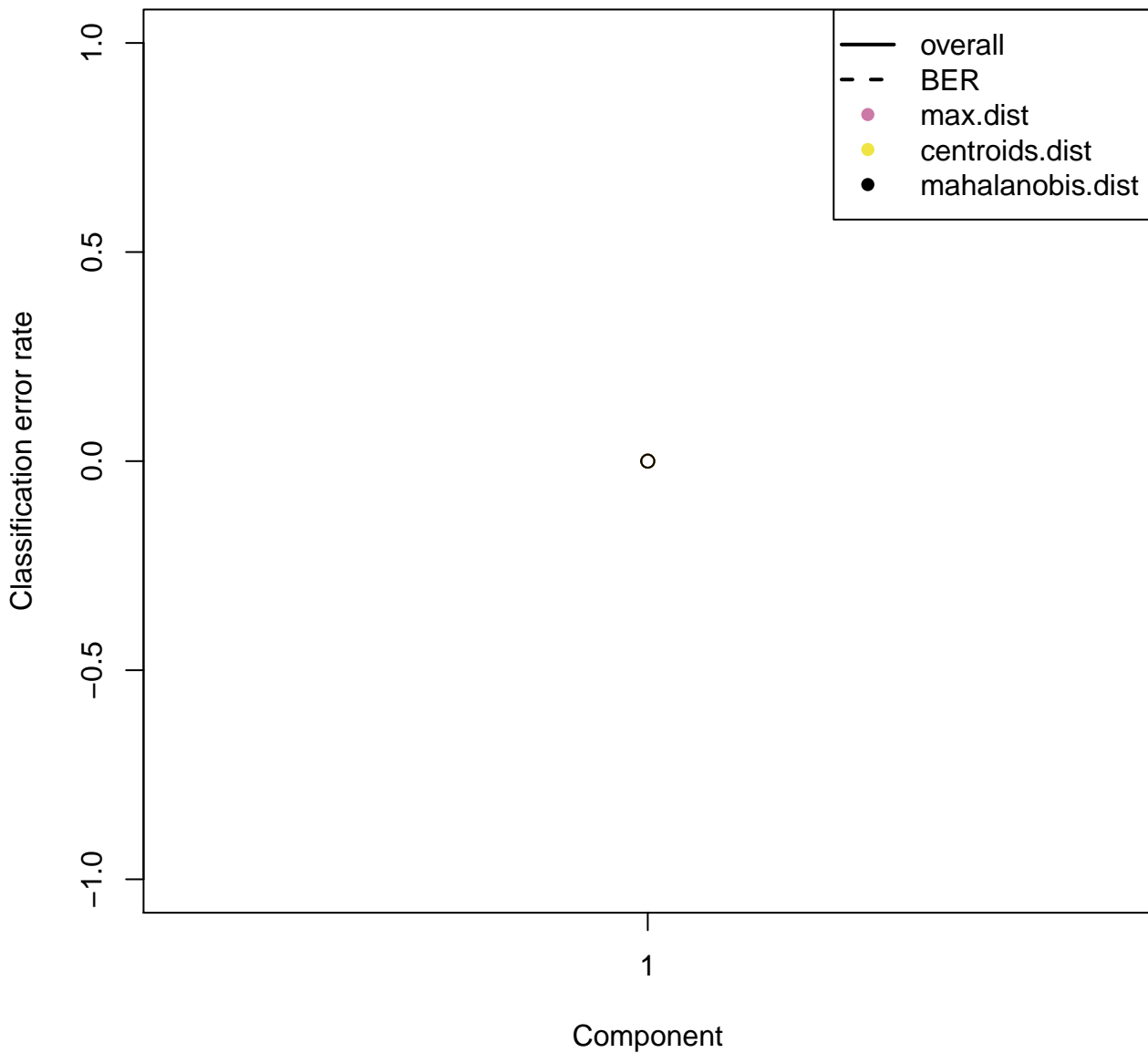


# Contribution on comp 1

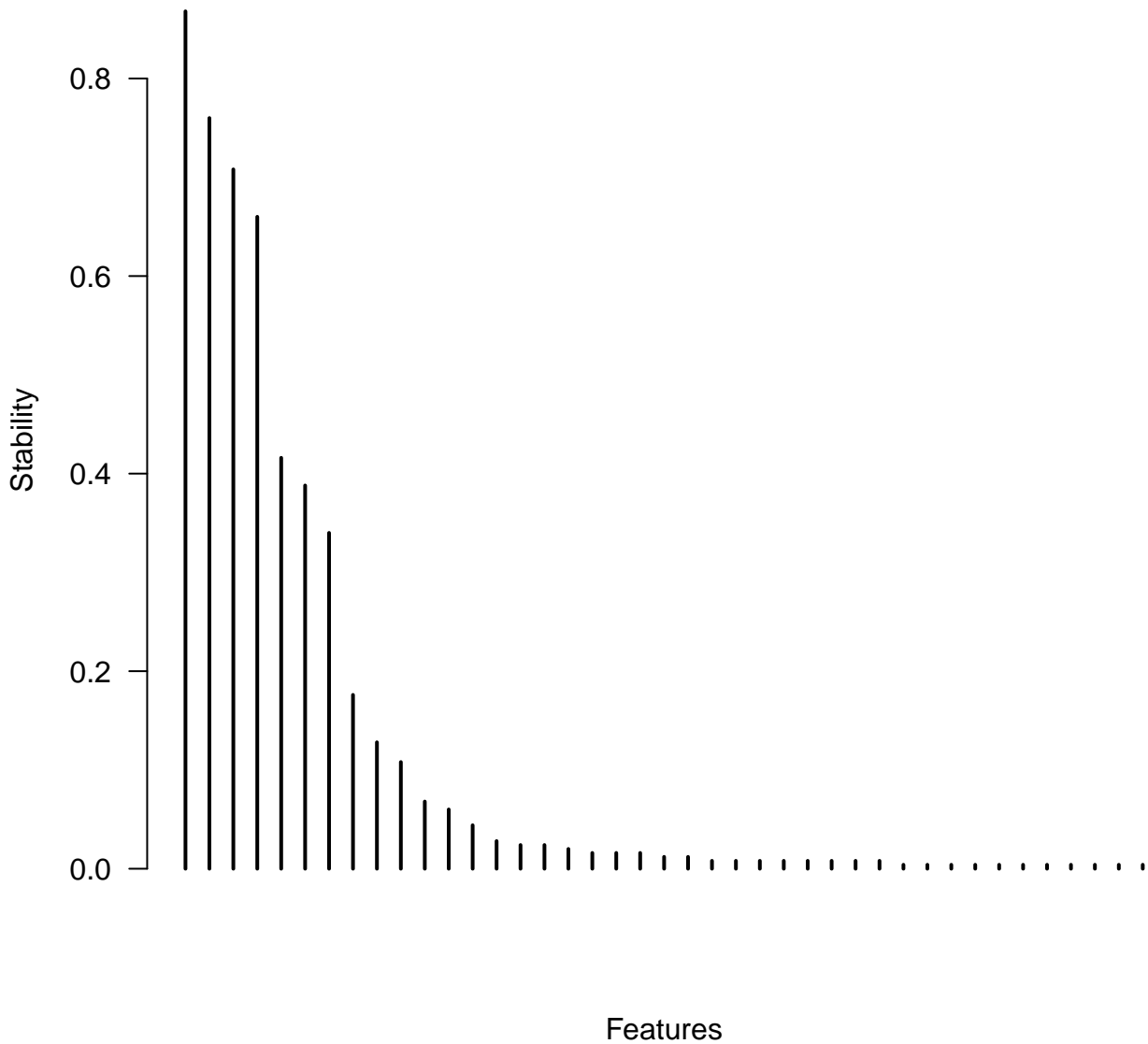


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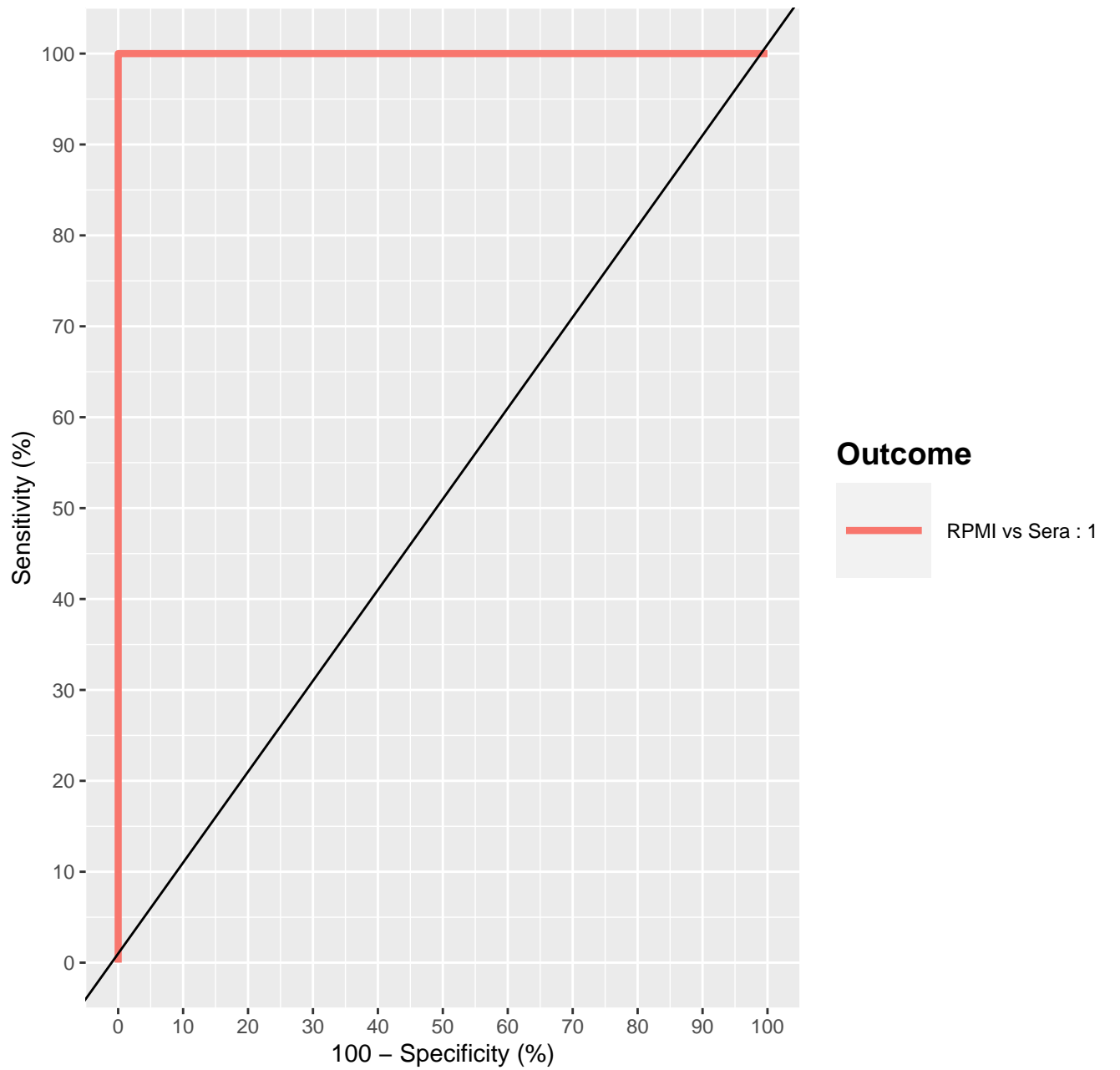




# Comp 1



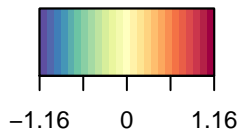
**ROC Curve Comp 1**





# sPLSDA

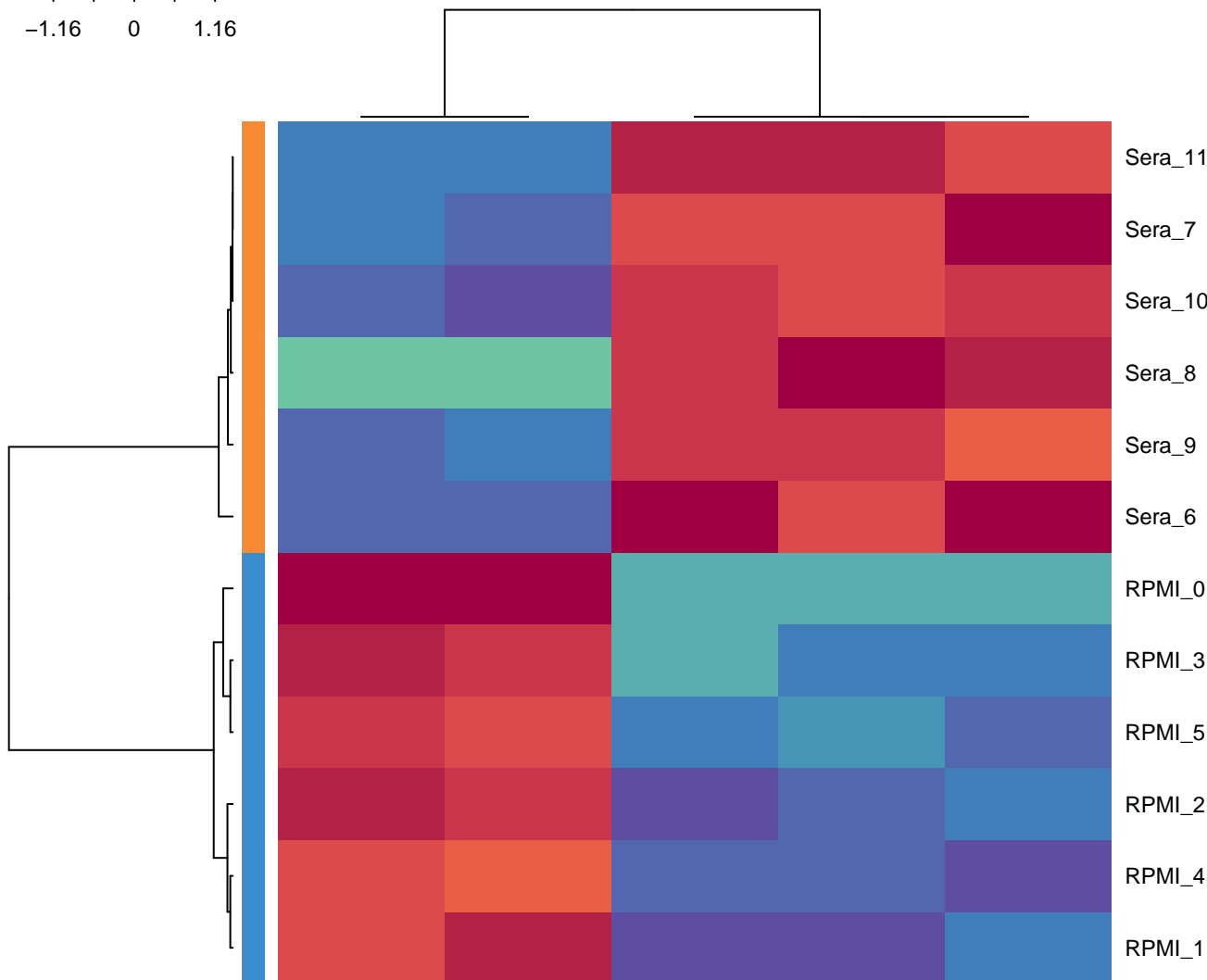
Color key



Status

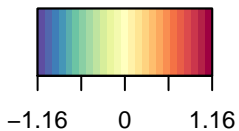
RPMI

Sera



# sPLSDA Component 1

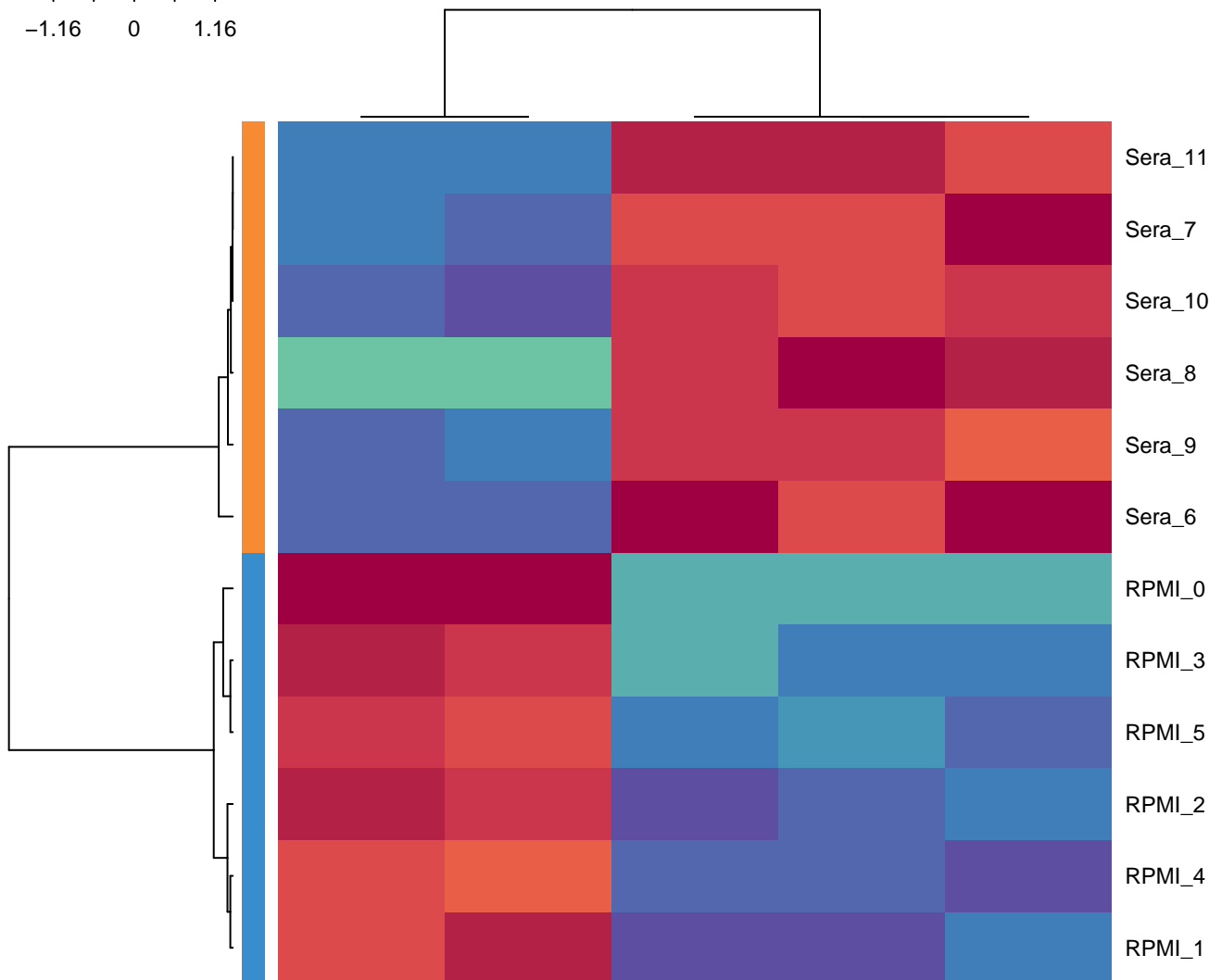
Color key



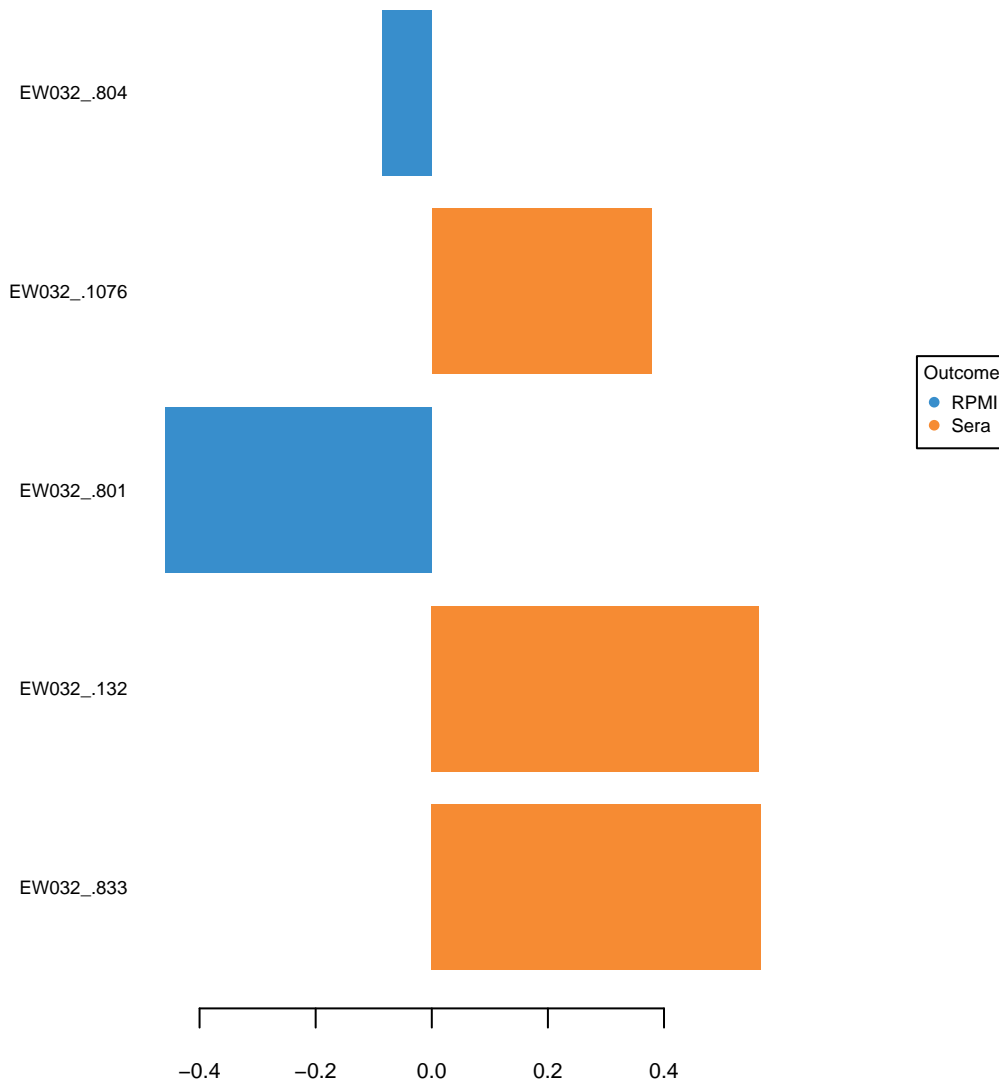
Status

RPMI

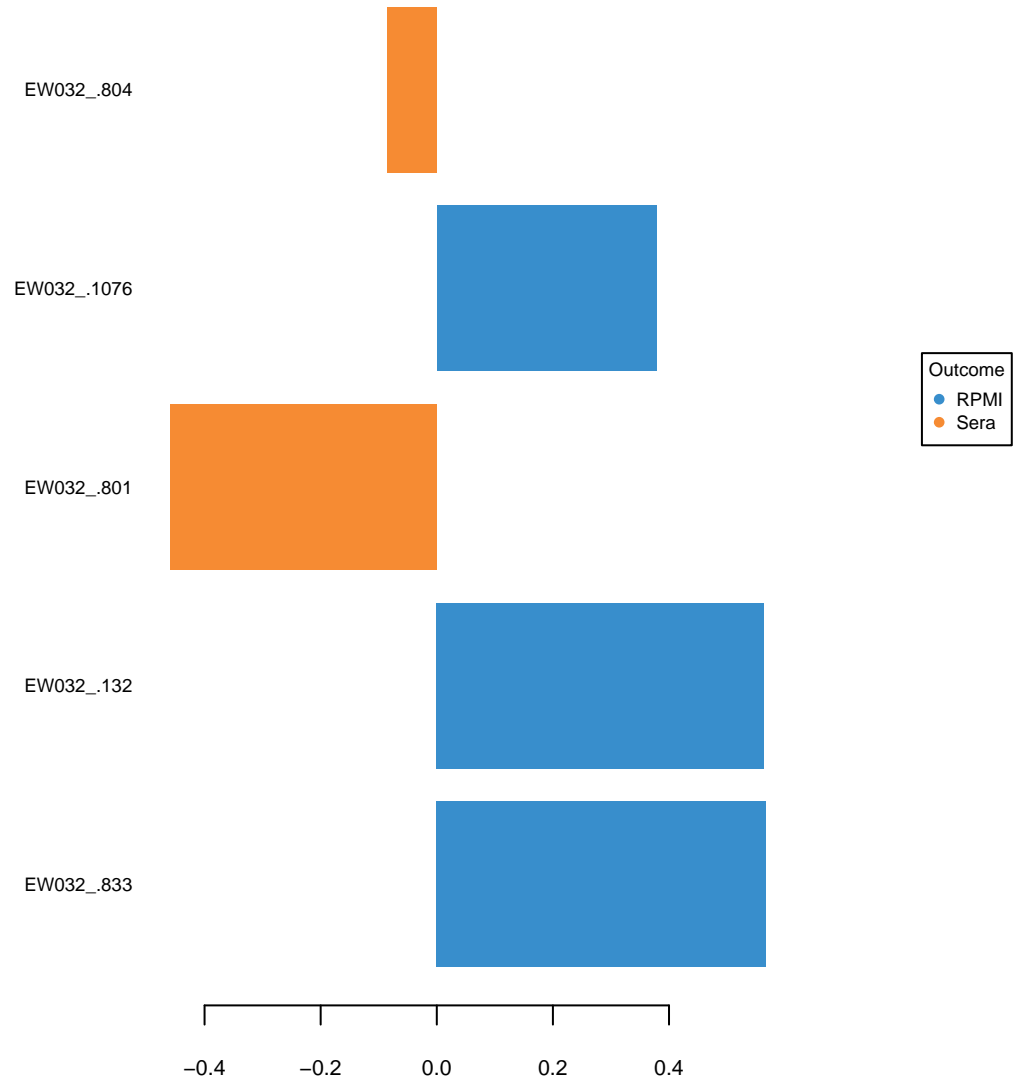
Sera



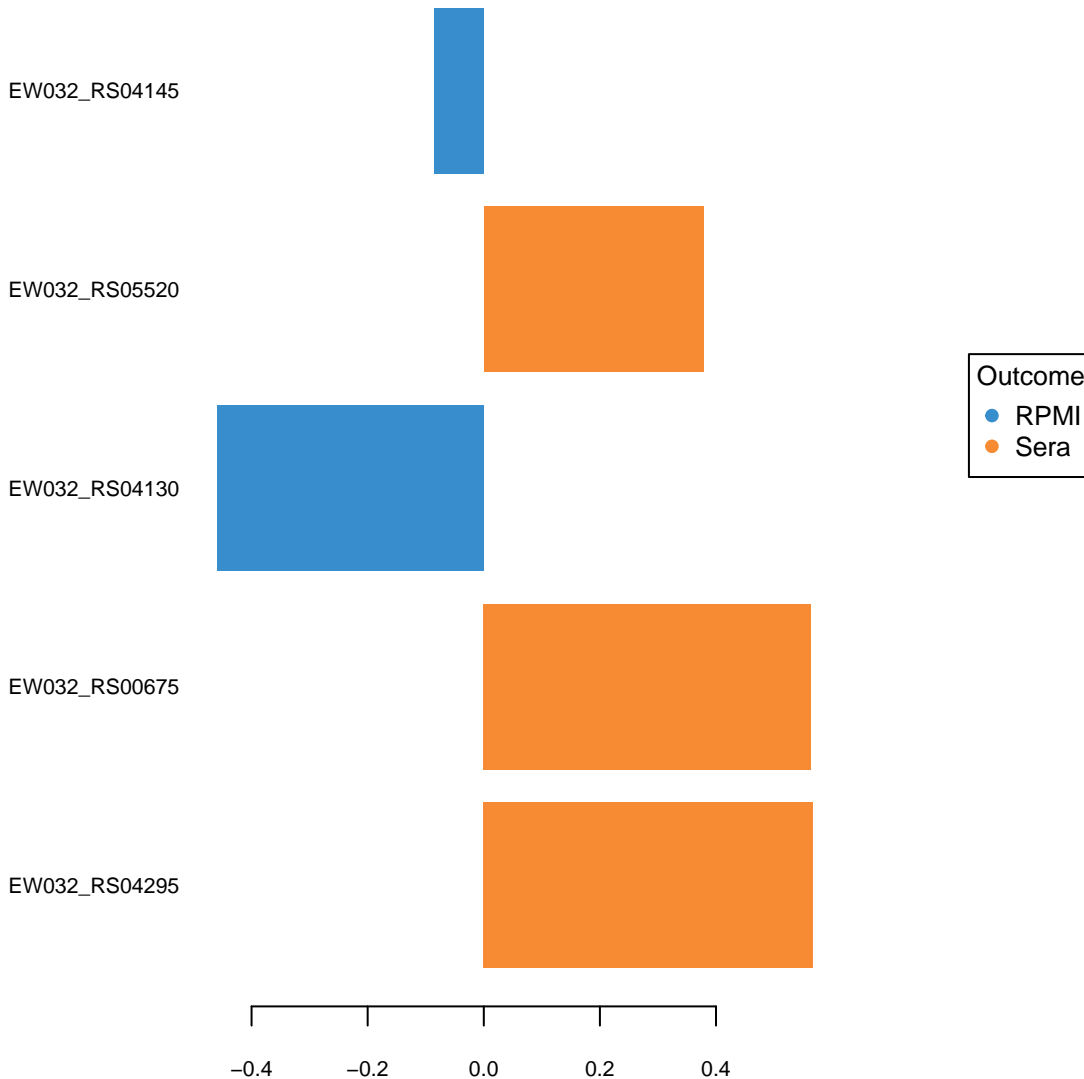
# RNA\_Seq 1 sPLSDA max loadings



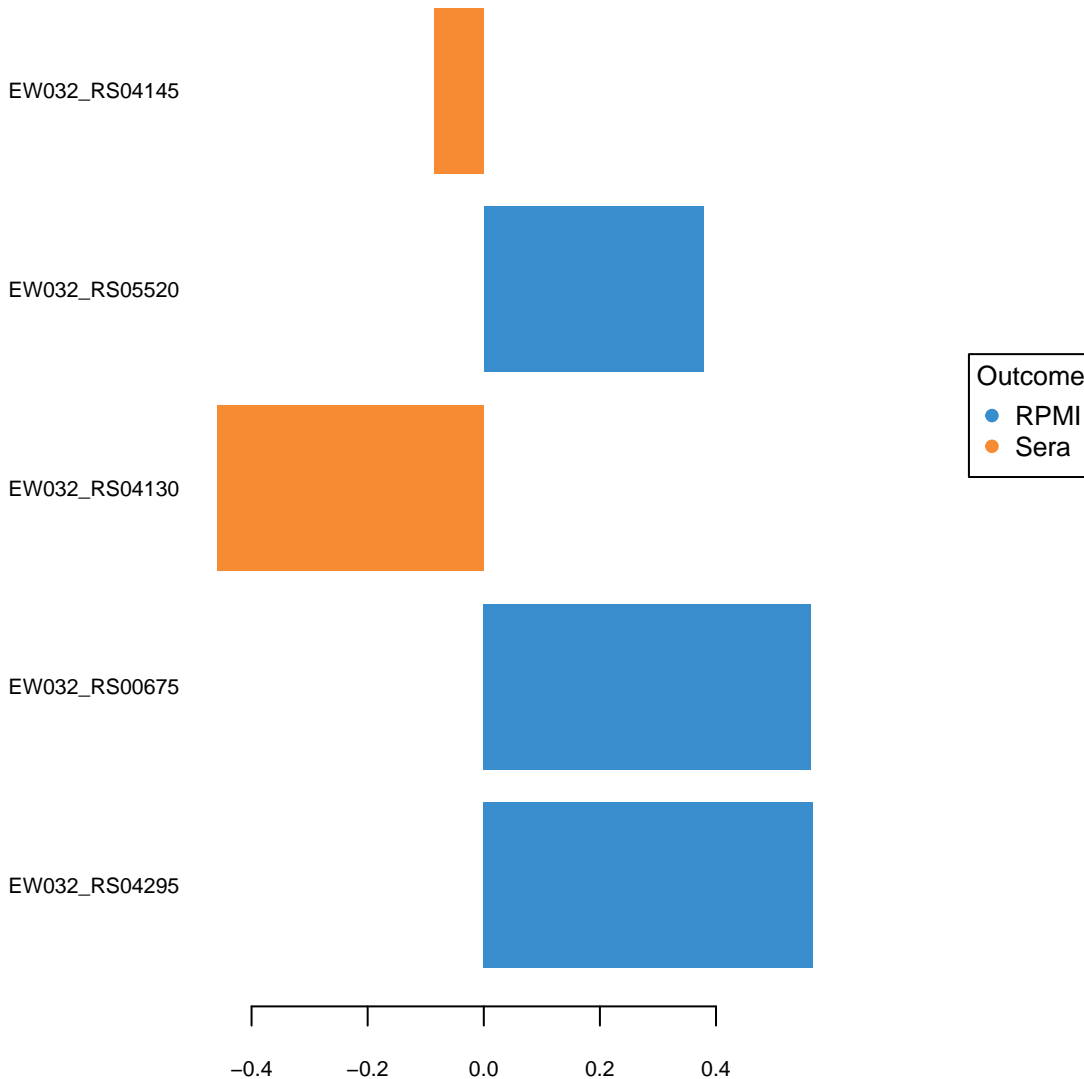
# RNA\_Seq 1 sPLSDA min loadings

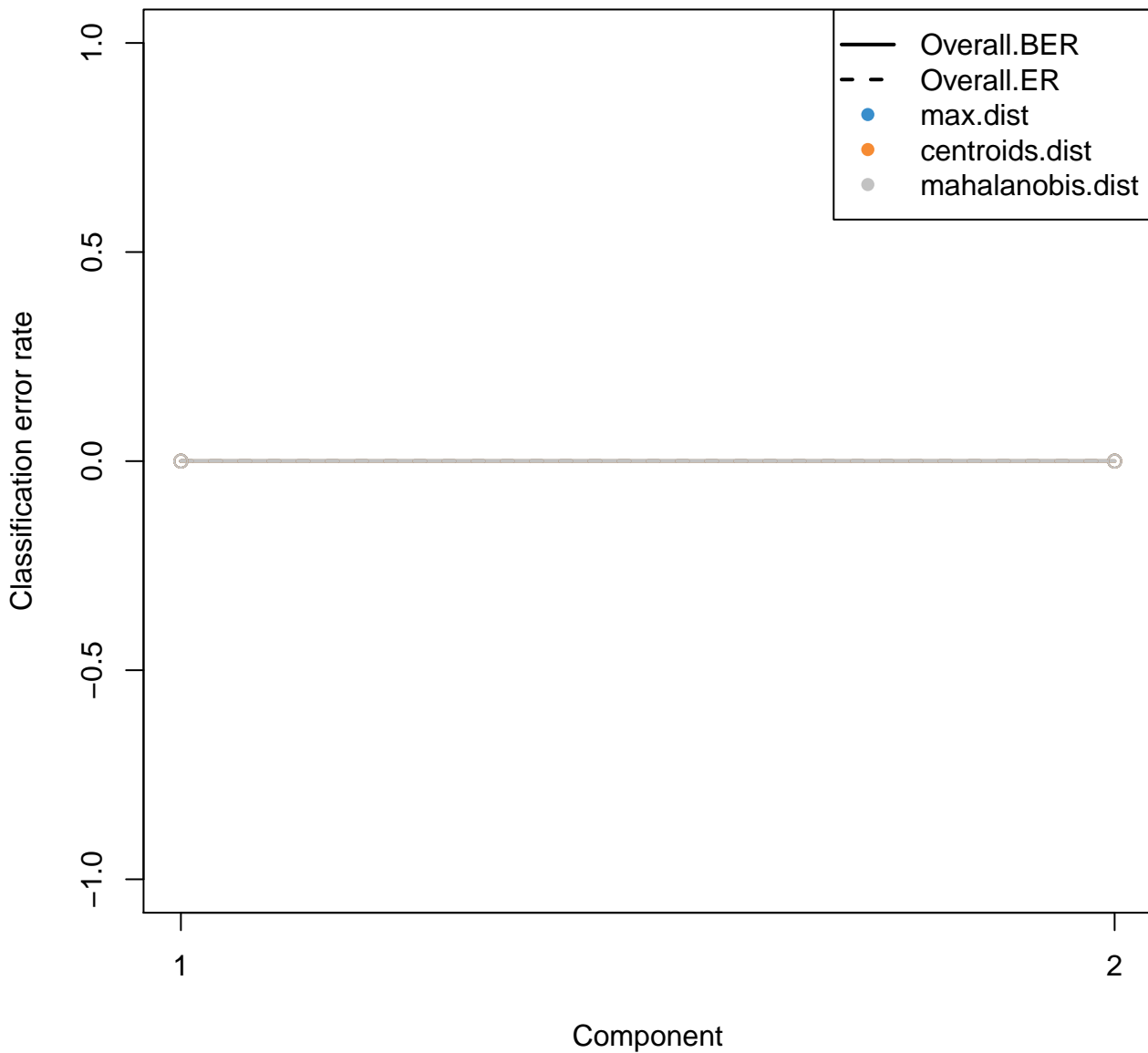


# Contribution on comp 1

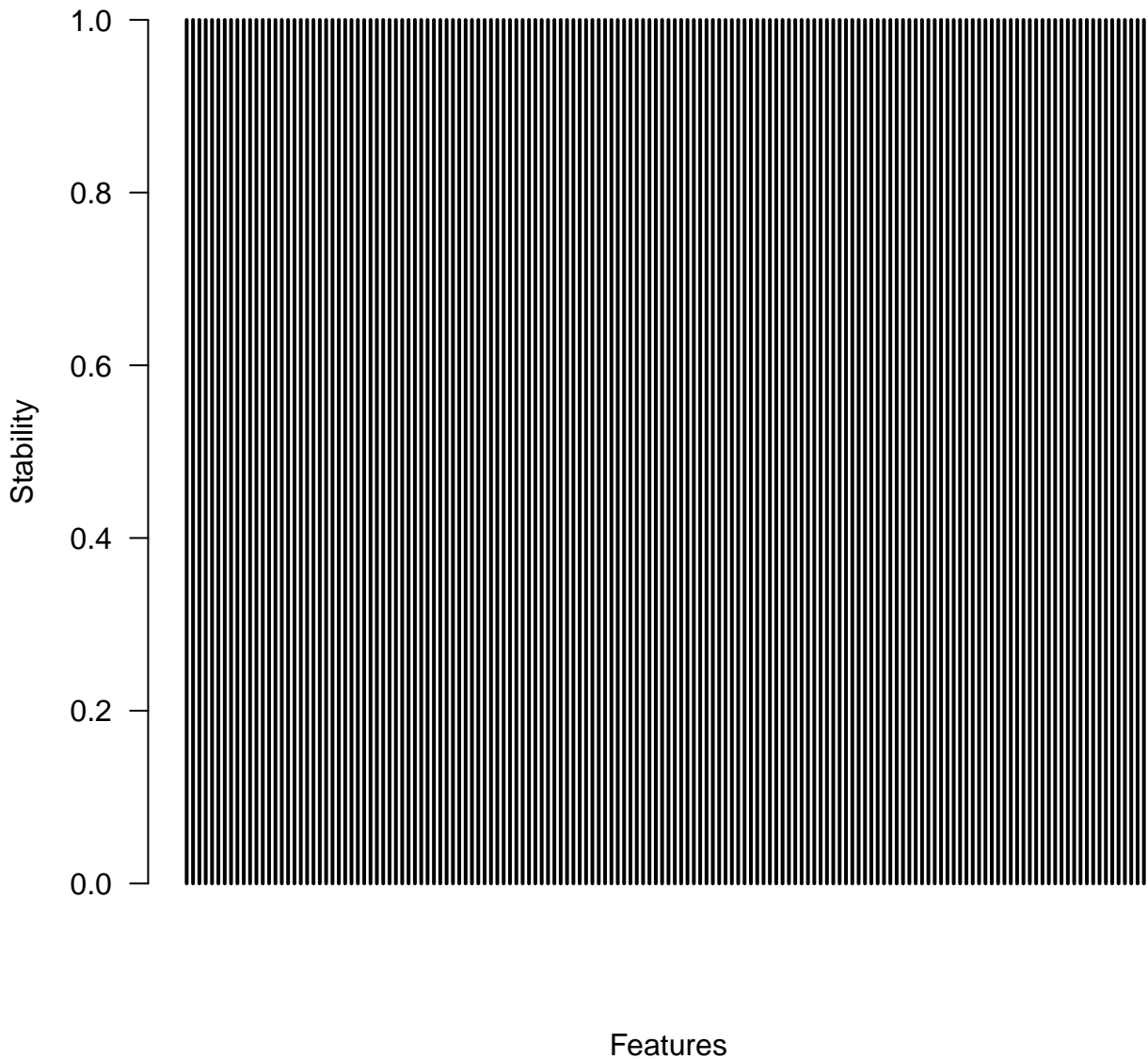


# Contribution on comp 1



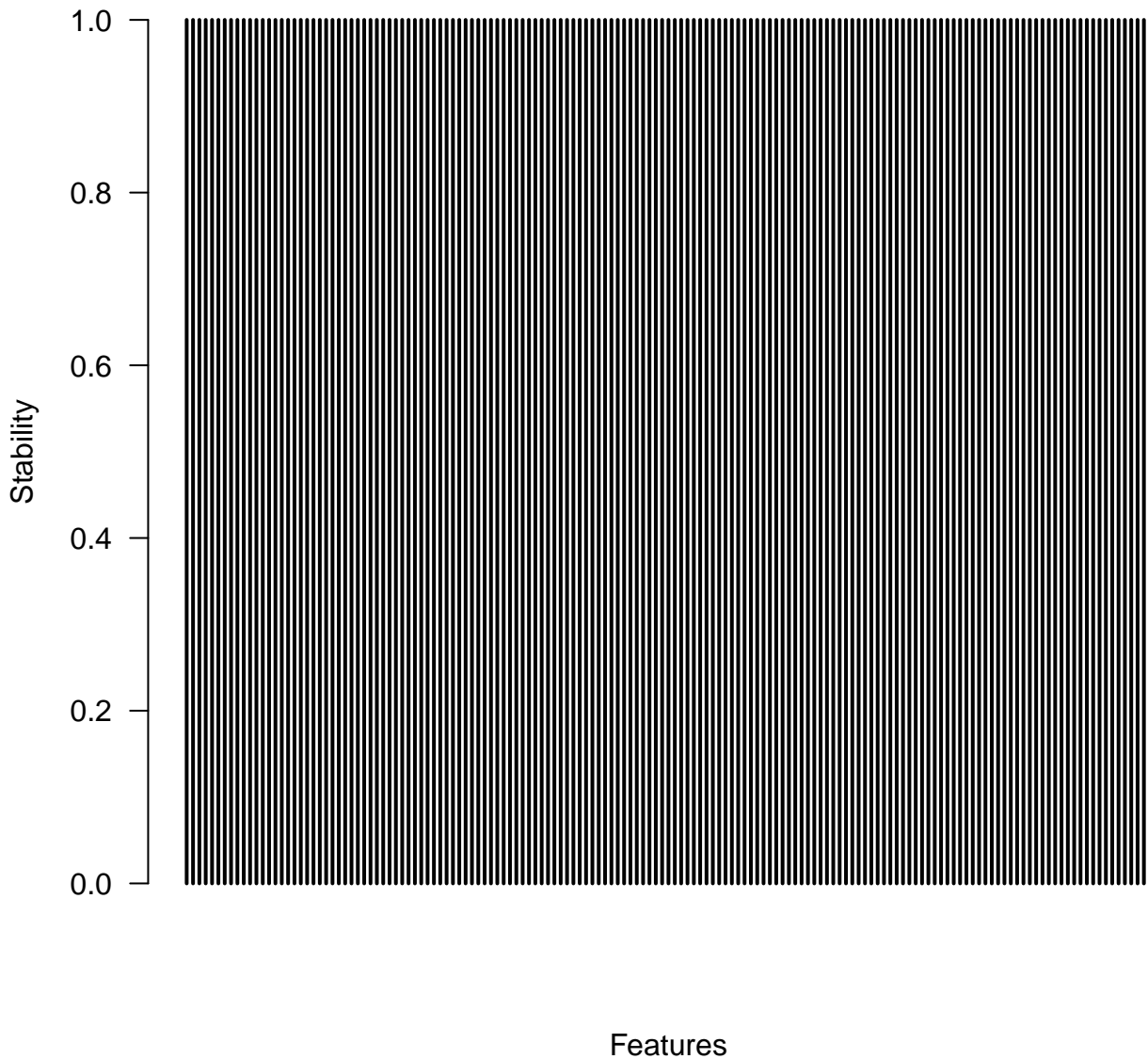


# Metabolomics Comp 1

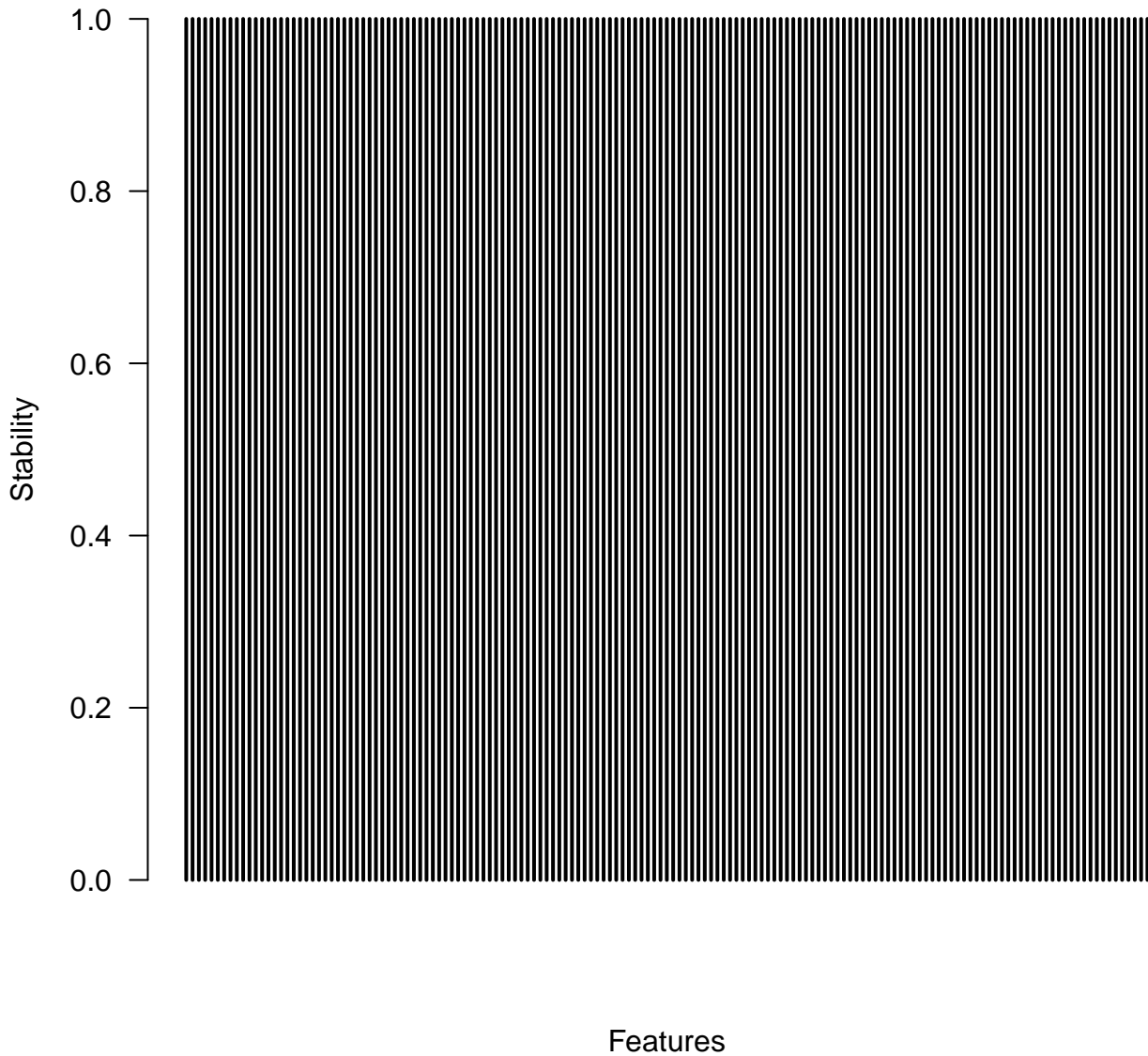




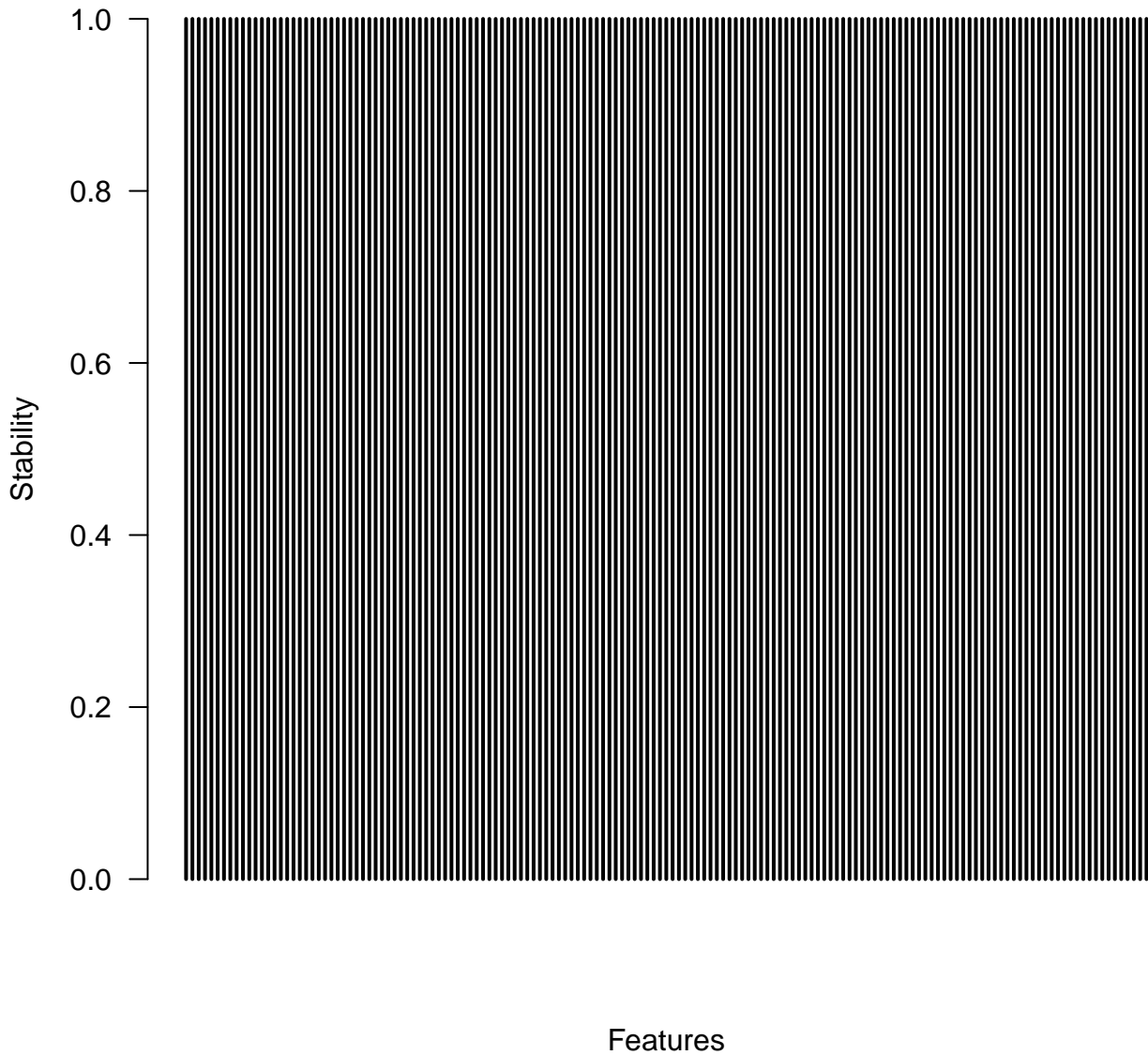
## Metabolomics Comp 2



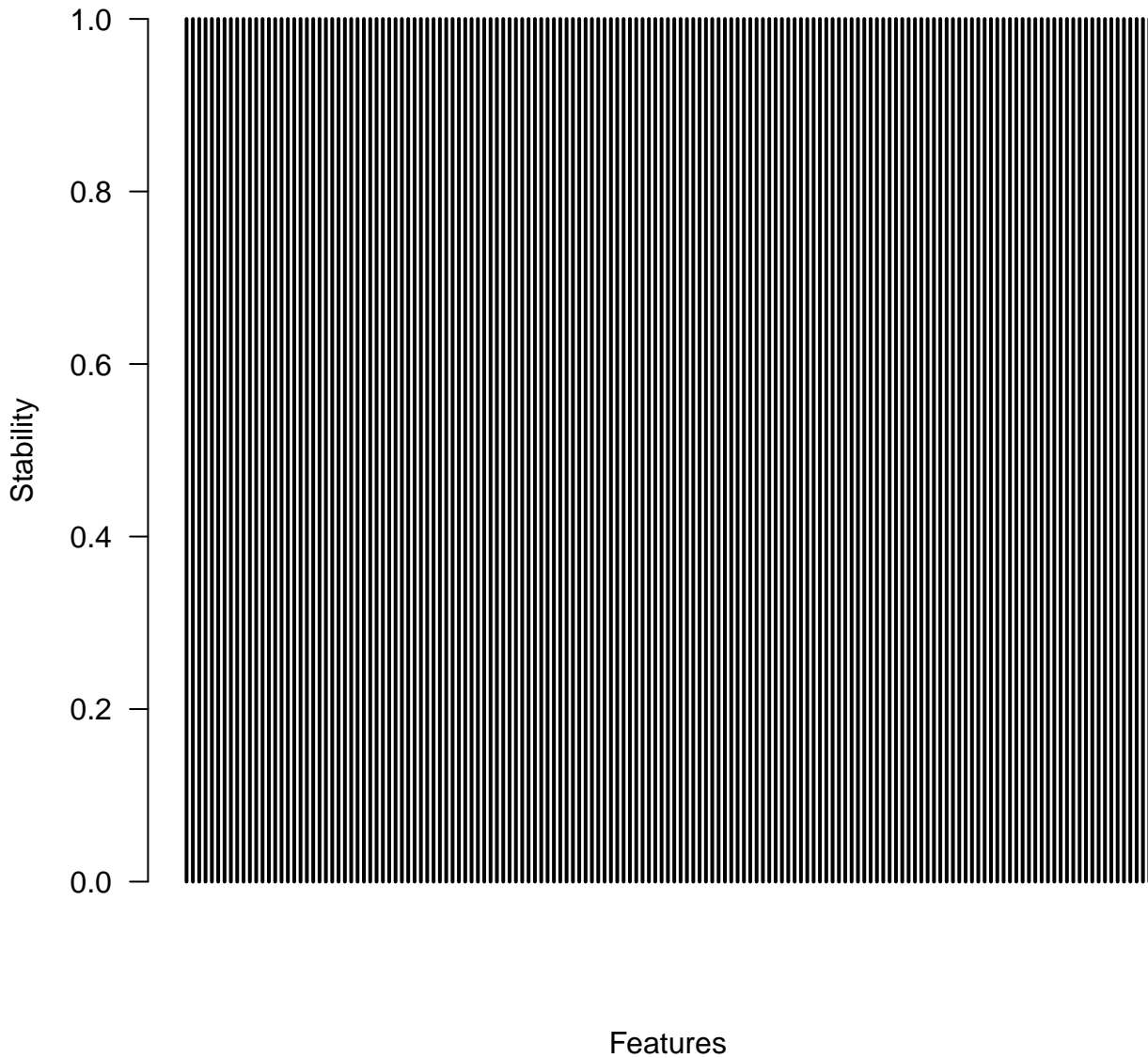
# Proteomics Comp 1



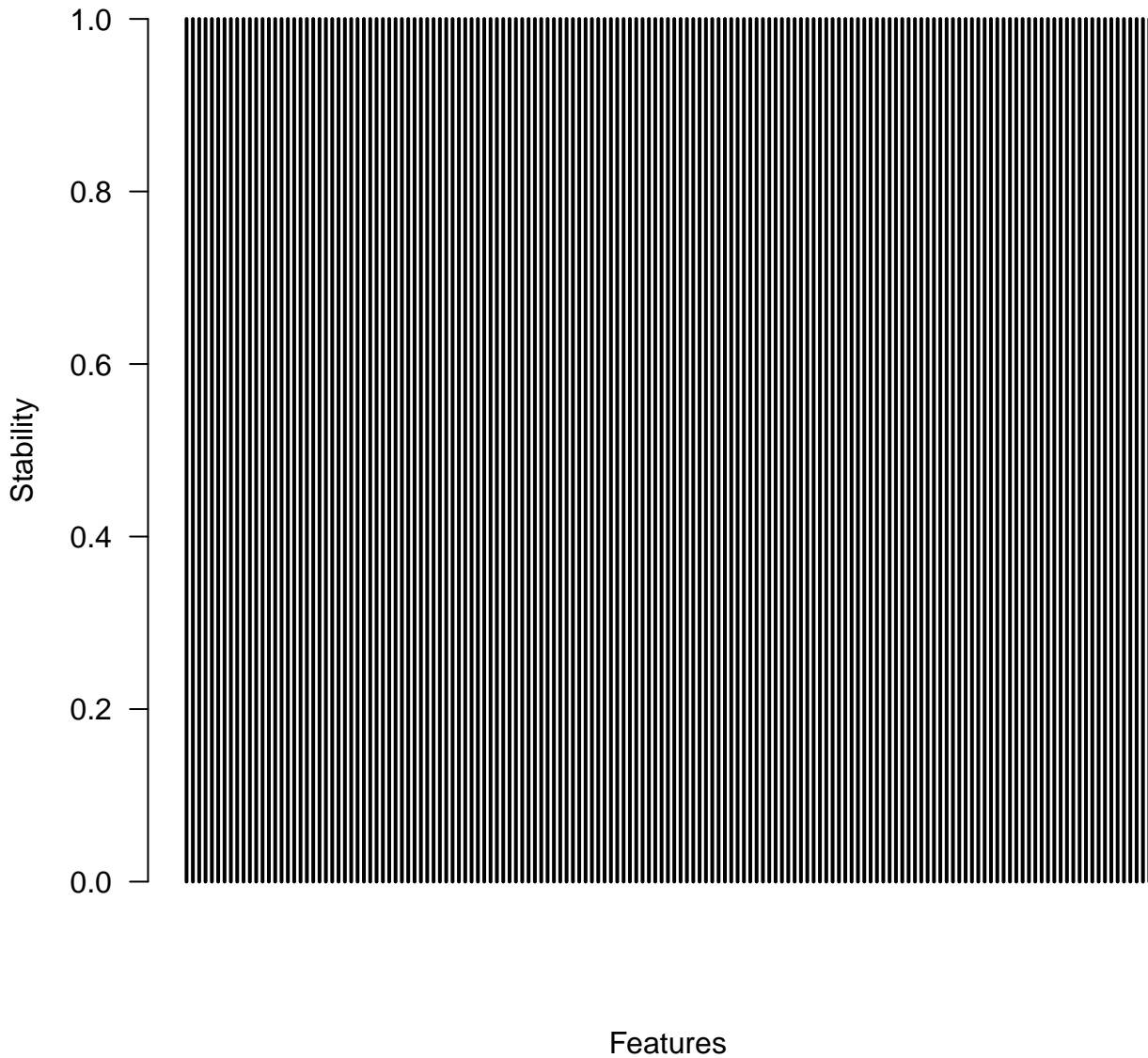
# Proteomics Comp 2



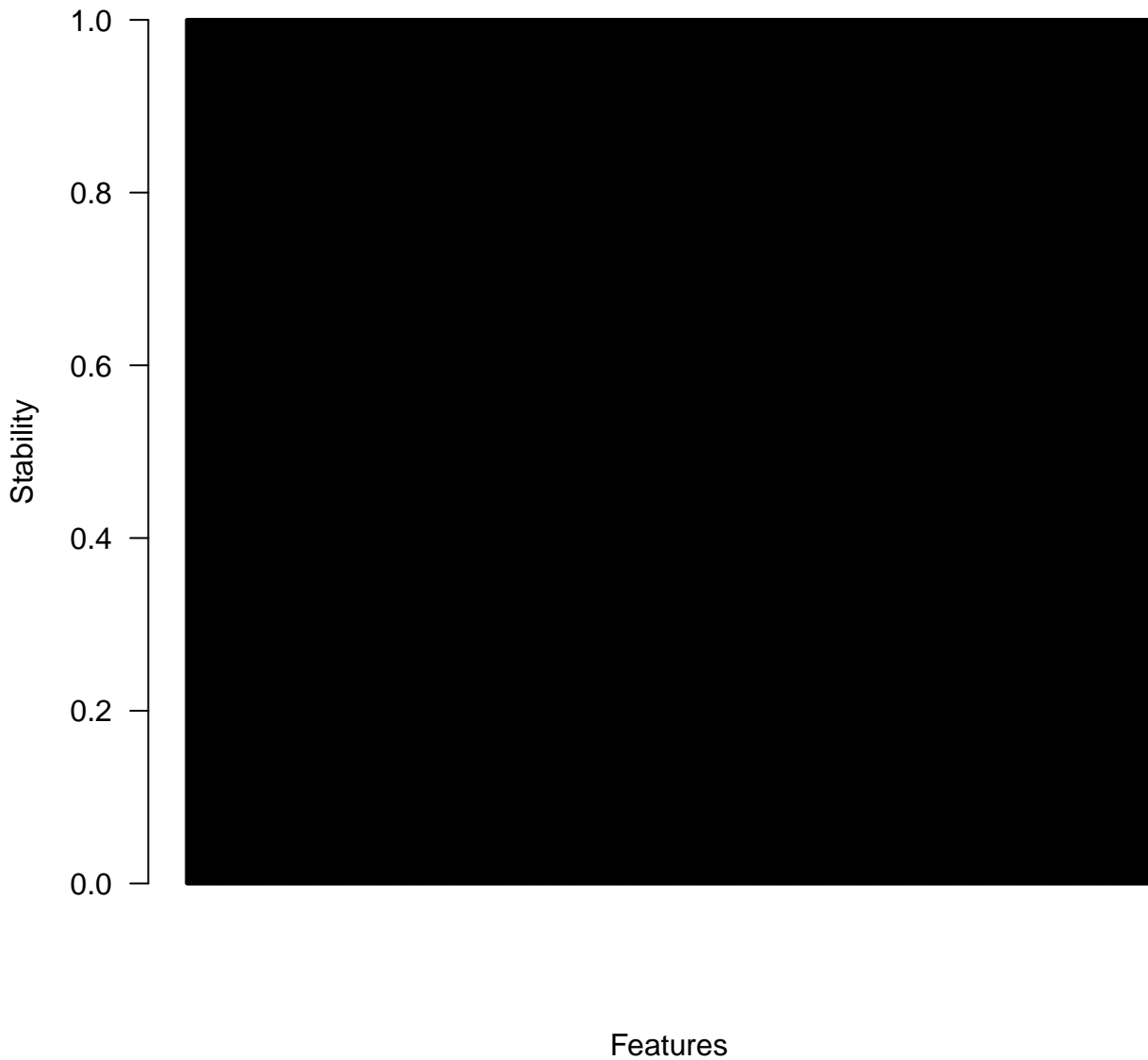
# RNA\_Seq Comp 1



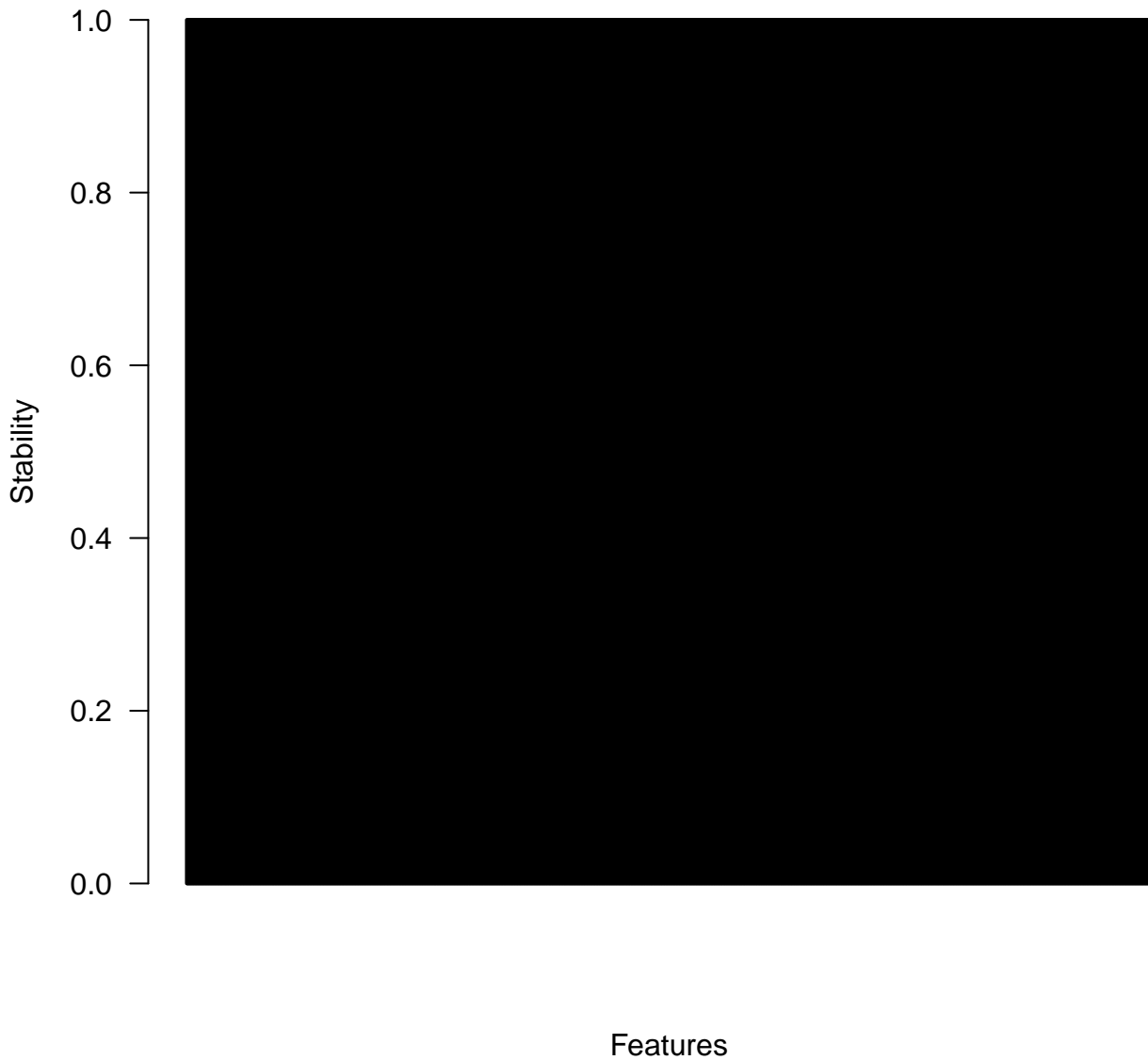
## RNA\_Seq Comp 2



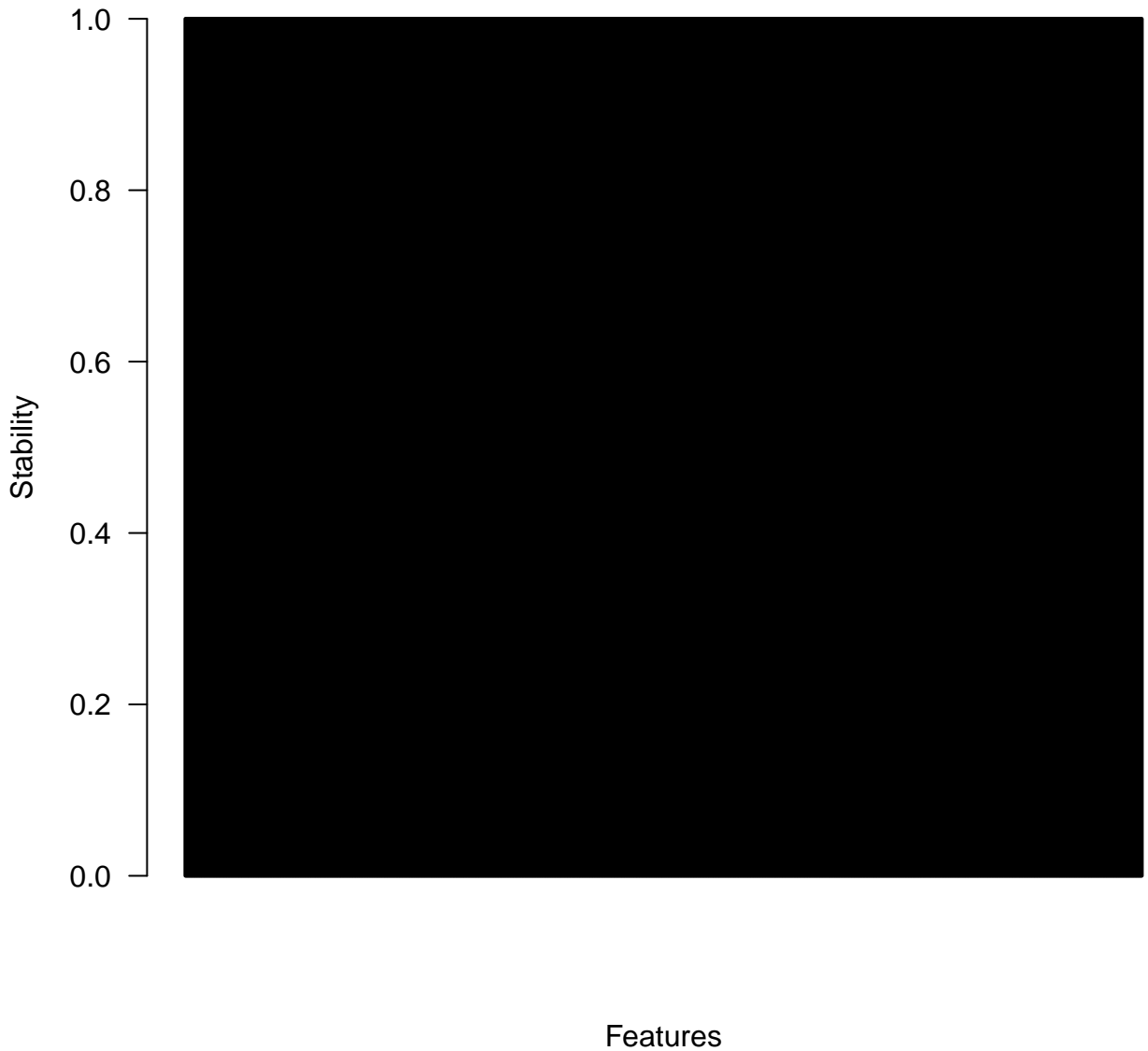
# Metabolomics Comp 1



## Metabolomics Comp 2

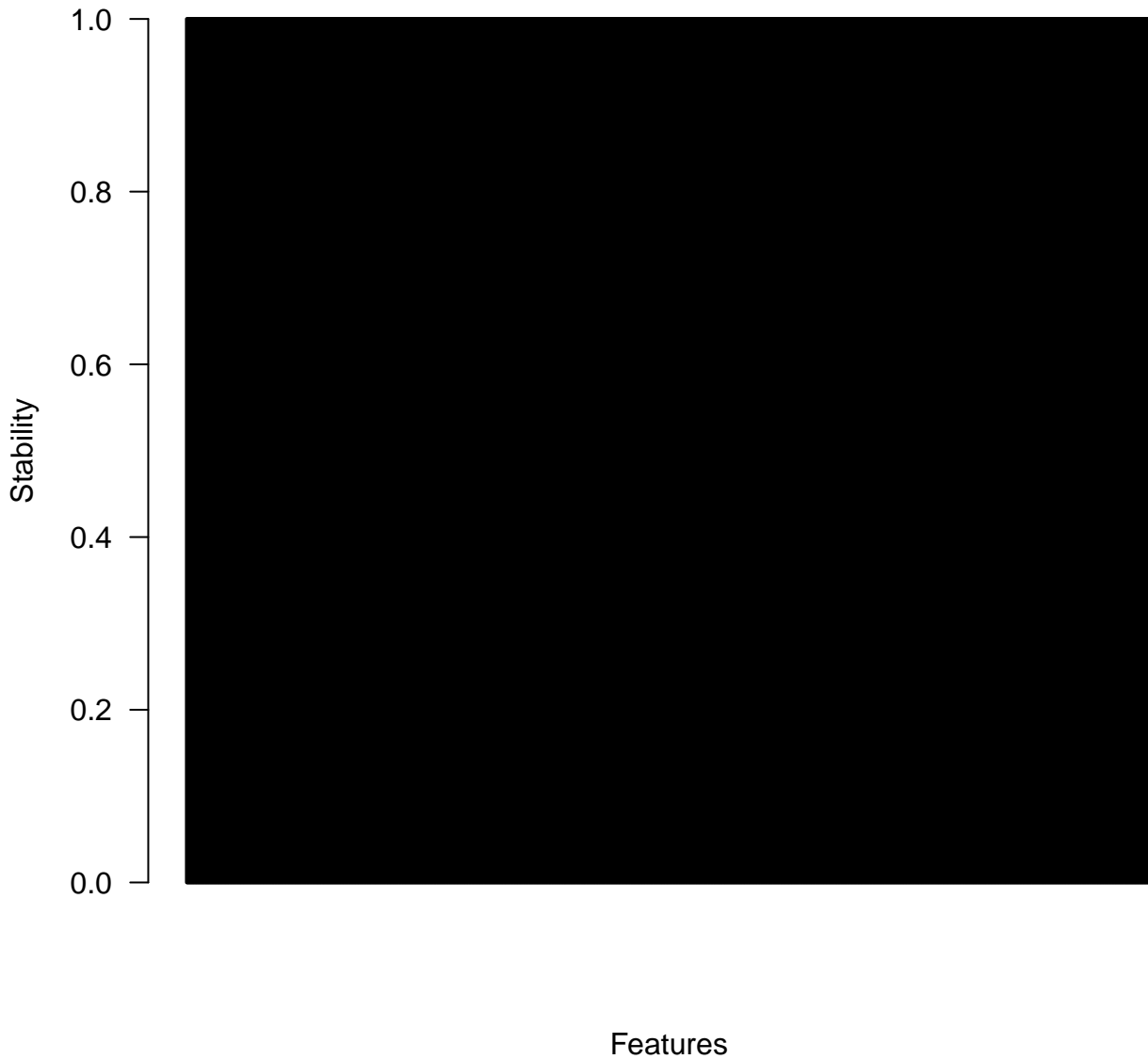


# Proteomics Comp 1

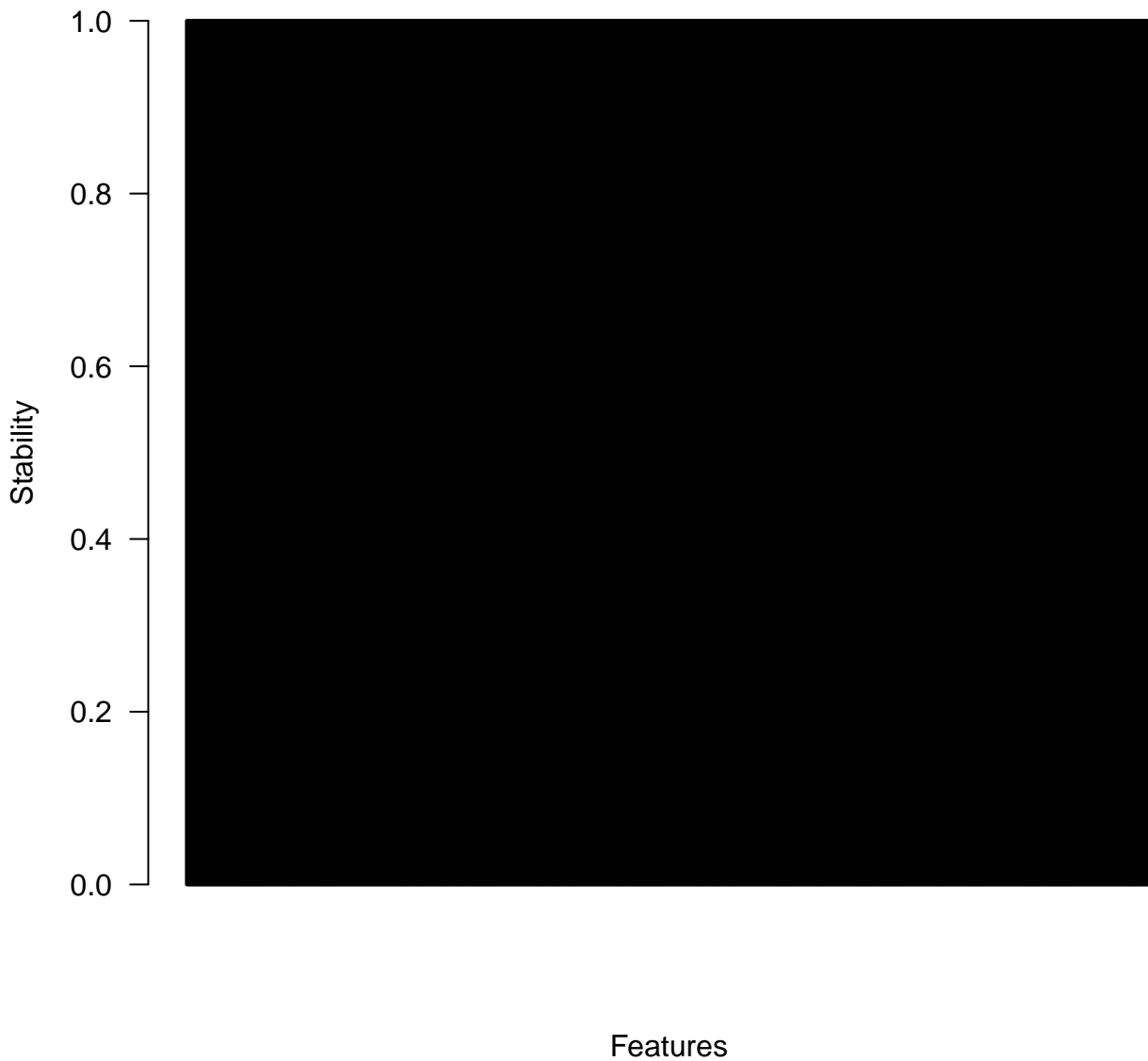




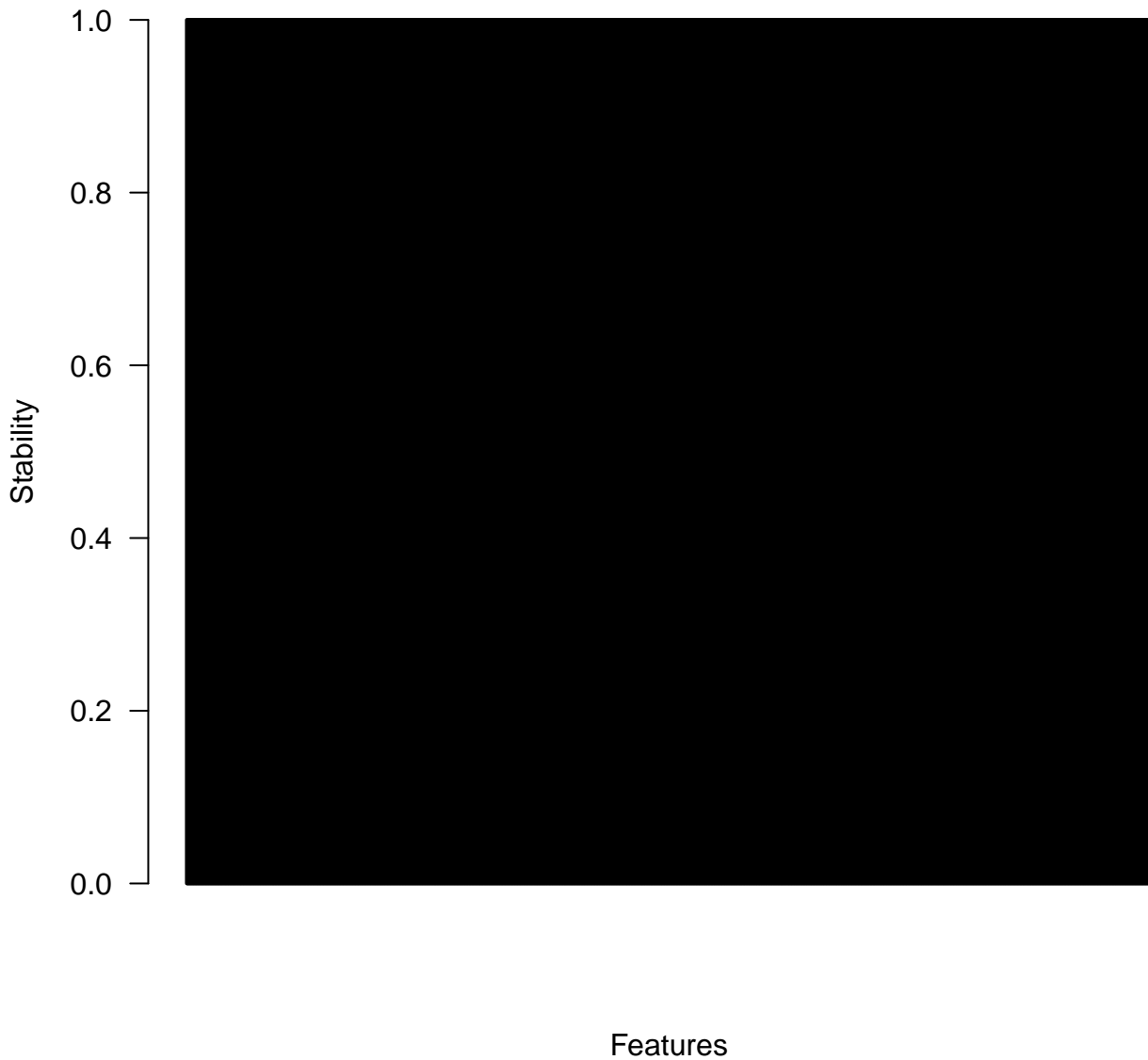
## Proteomics Comp 2



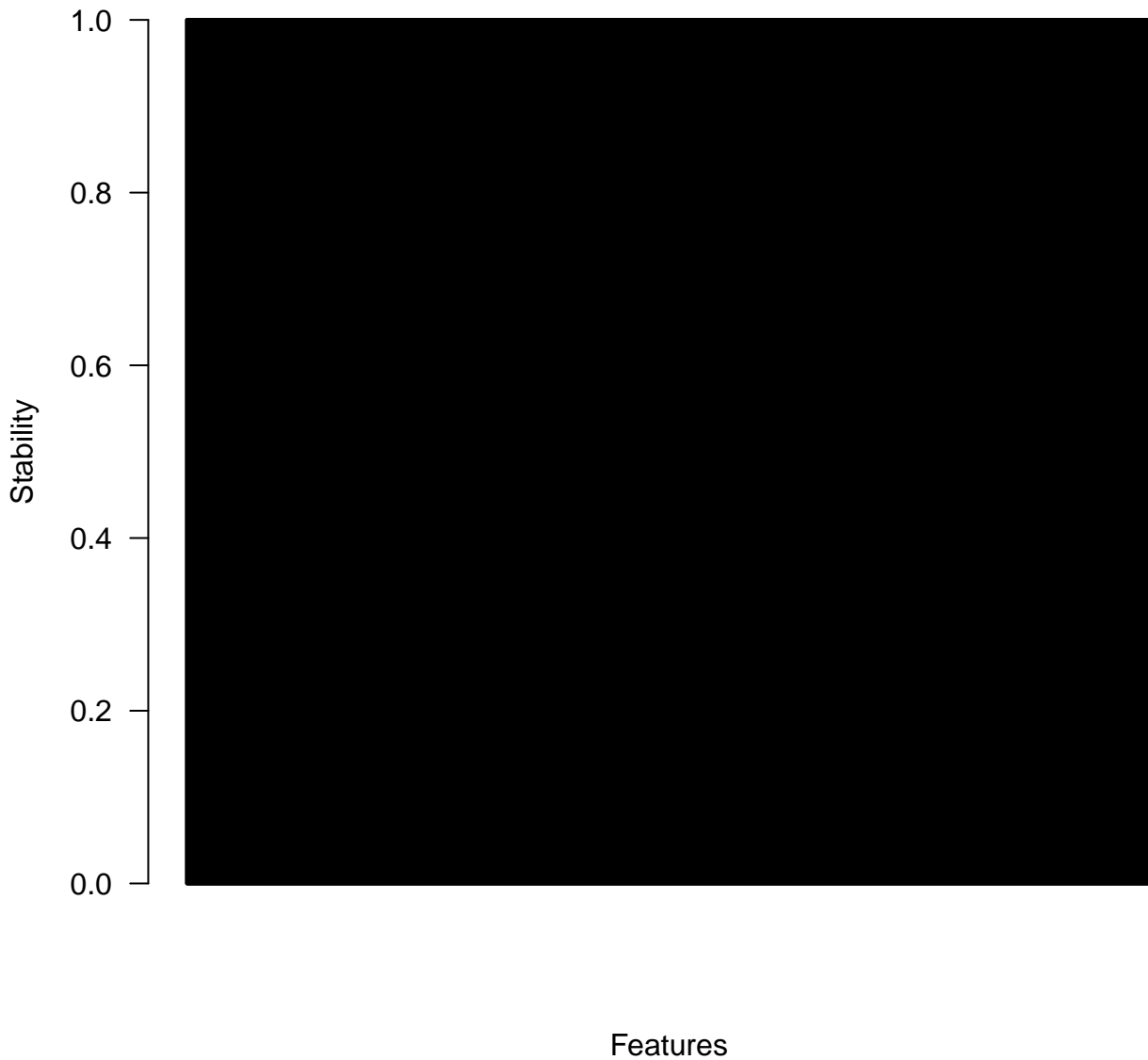
# RNA\_Seq Comp 1



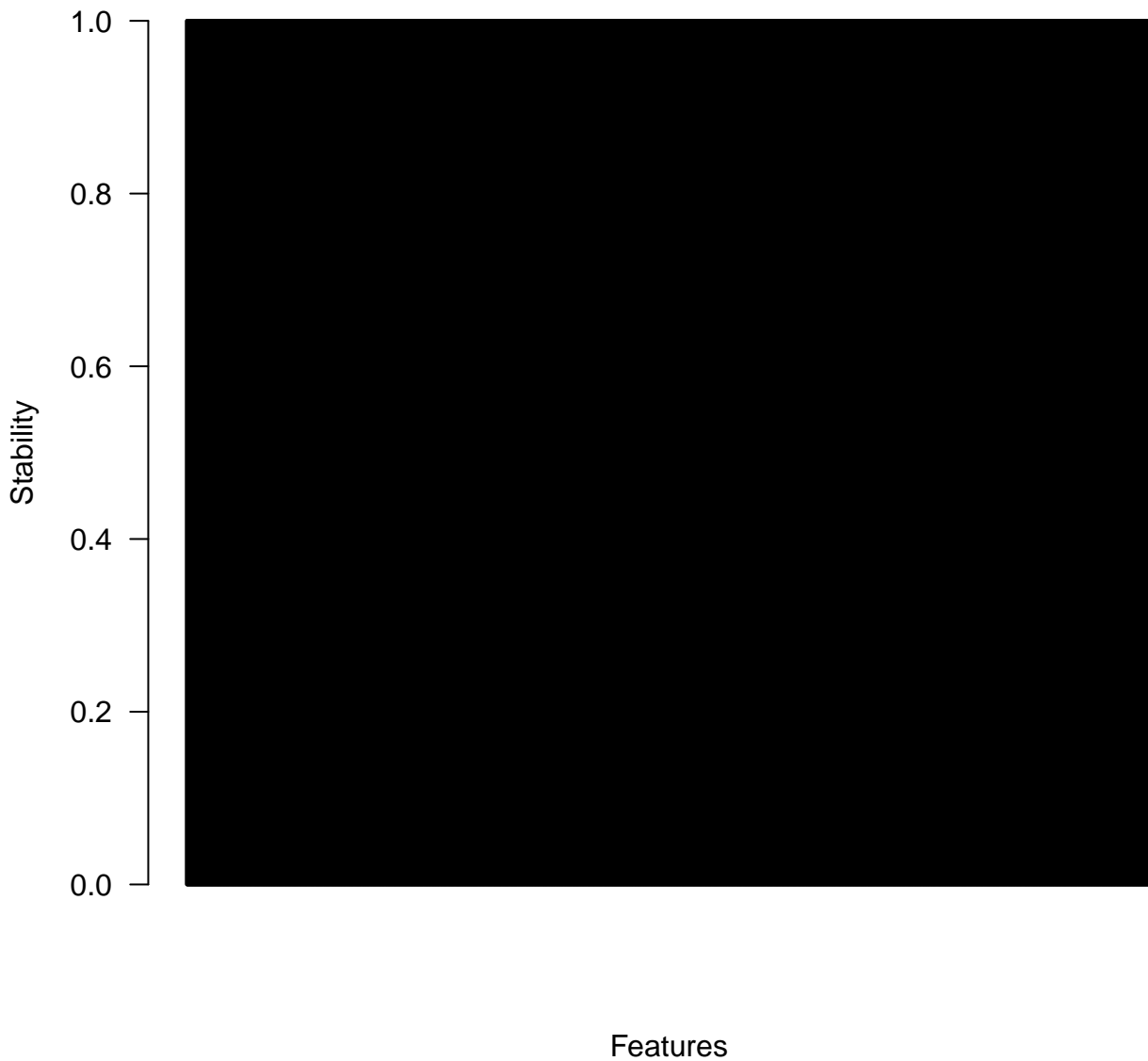
## RNA\_Seq Comp 2



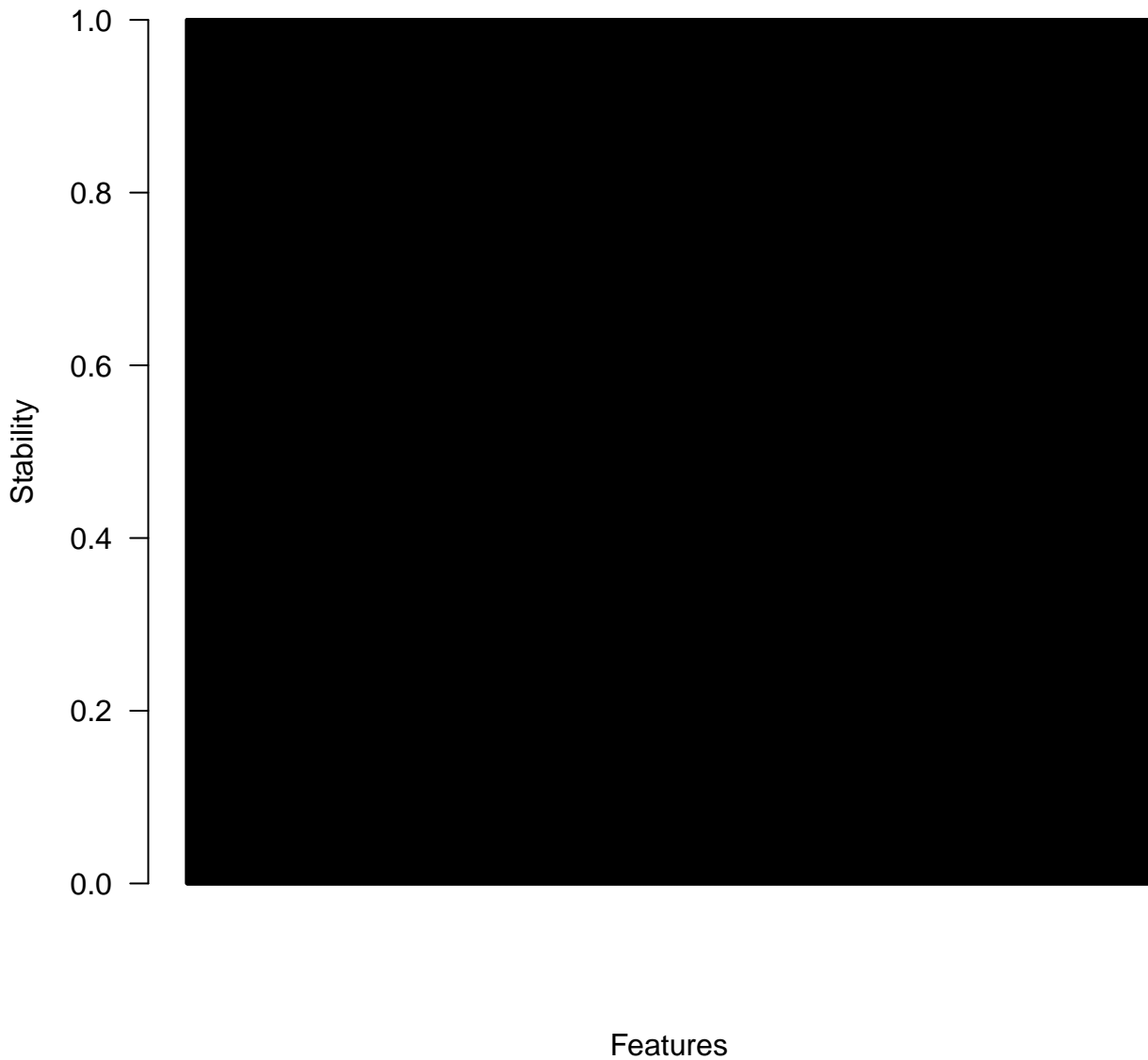
# Metabolomics Comp 1



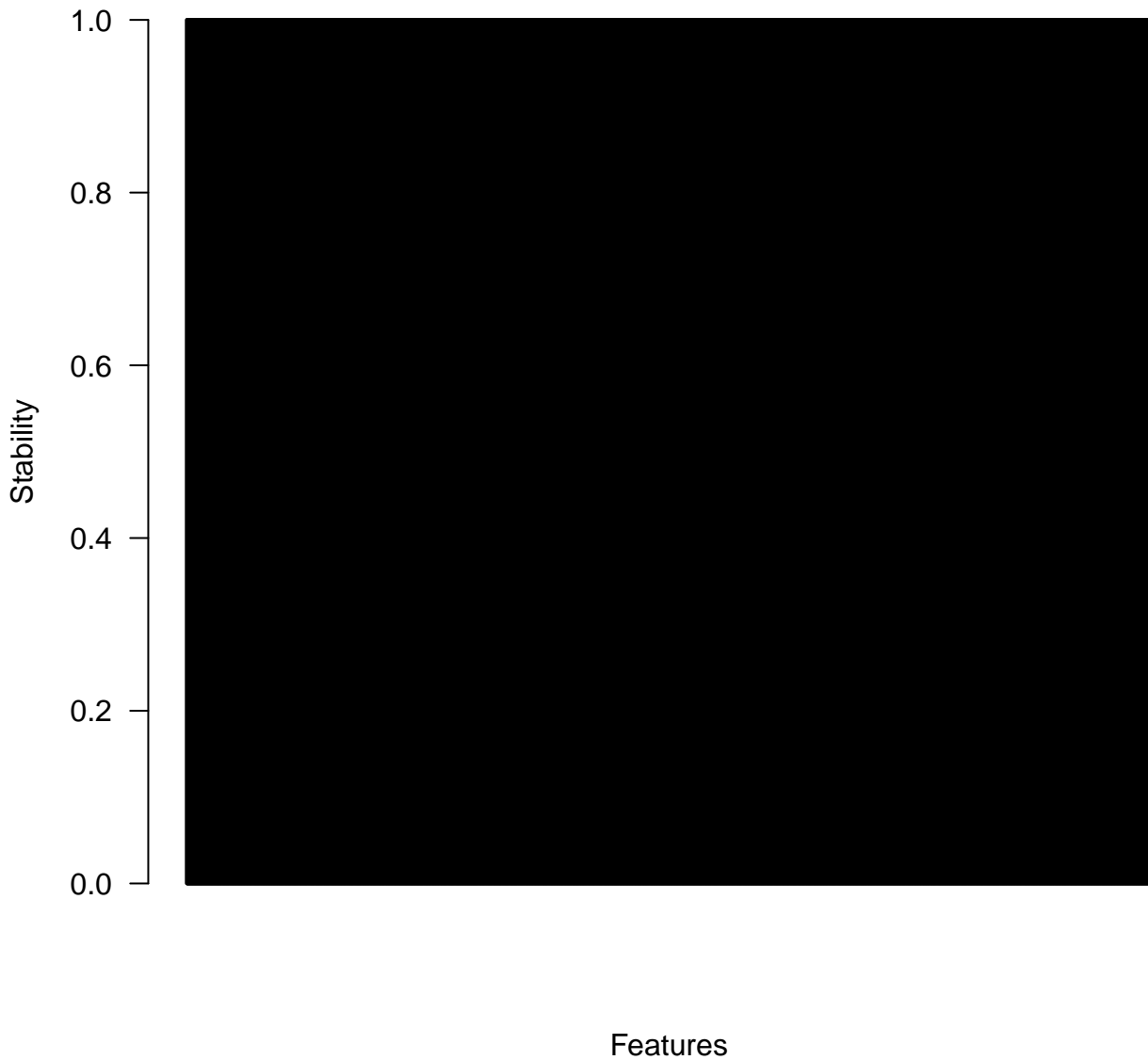
## Metabolomics Comp 2



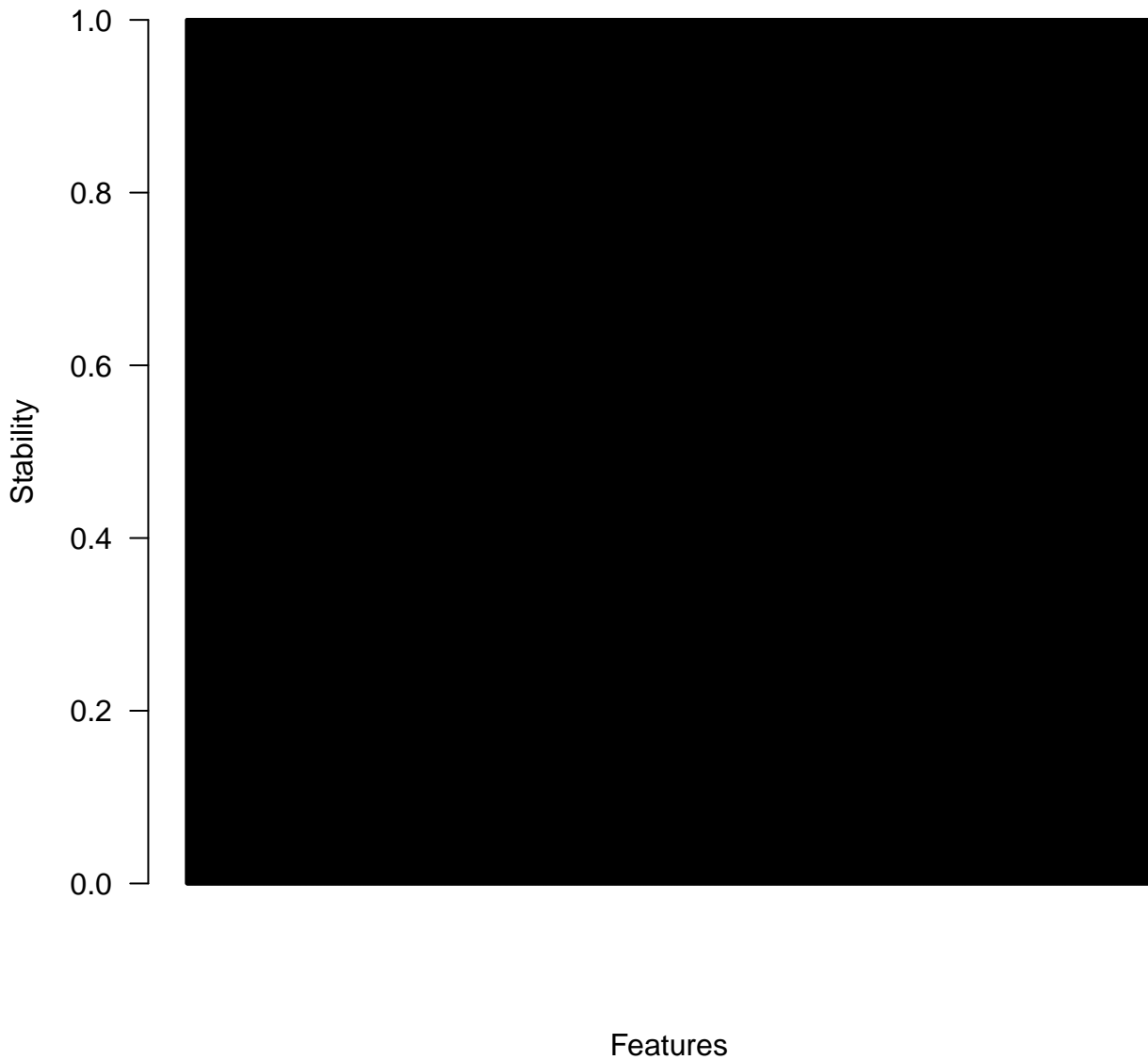
# Proteomics Comp 1



## Proteomics Comp 2

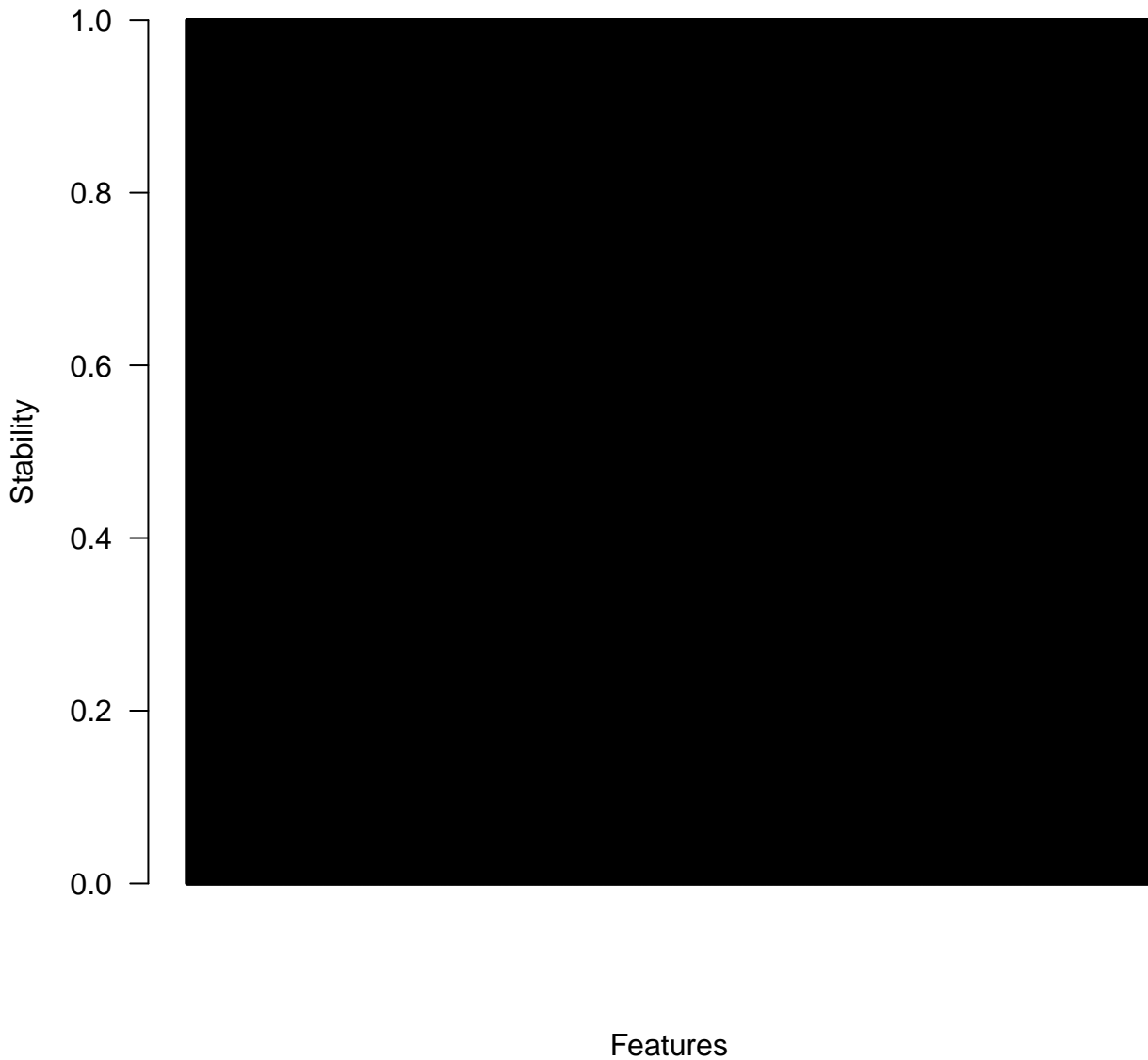


# RNA\_Seq Comp 1

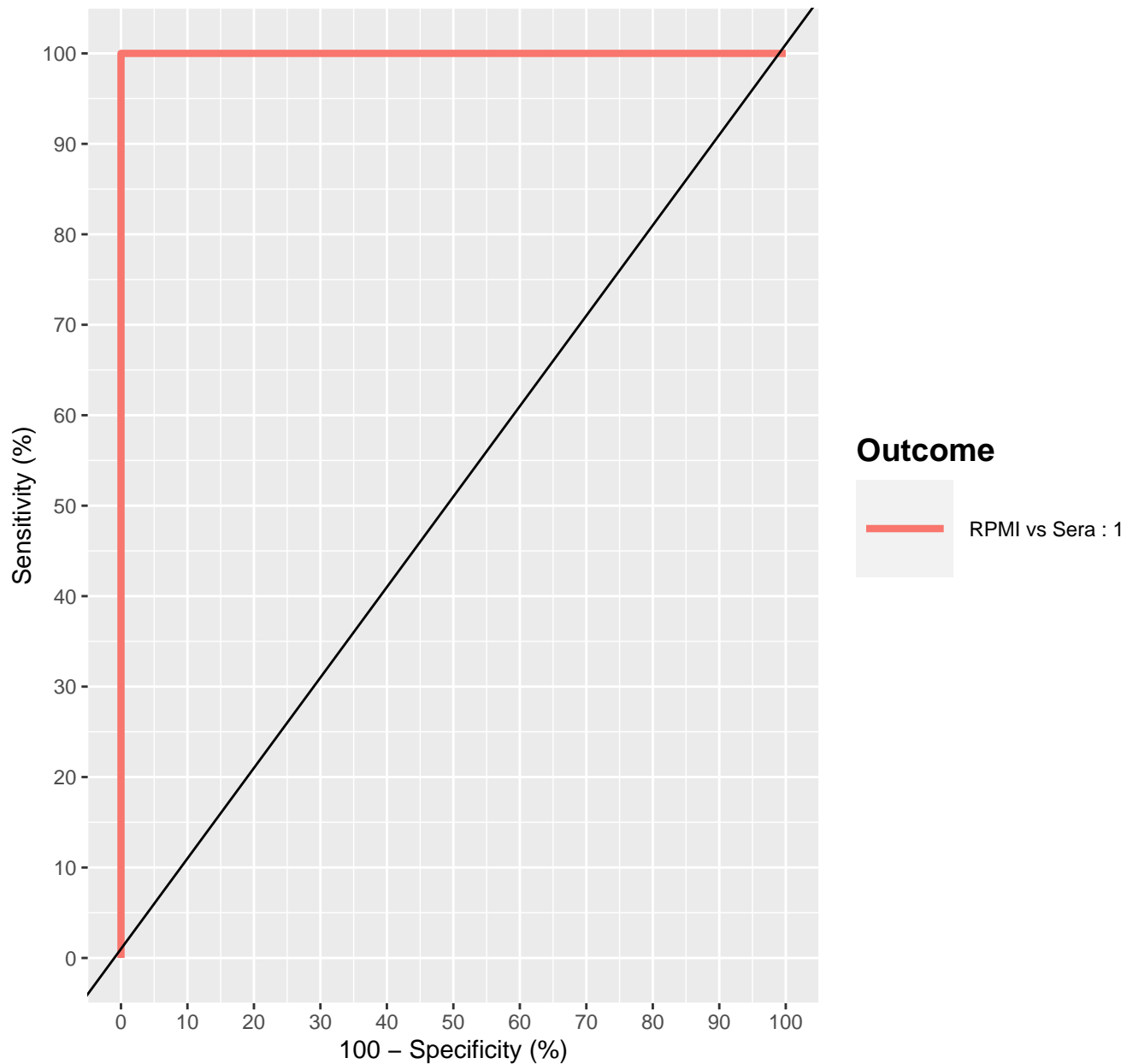


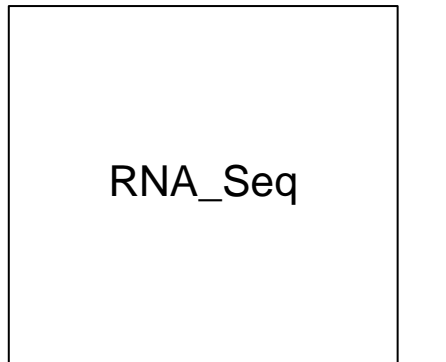
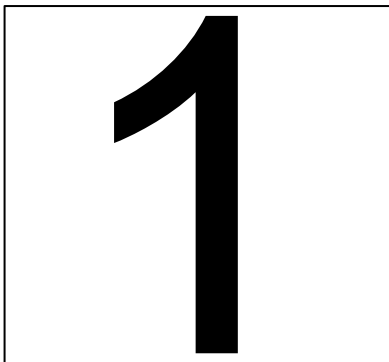
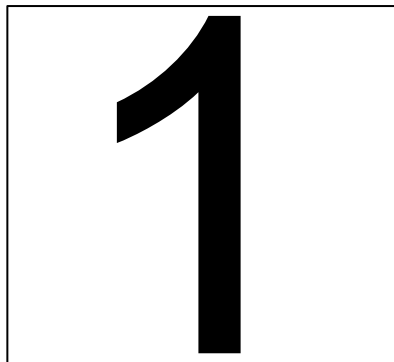
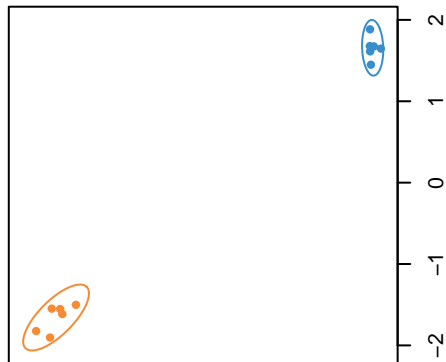
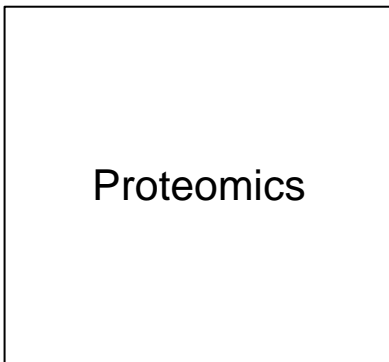
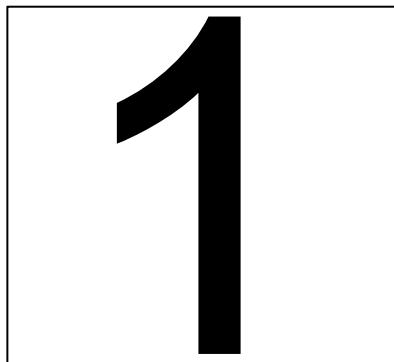
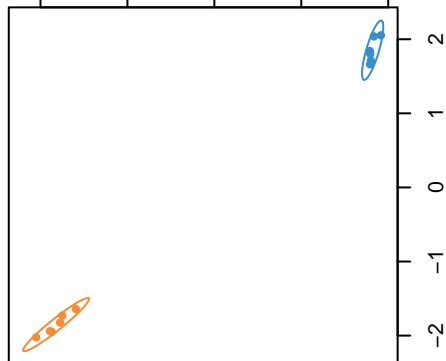
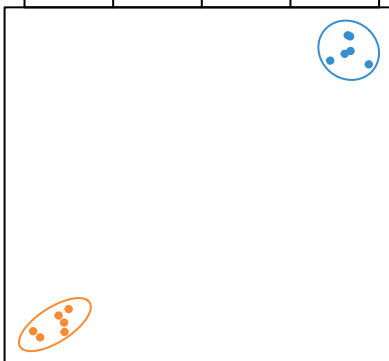
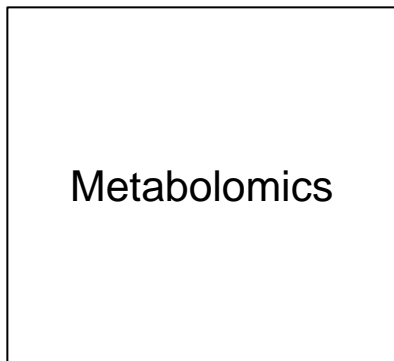


## RNA\_Seq Comp 2



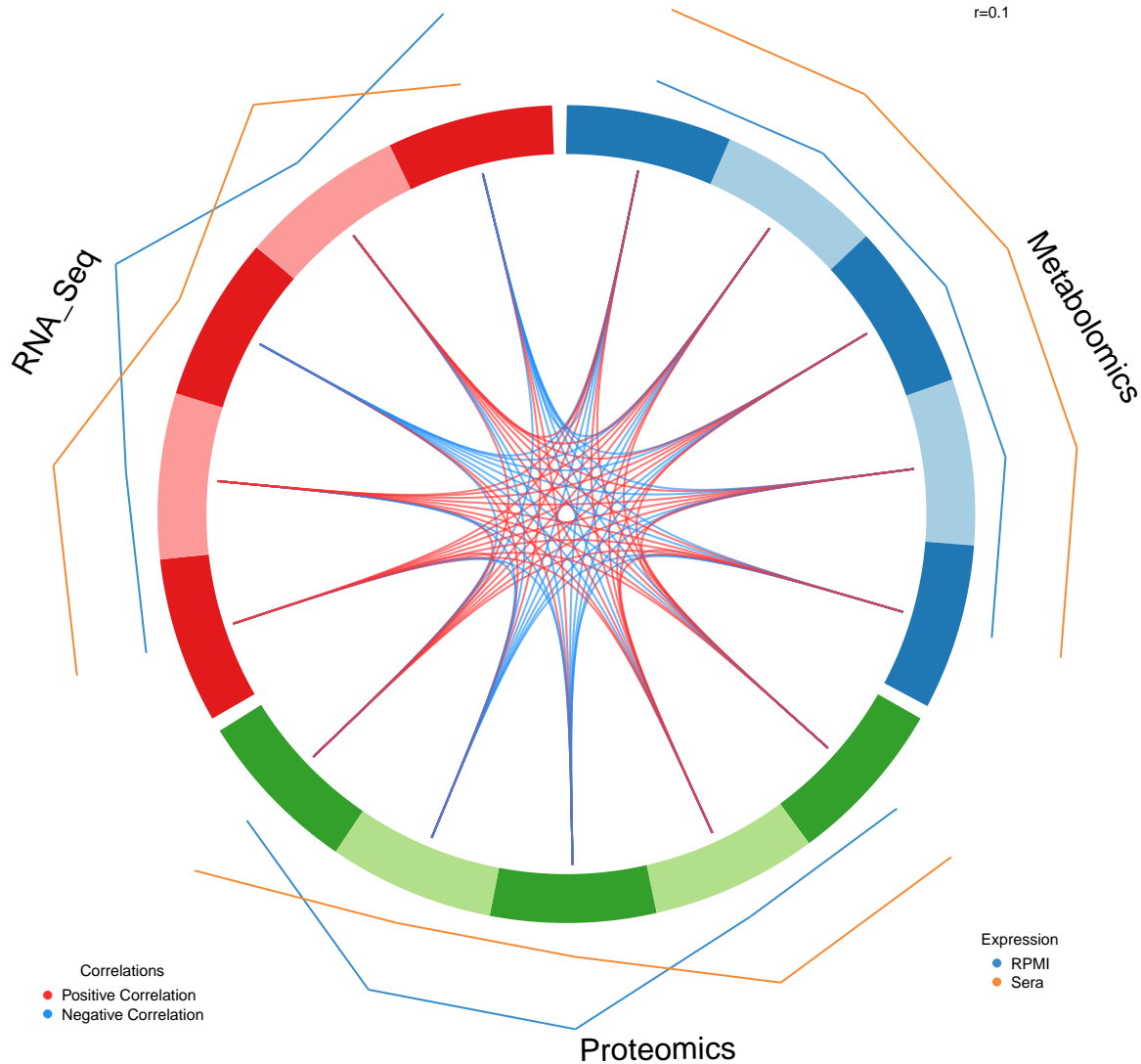
**ROC Curve**  
**Block: Metabolomics, comp: 1**





Comp 1

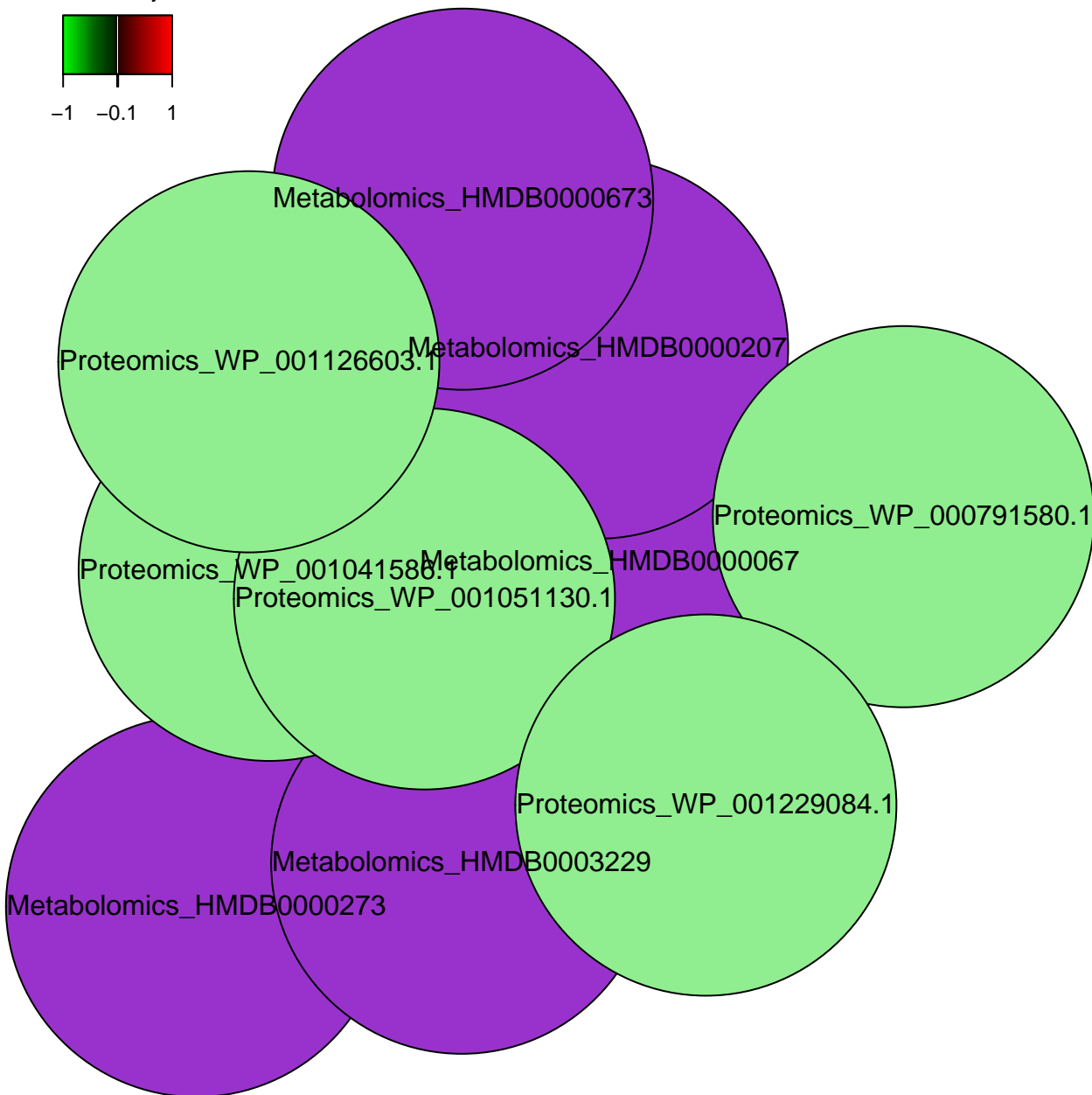
Correlation cut-off  
 $r=0.1$



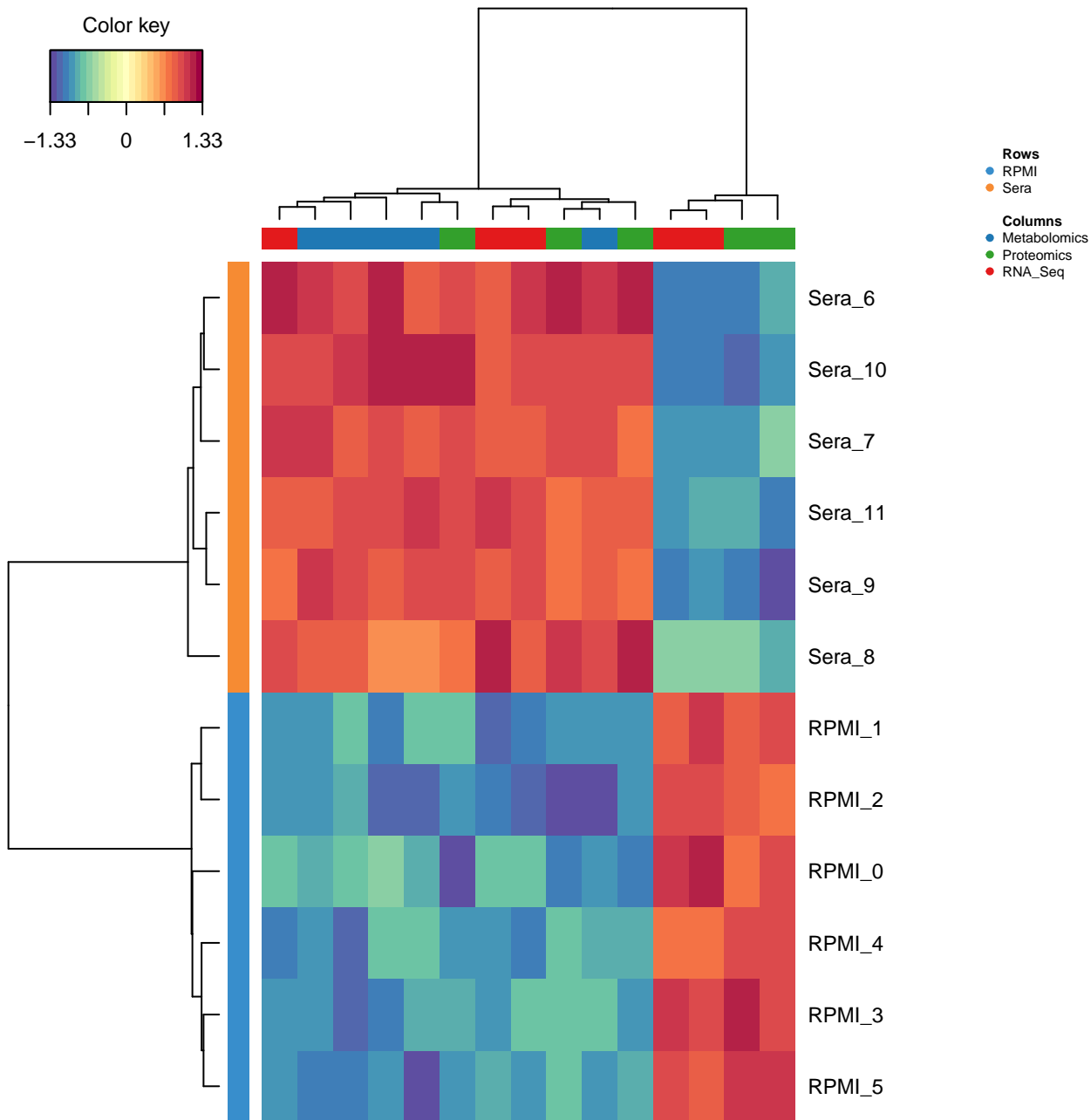
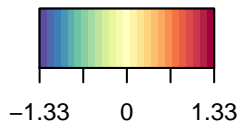
Color key



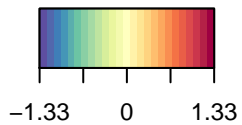
-1 -0.1 1



Color key



Color key

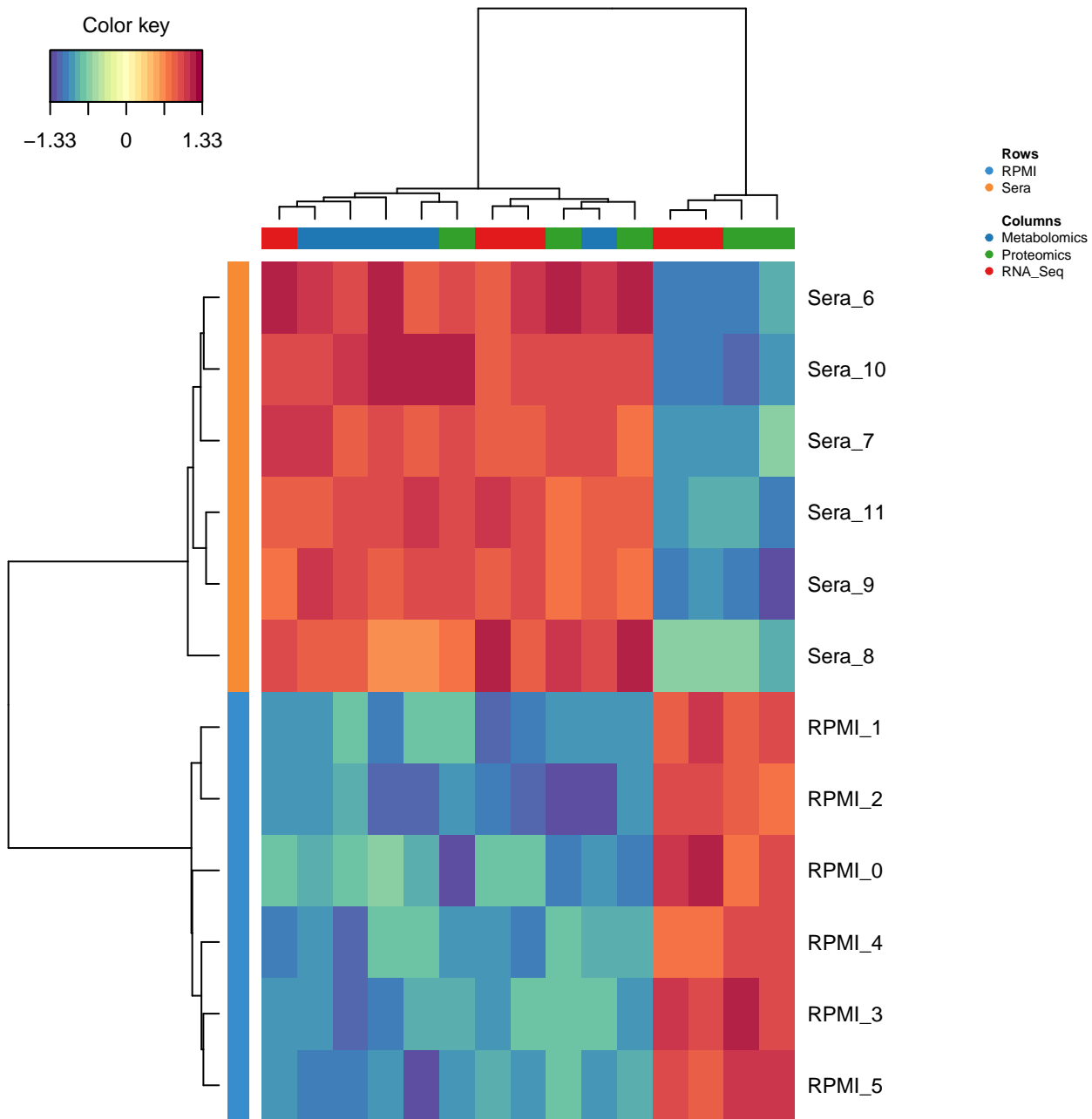


Rows

- RPMI
- Sera

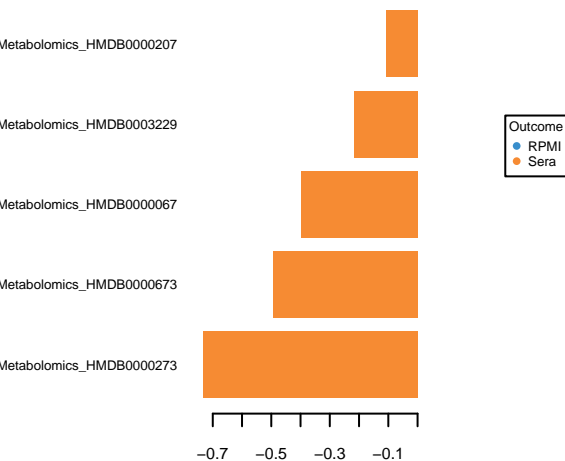
Columns

- Metabolomics
- Proteomics
- RNA\_Seq

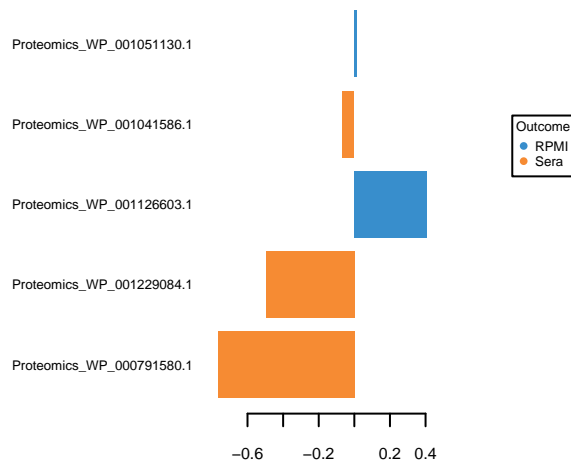


# 1 DIABLO max loadings

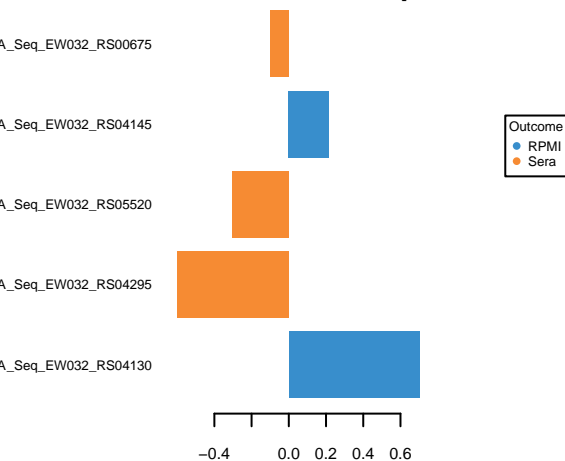
Contribution on comp 1  
Block 'Metabolomics'



Contribution on comp 1  
Block 'Proteomics'



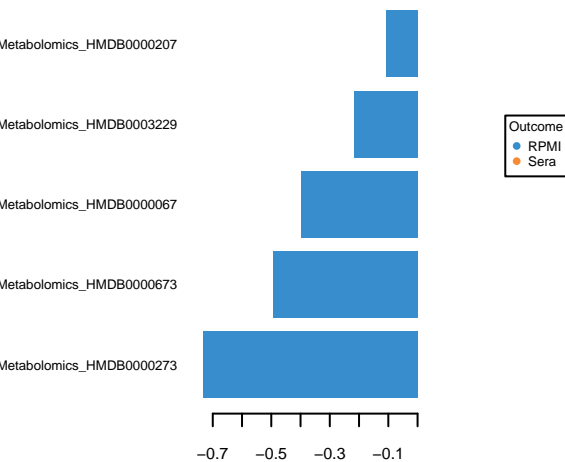
Contribution on comp 1  
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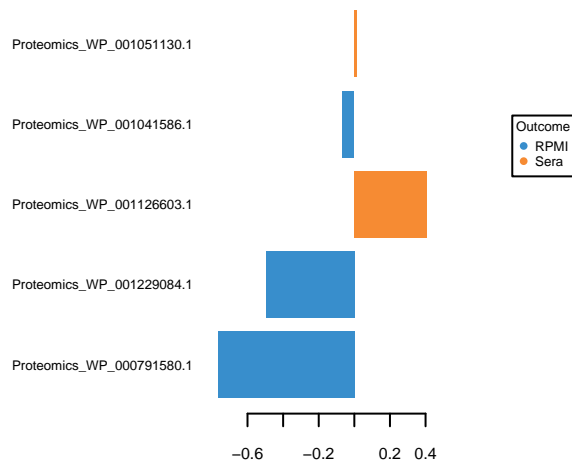


# 1 DIABLO min loadings

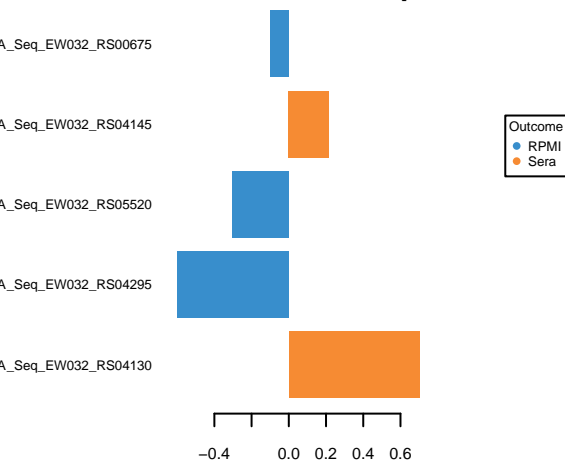
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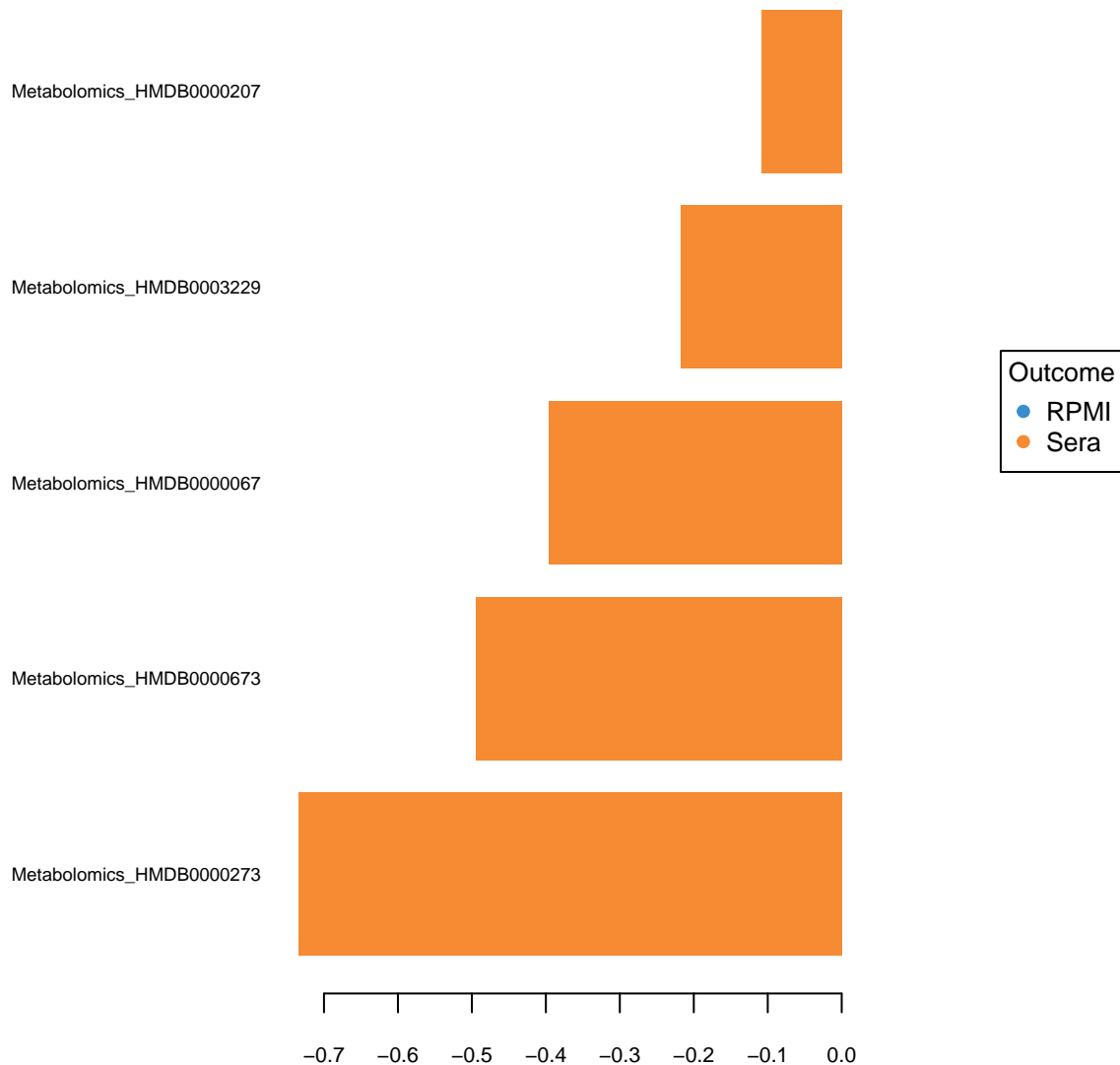
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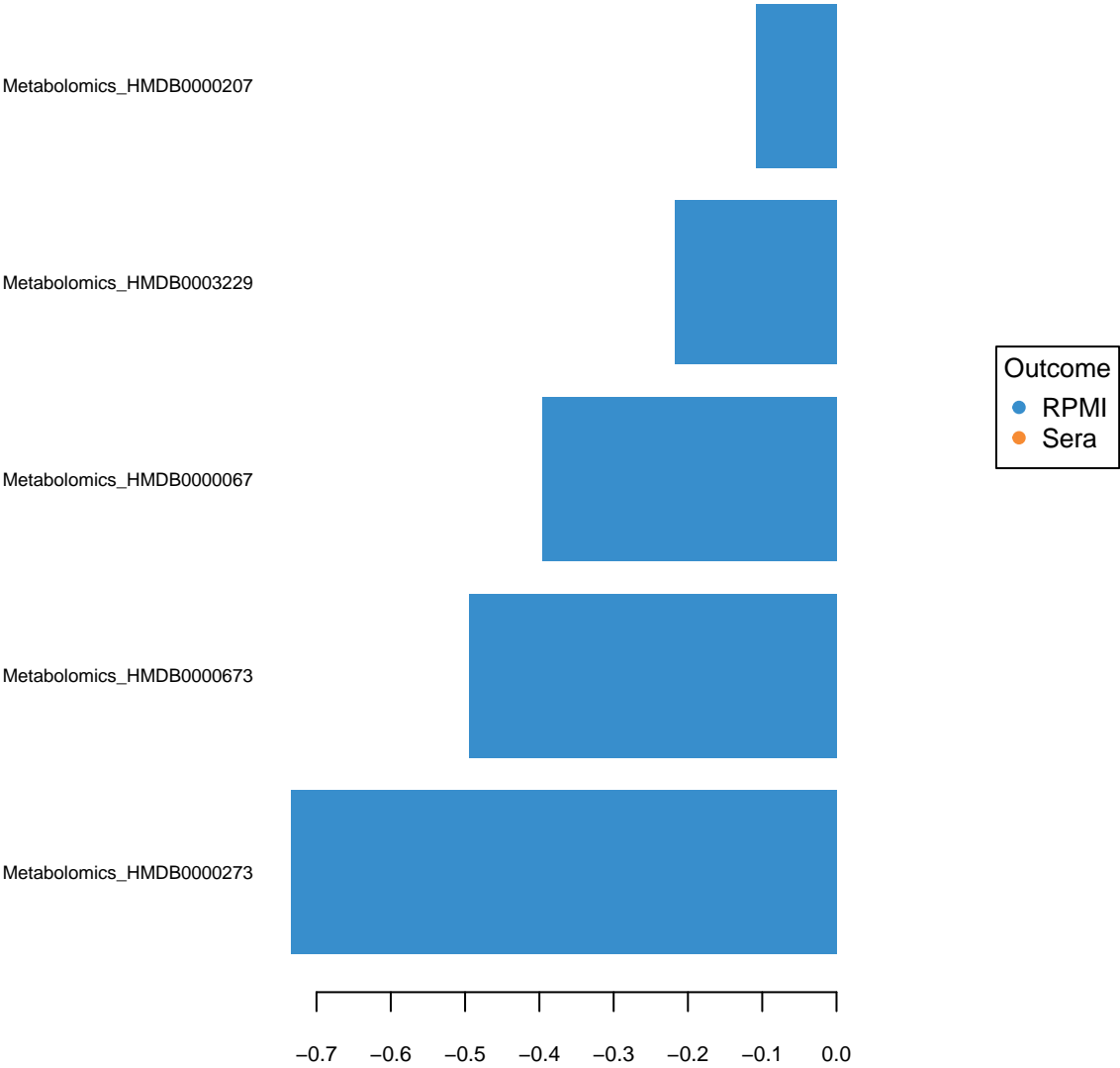
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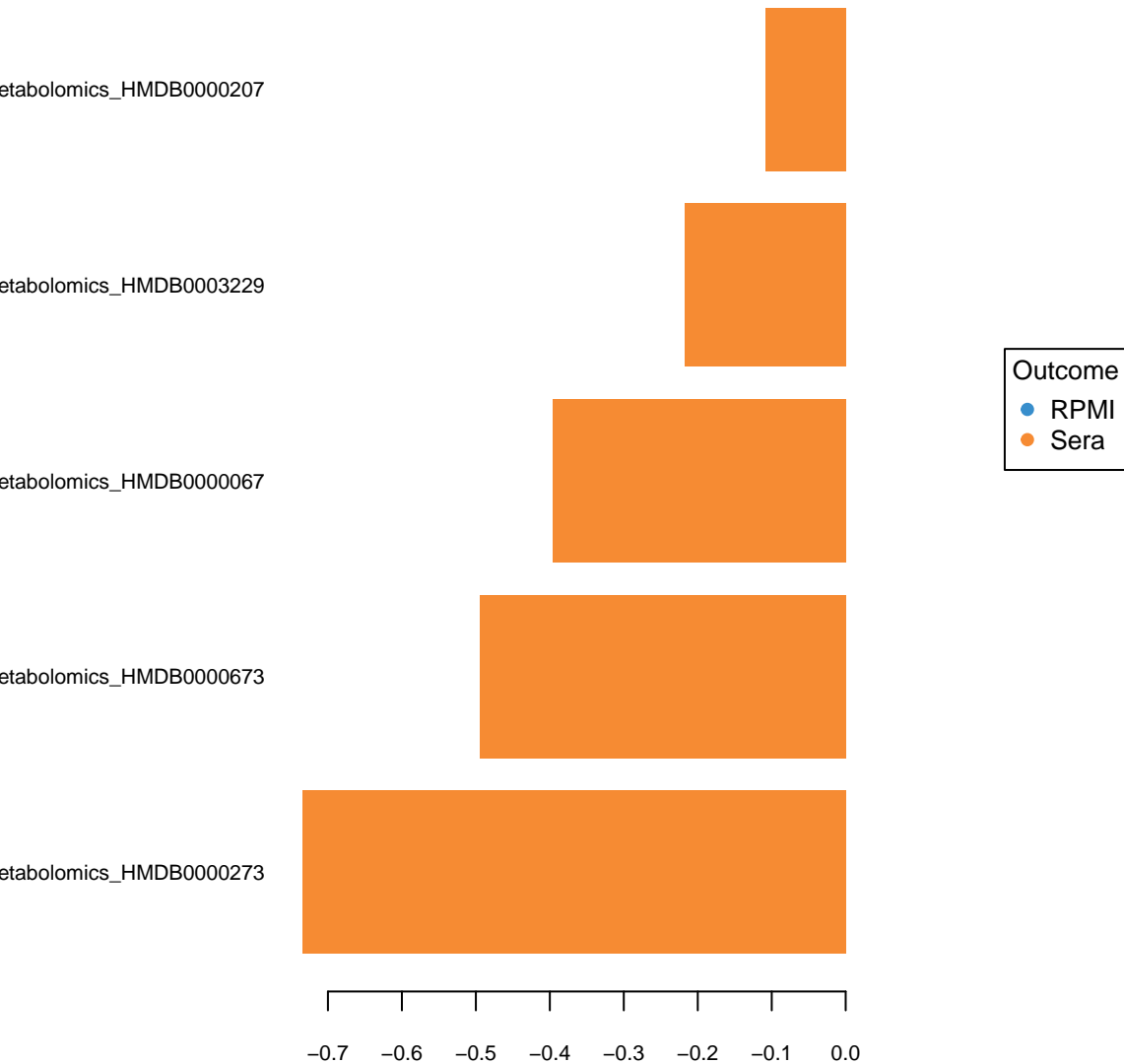
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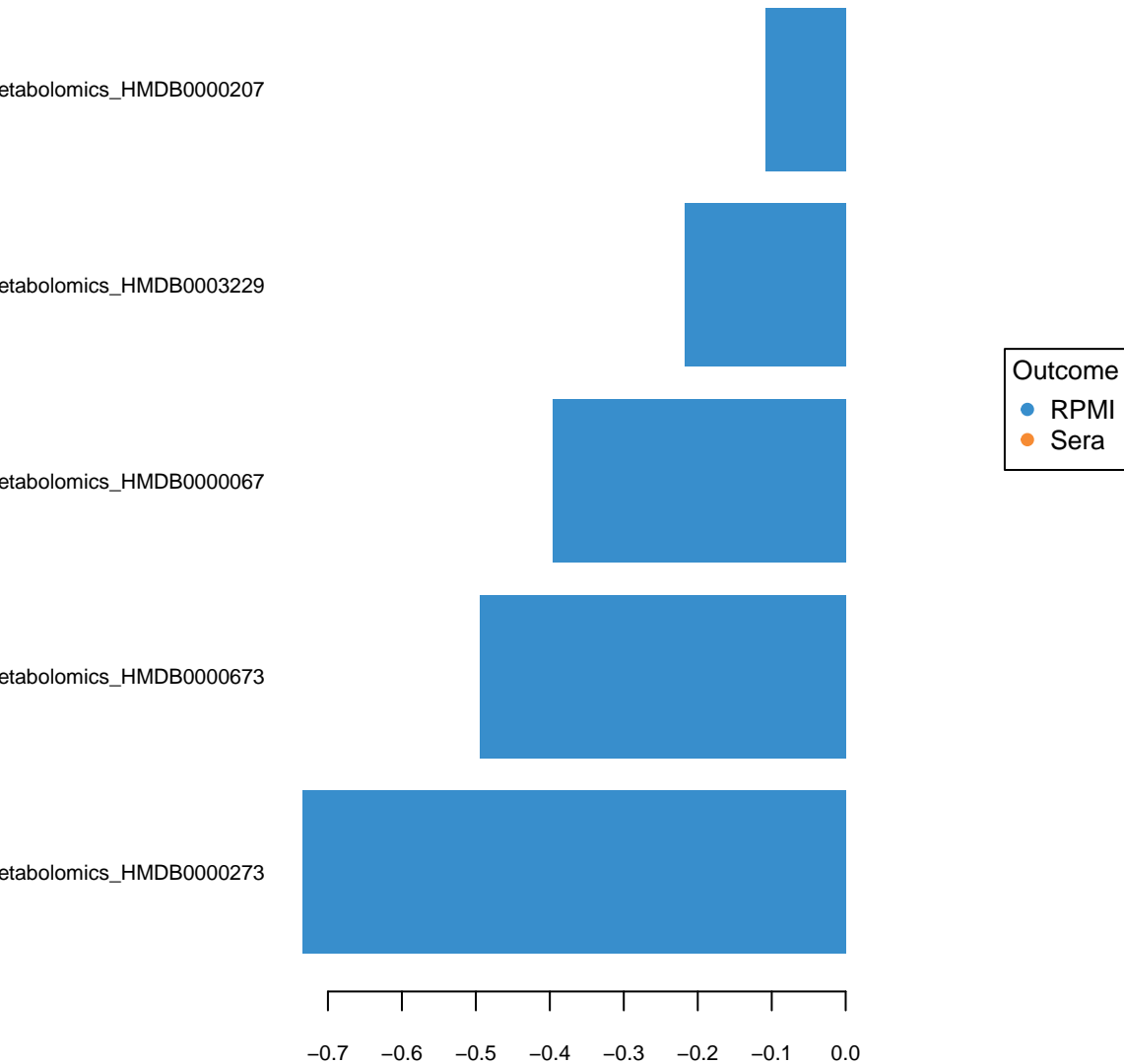
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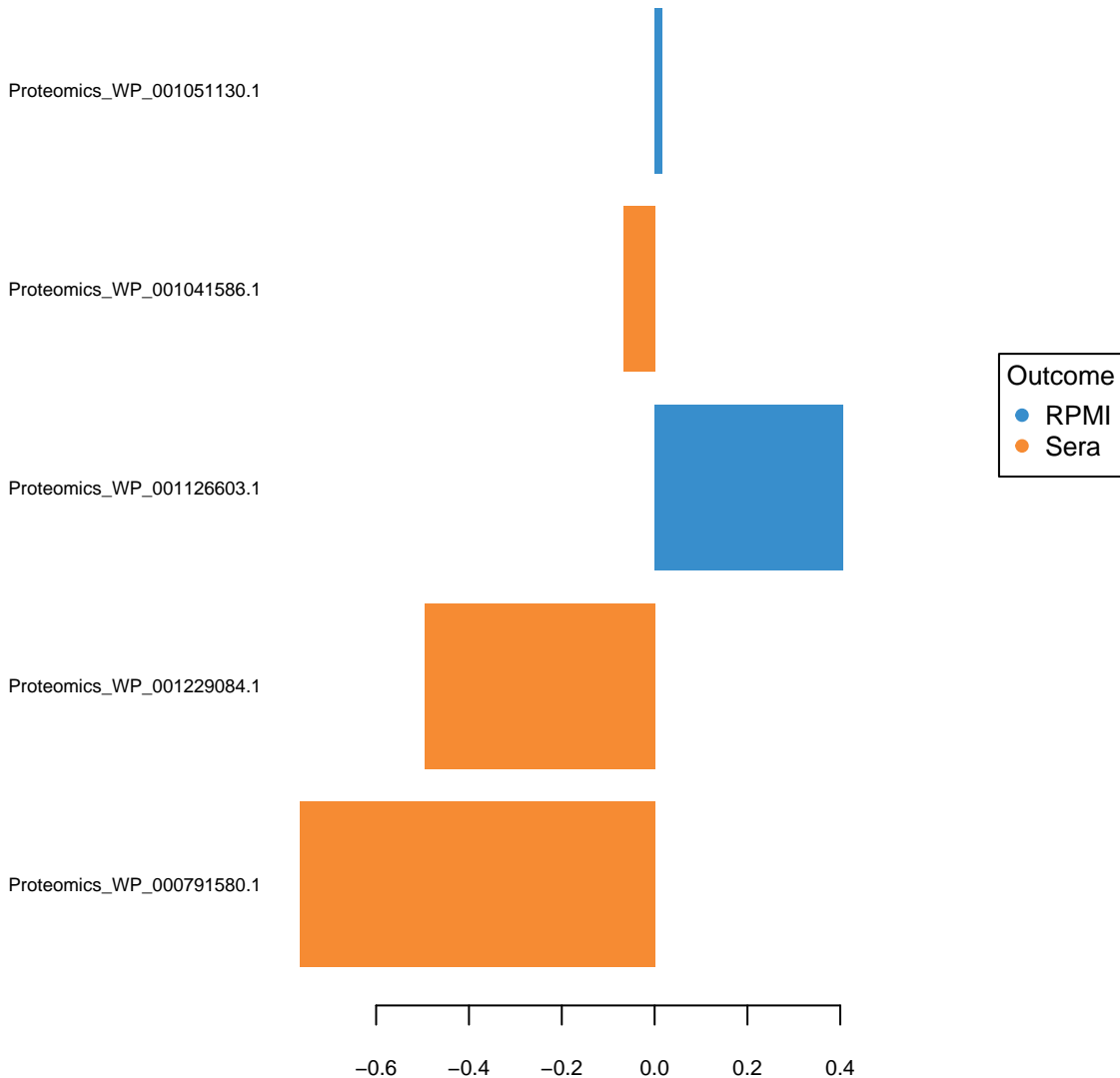
# Contribution on comp 1



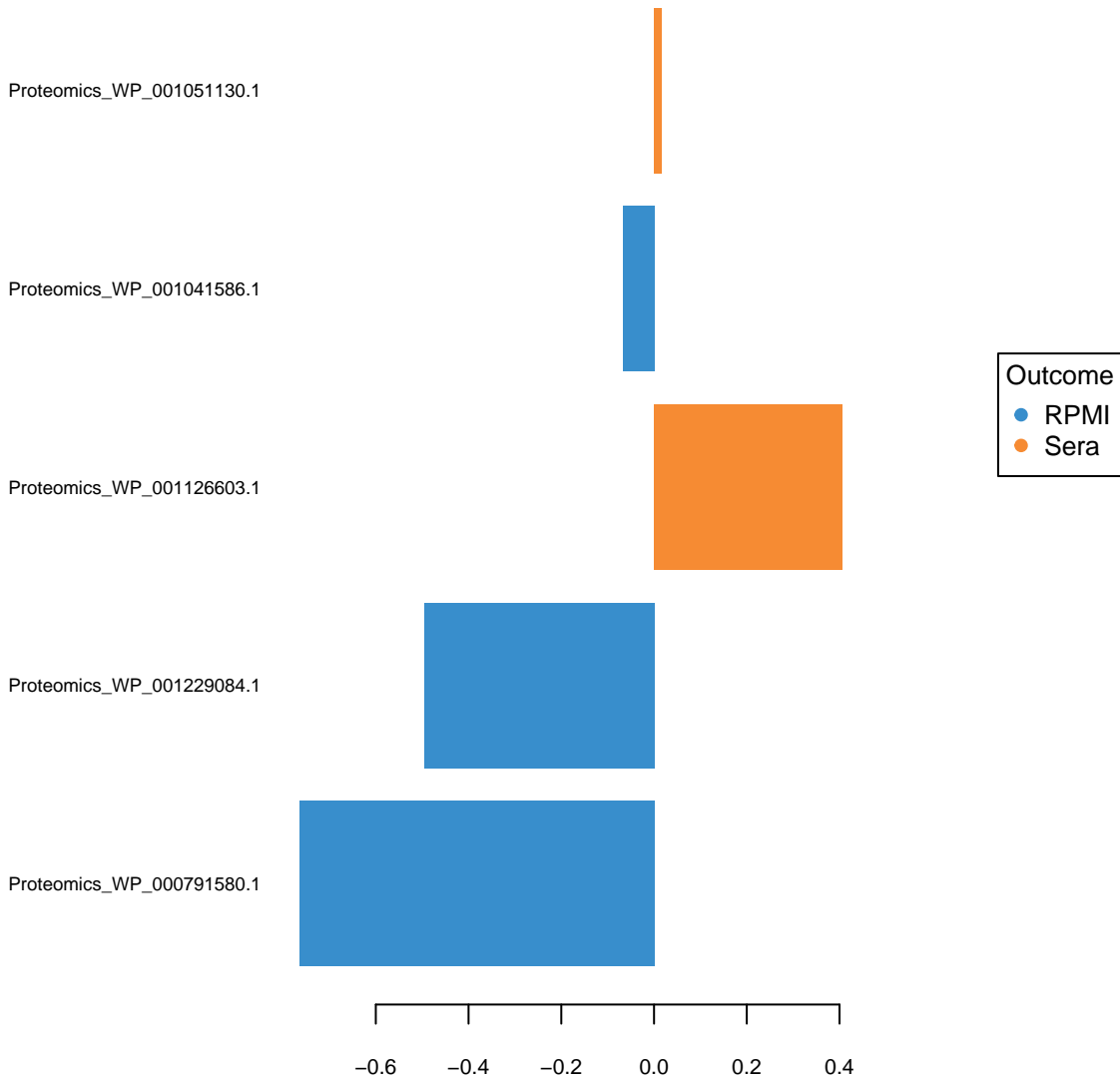
# Contribution on comp 1



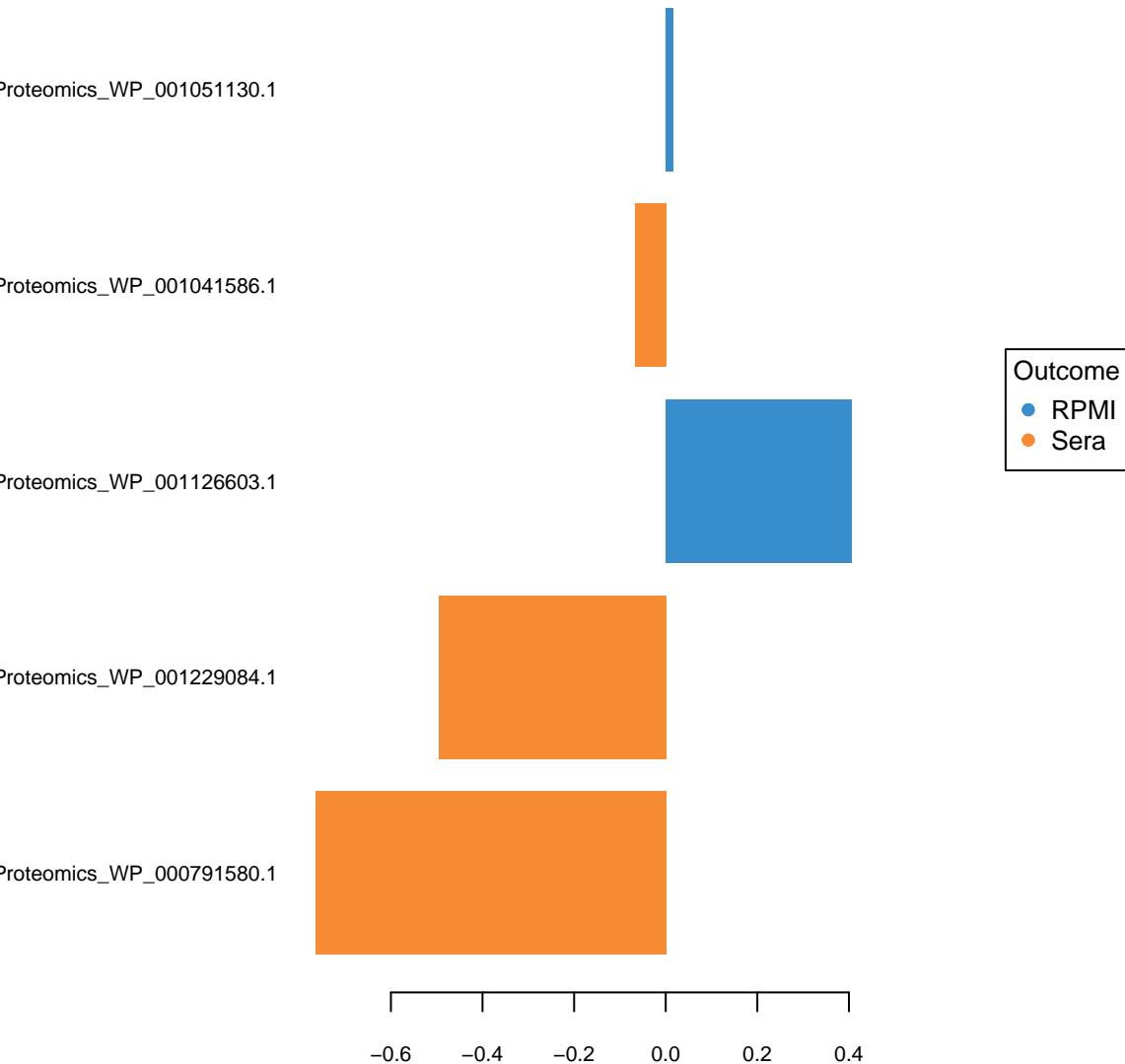
# 1 Proteomics DIABLO max load



# 1 Proteomics DIABLO min load

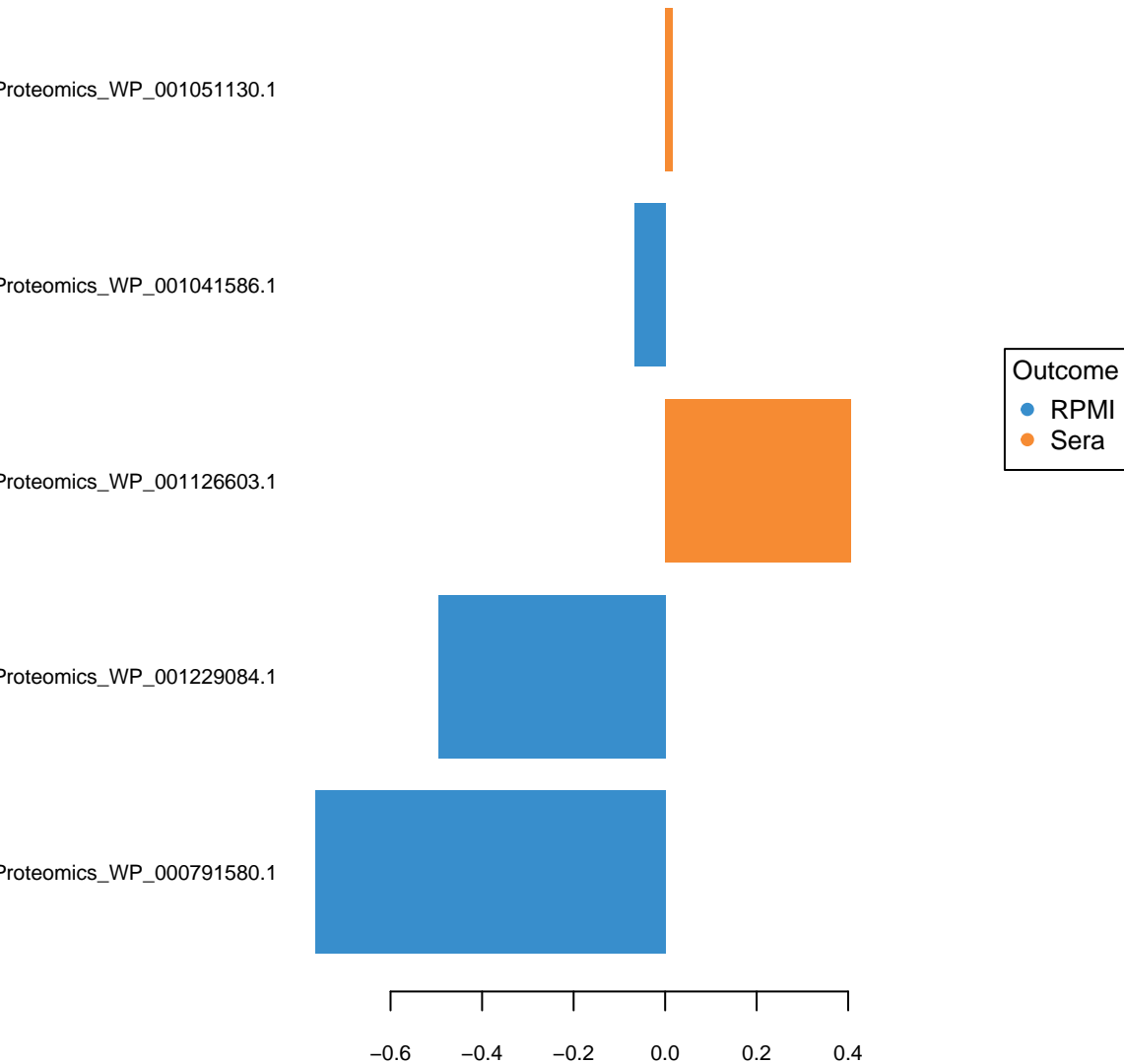


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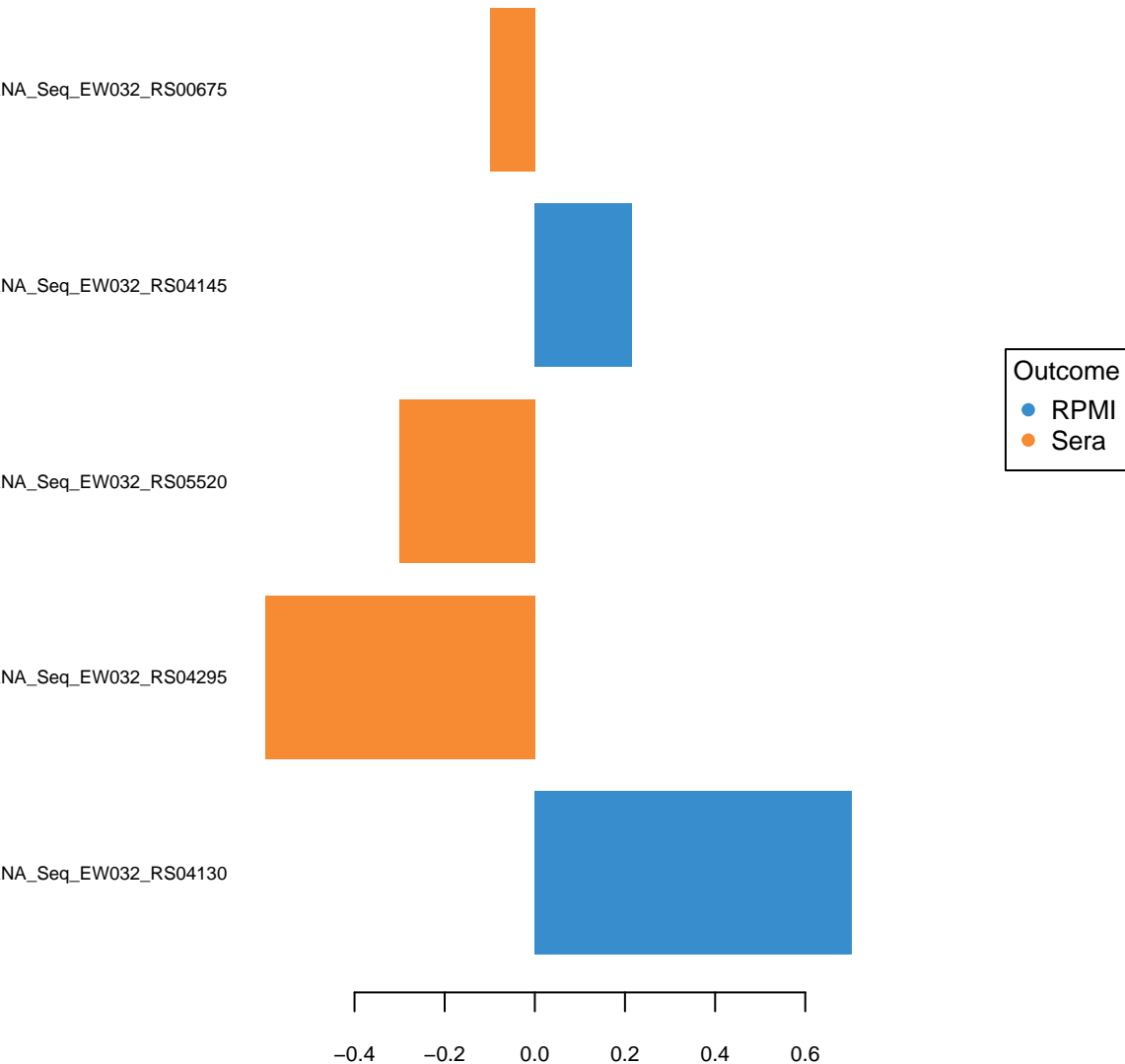




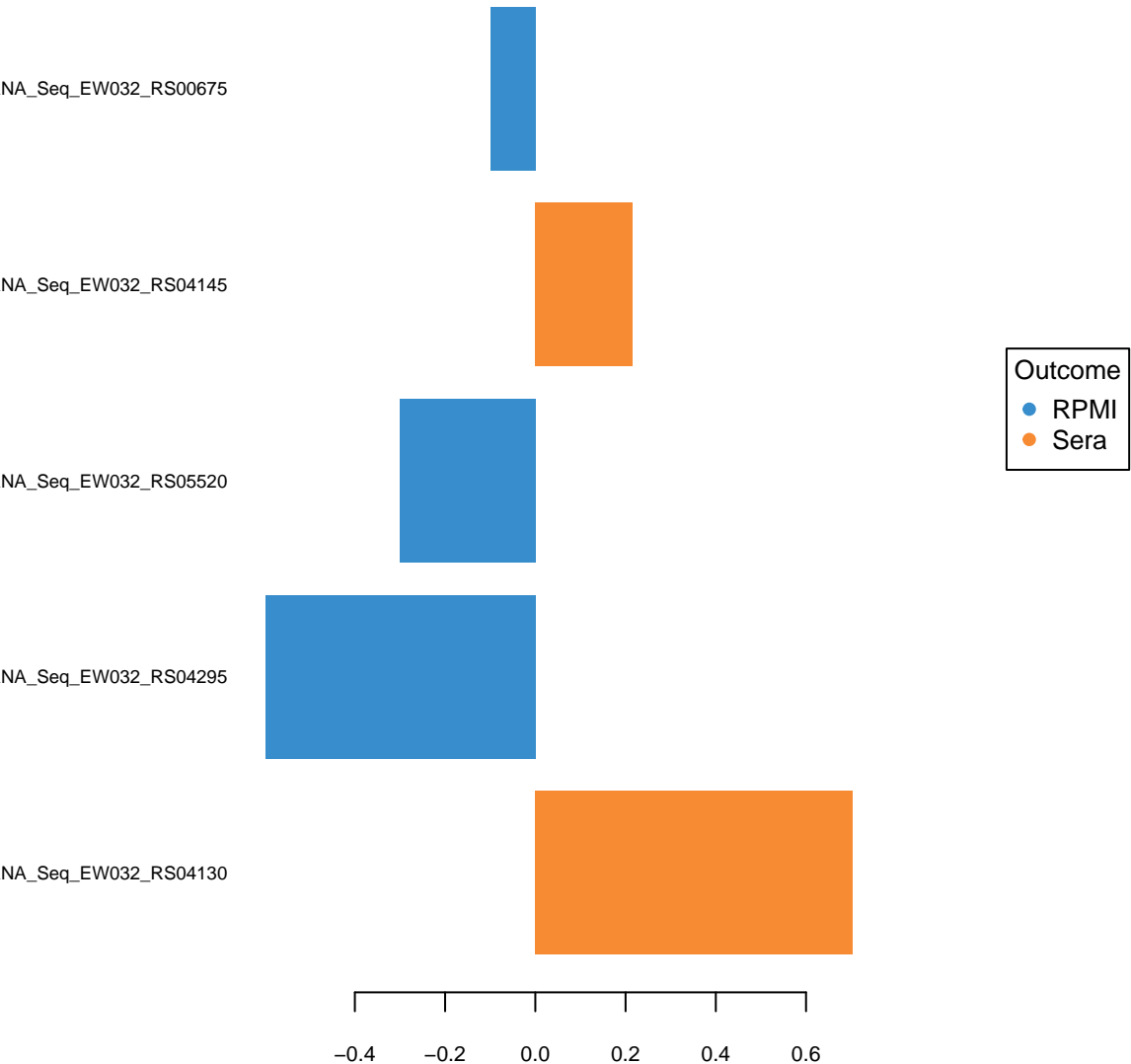
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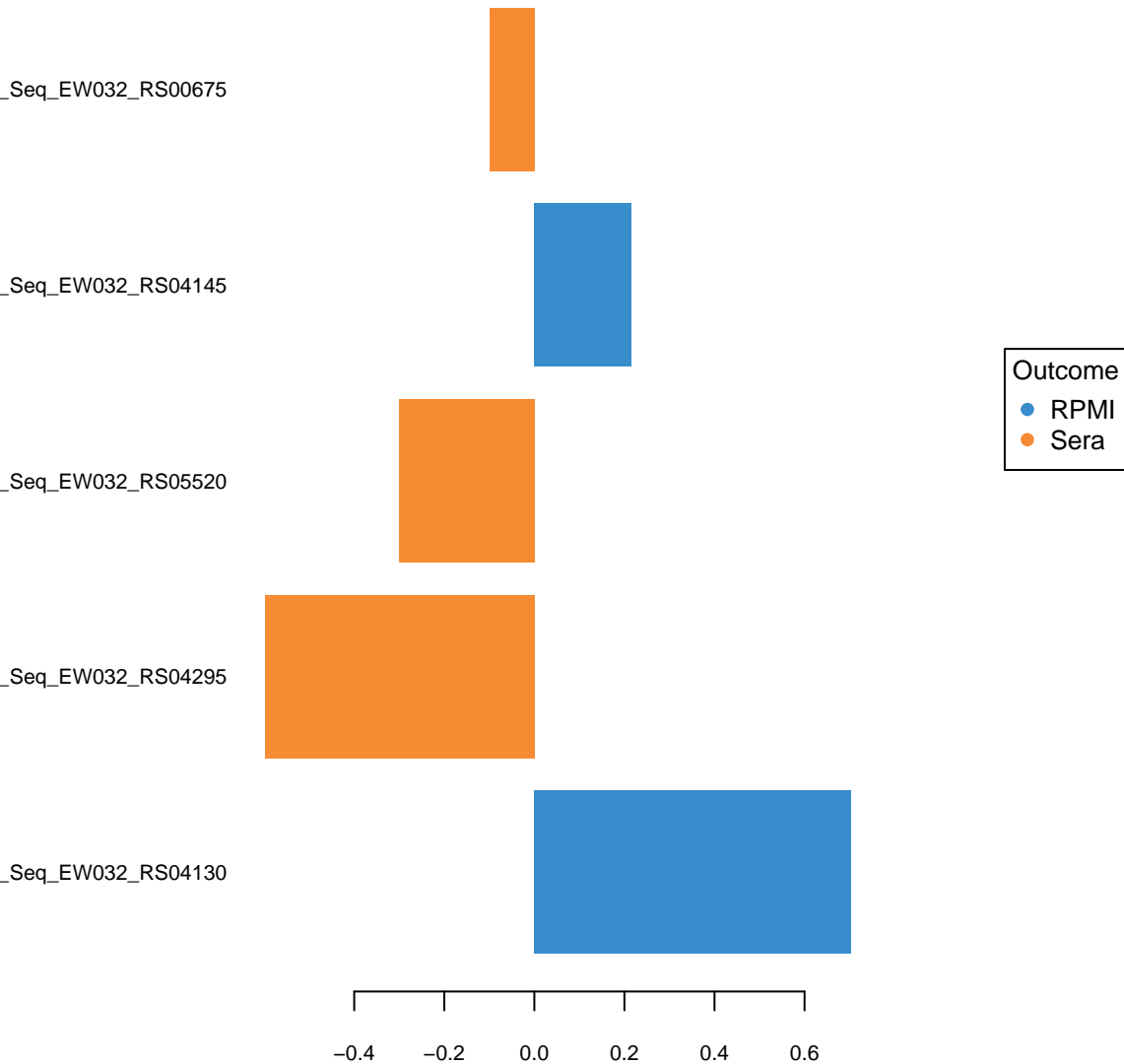
# 1 RNA\_Seq DIABLO max load



# 1 RNA\_Seq DIABLO min load



# Contribution on comp 1



# Contribution on comp 1

