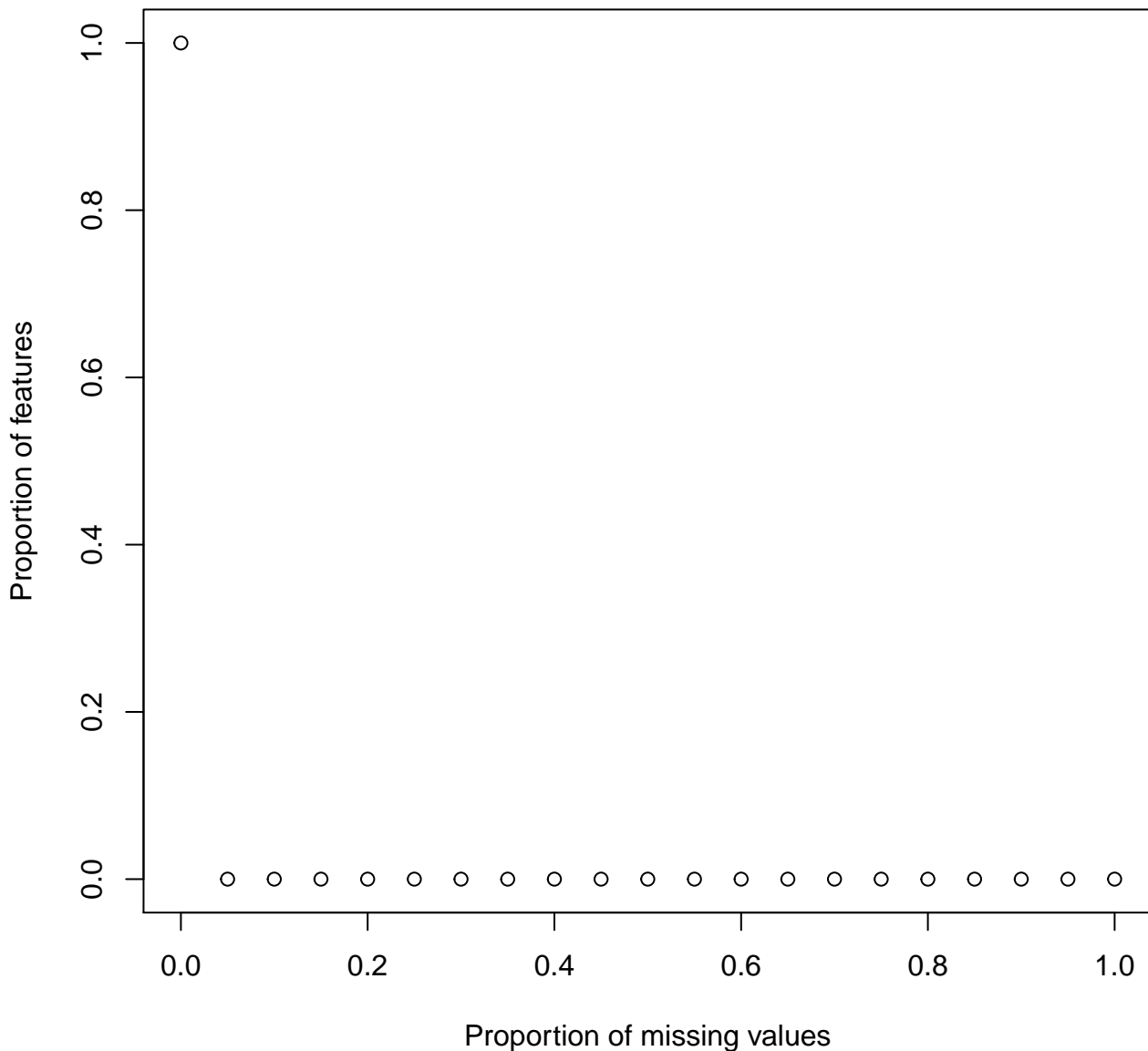
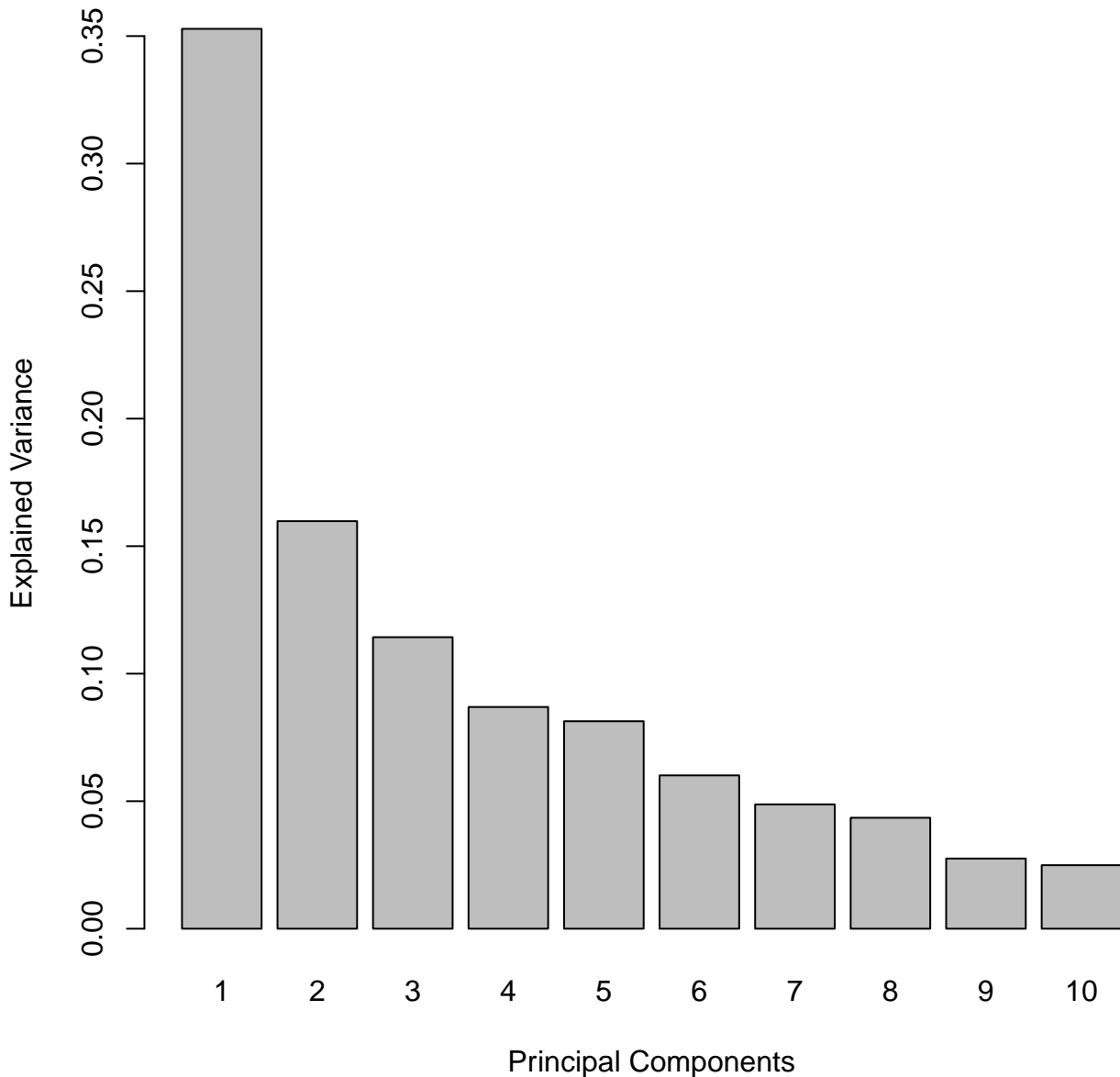


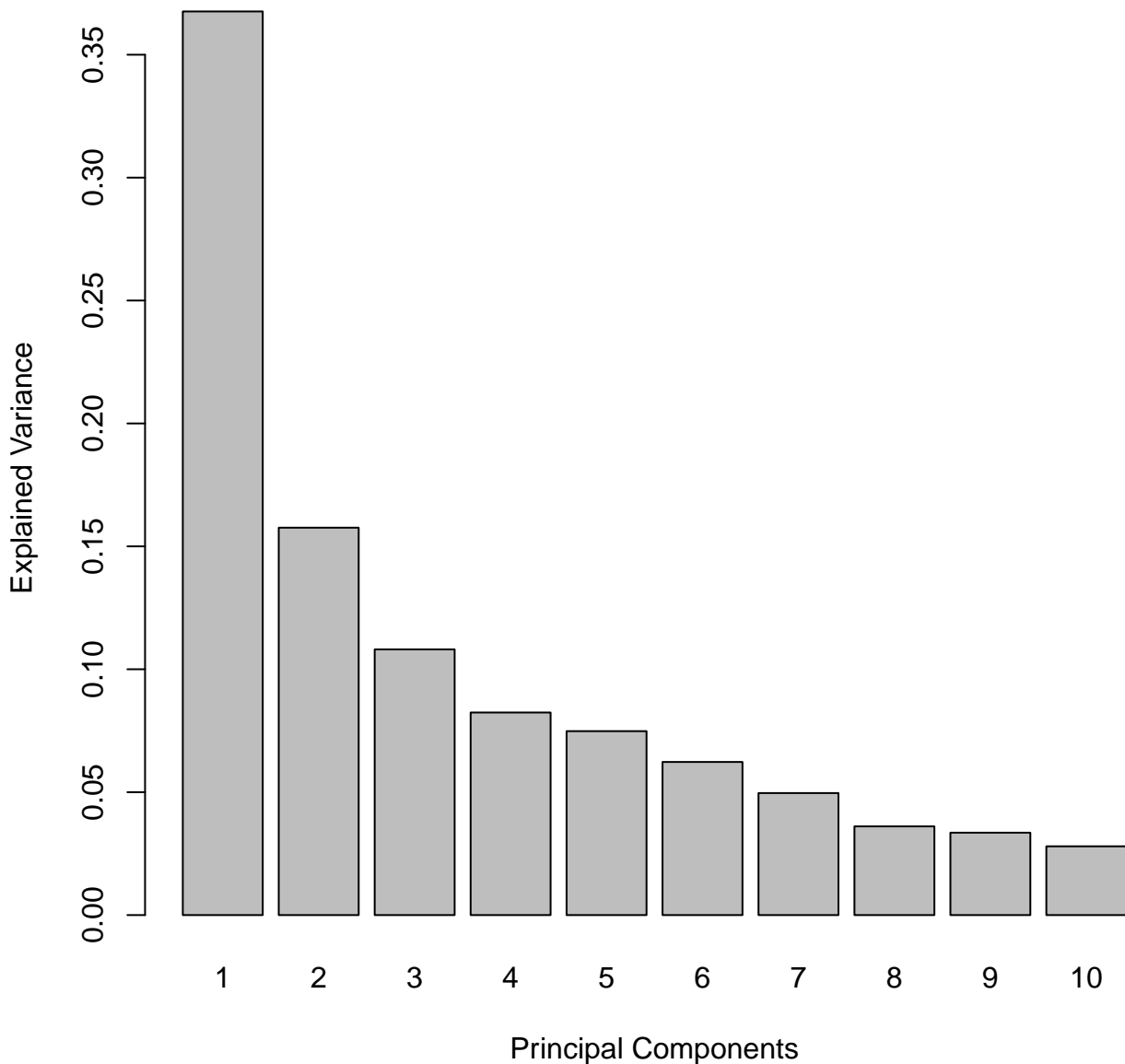
RNA_Seq missing value proportions for unfiltered data



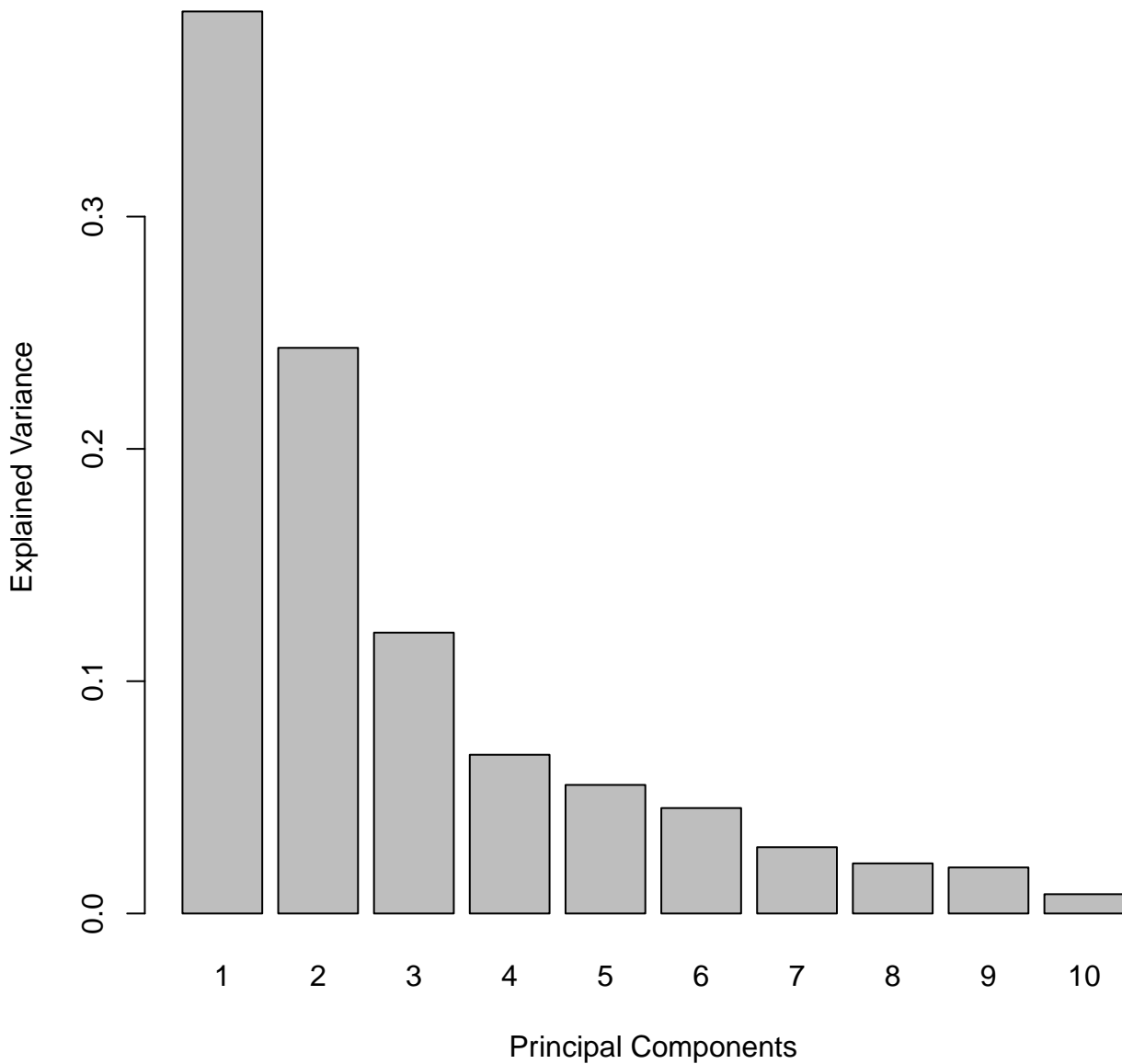
Metabolomics screeplot



Proteomics screeplot



RNA_Seq screeplot



**No Impute n_PCs = 10
Metabolomics PCs (1,2)**

PC2: 16% expl. var

PC1: 35% expl. var

Class

○ RPMI
△ Sera

10

5

0

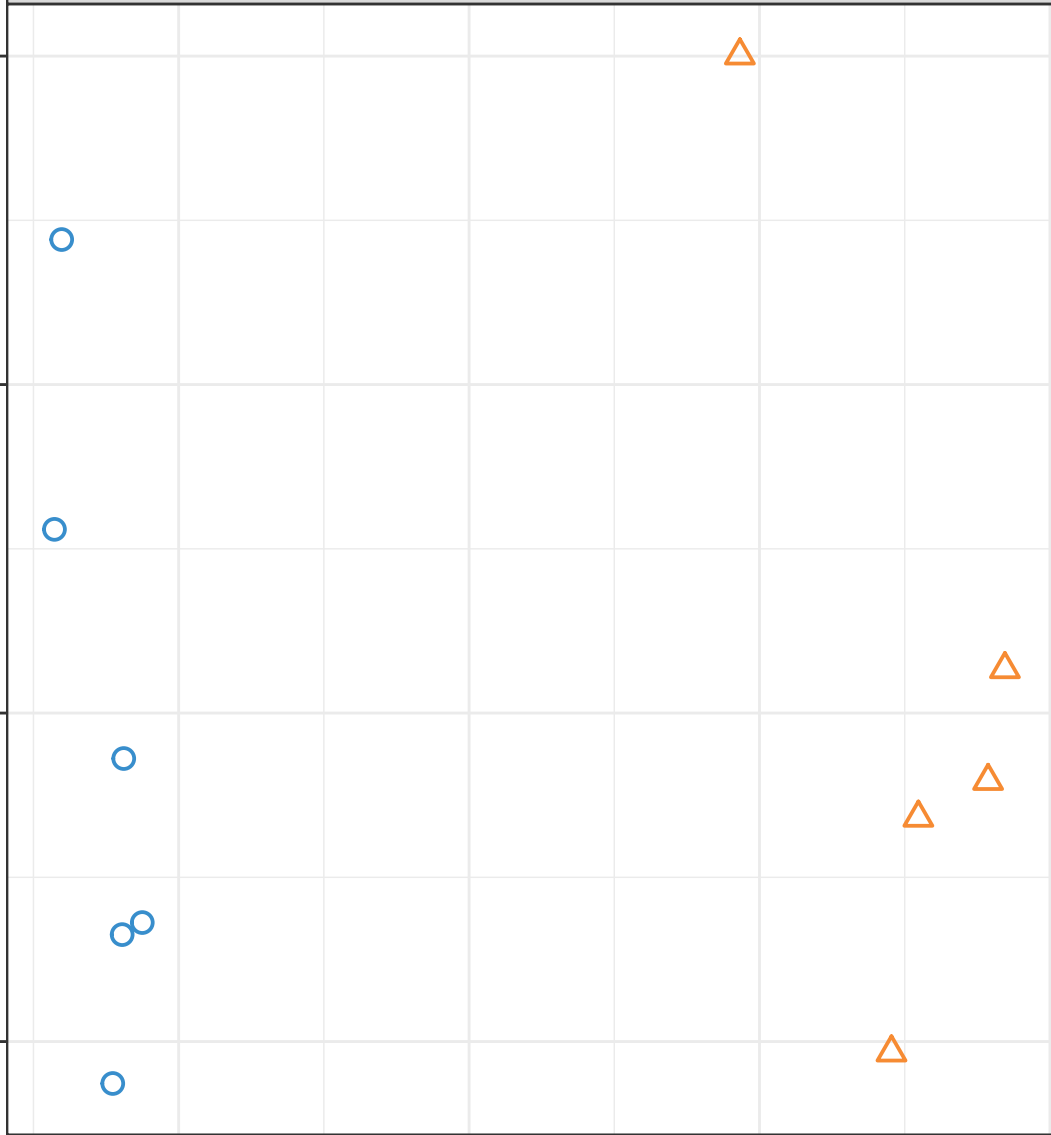
-5

-5

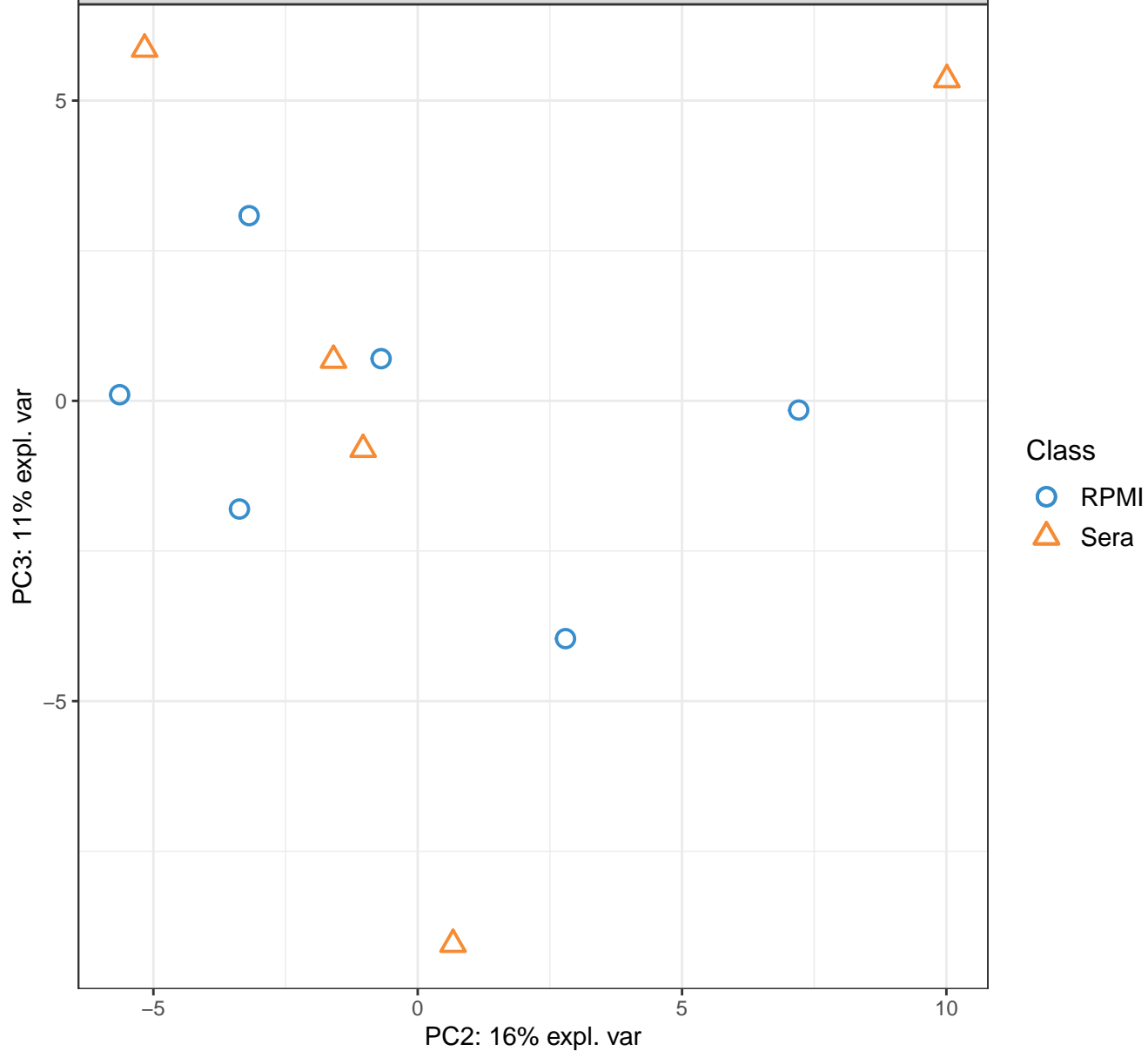
0

5

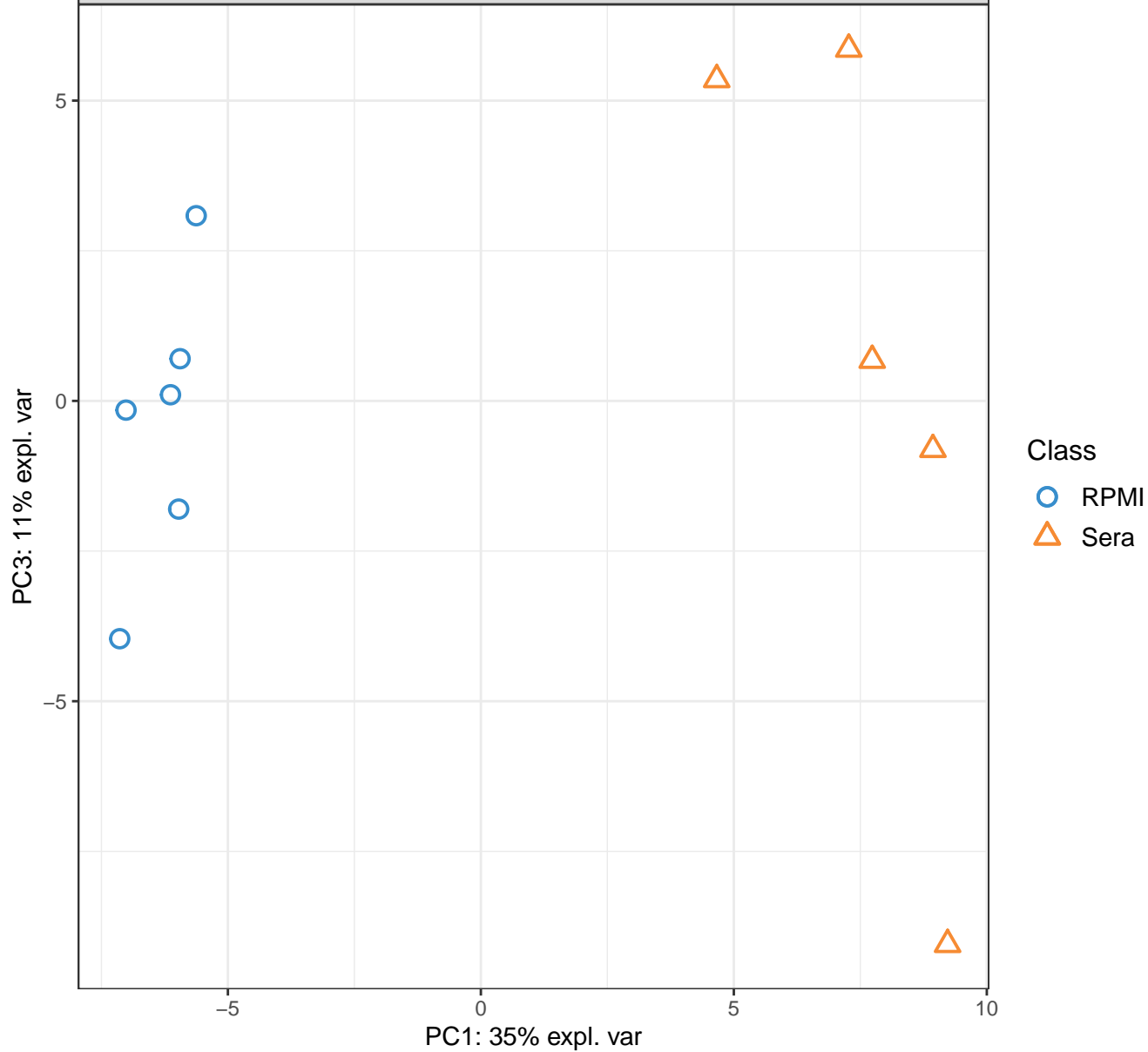
10



No Impute n_PCs = 10
Metabolomics PCs (2,3)



No Impute n_PCs = 10
Metabolomics PCs (1,3)



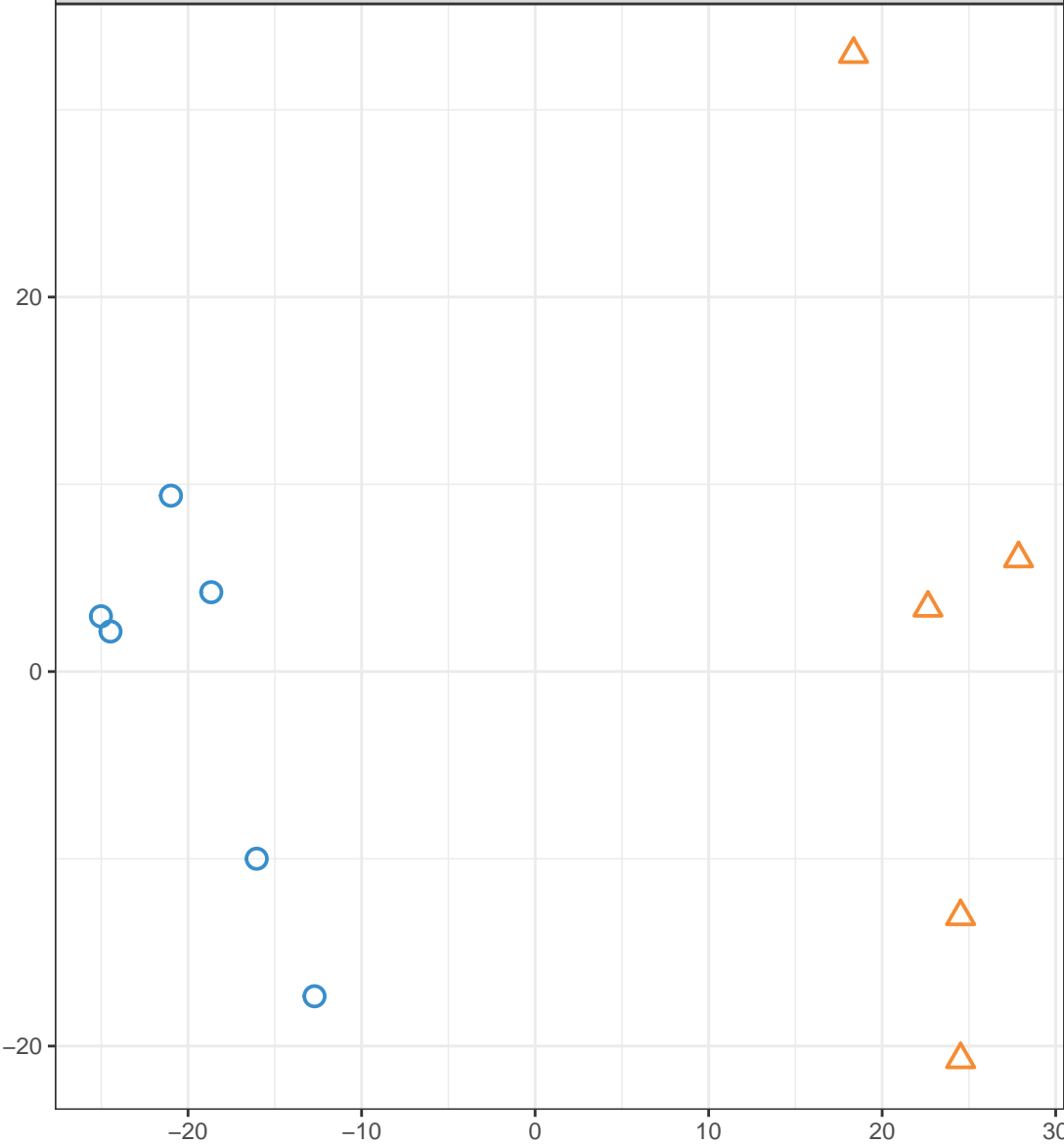
No Impute n_PCs = 10
Proteomics PCs (1,2)

PC2: 16% expl. var

PC1: 37% expl. var

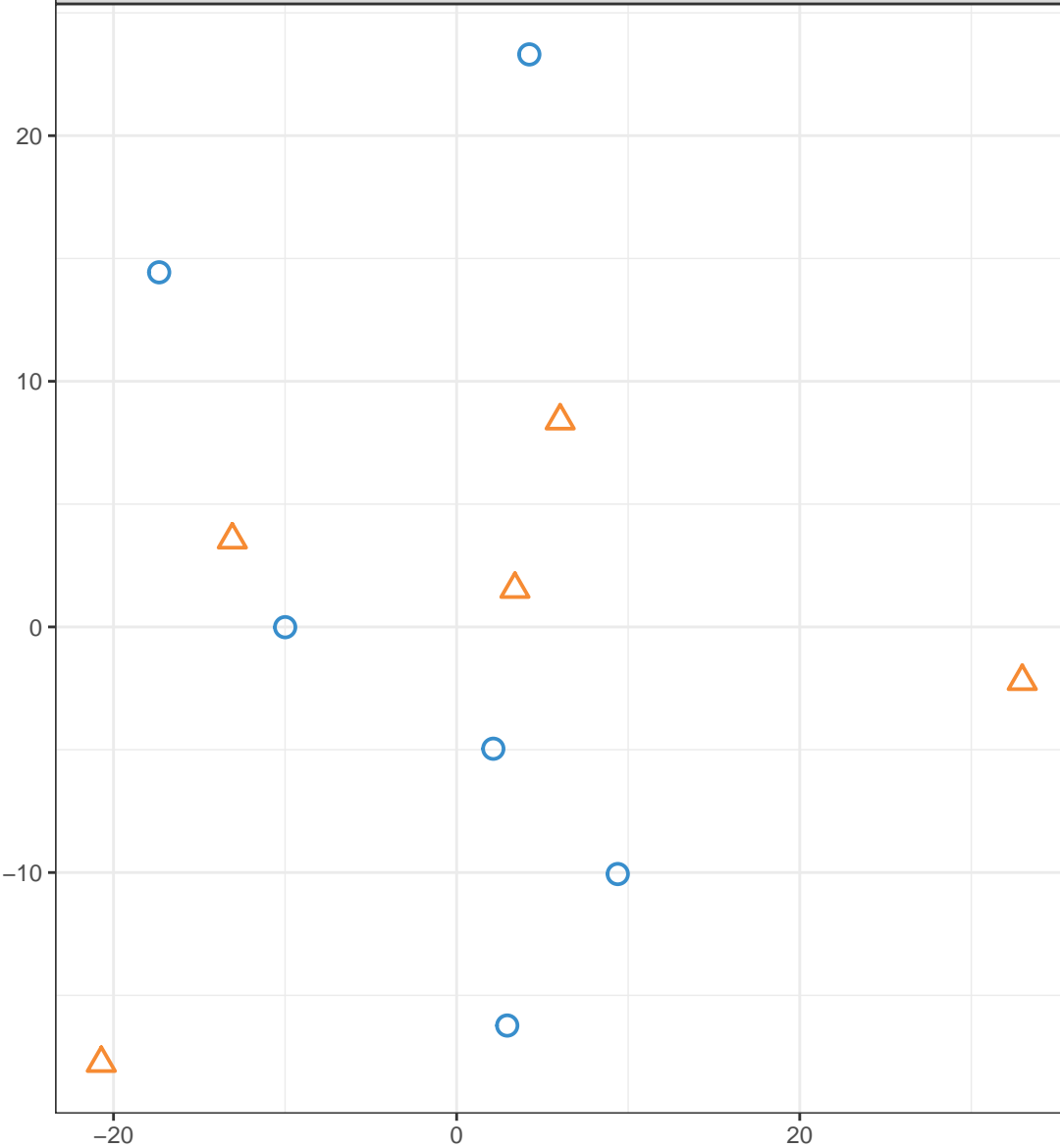
Class

○ RPMI
△ Sera



No Impute n_PCs = 10
Proteomics PCs (2,3)

PC3: 11% expl. var

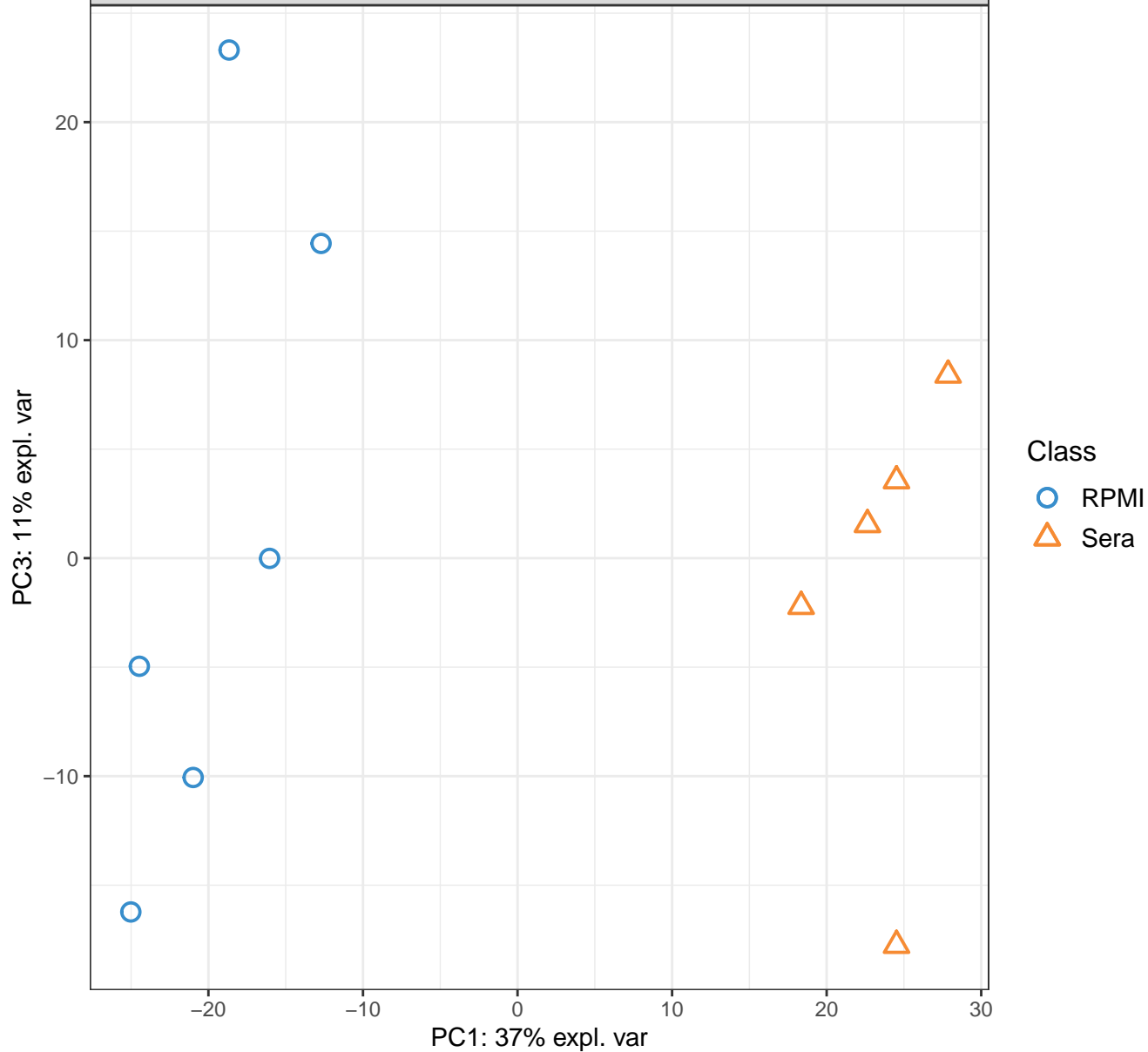


Class

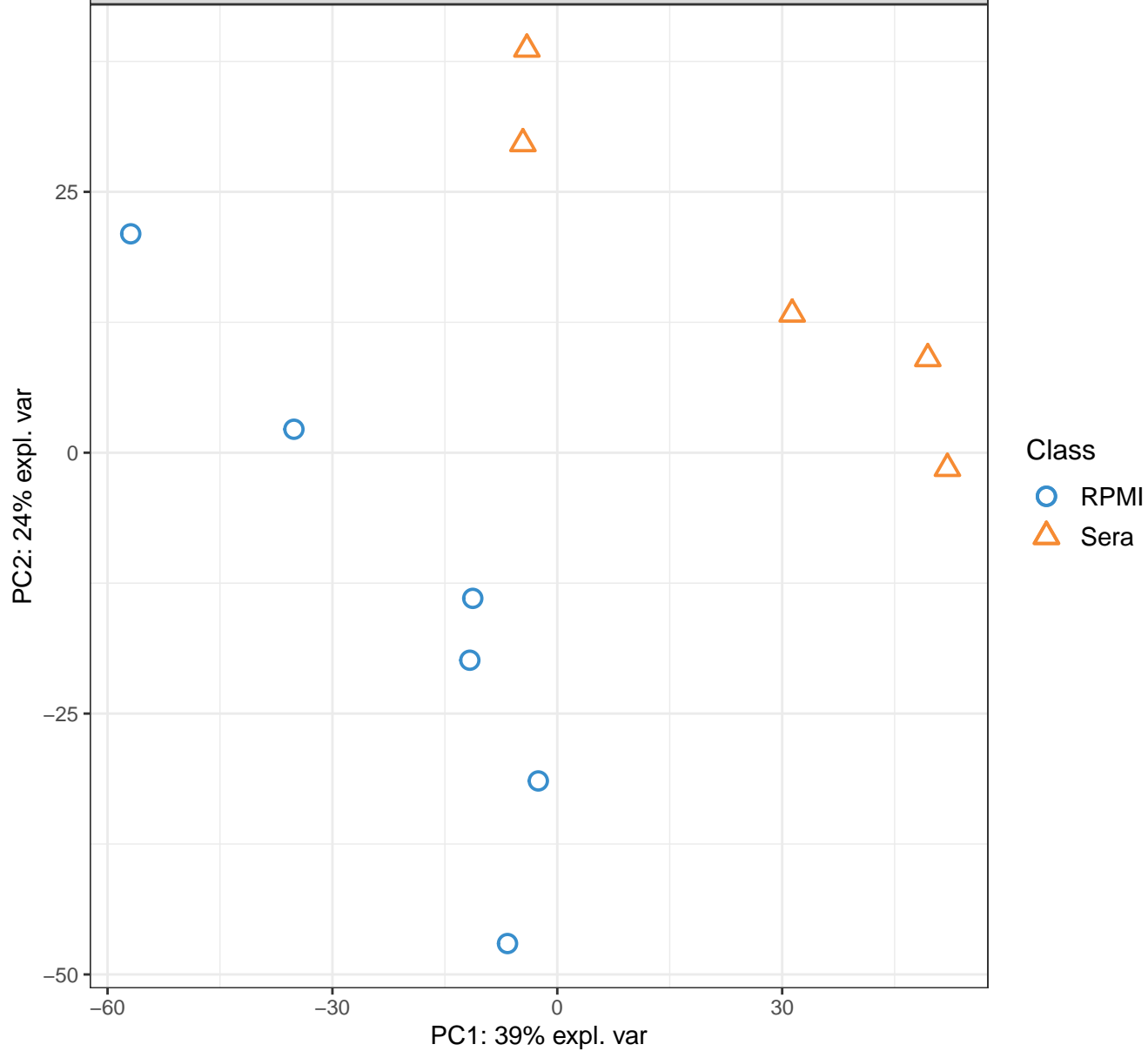
○ RPMI
△ Sera

PC2: 16% expl. var

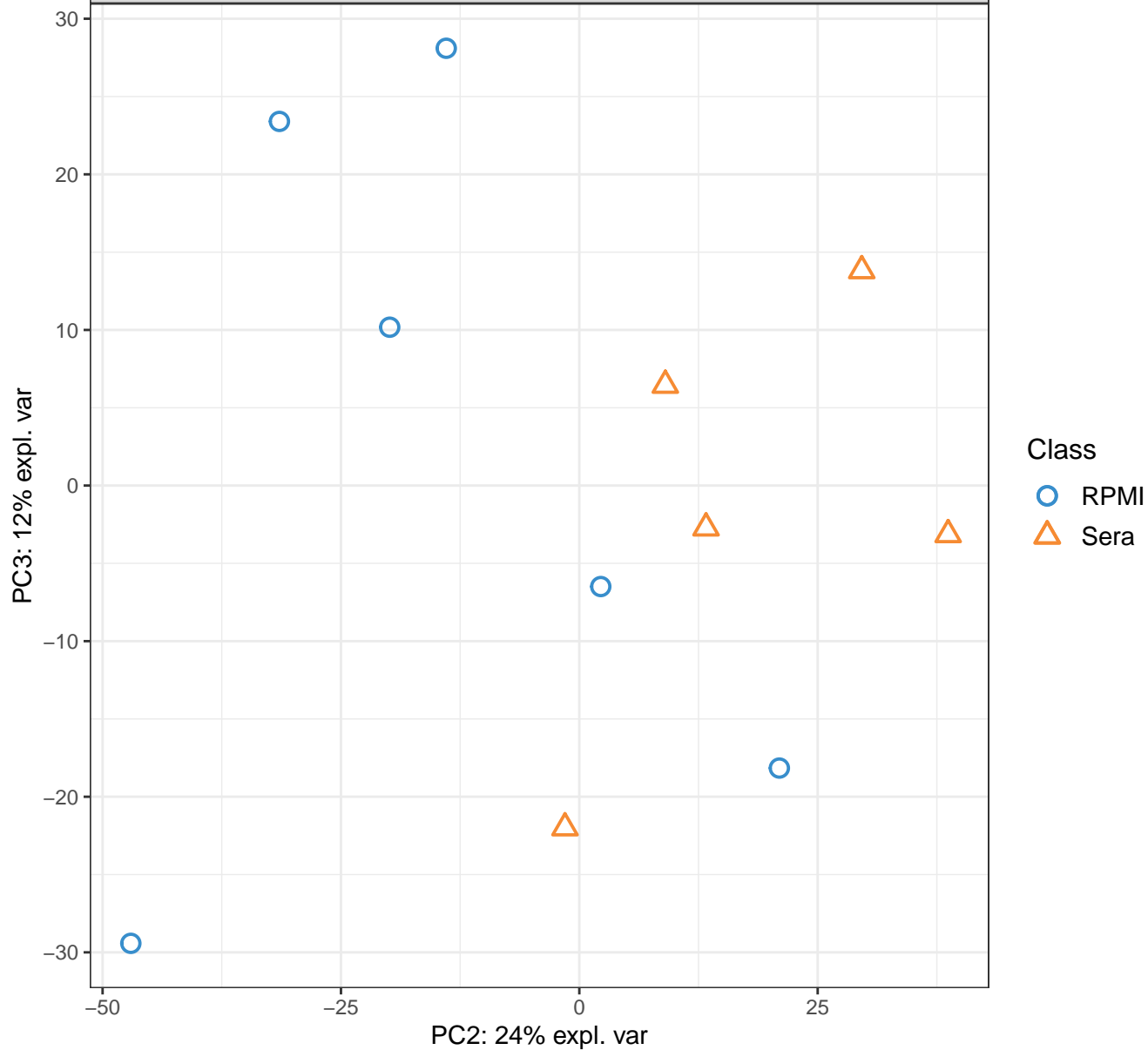
**No Impute n_PCs = 10
Proteomics PCs (1,3)**



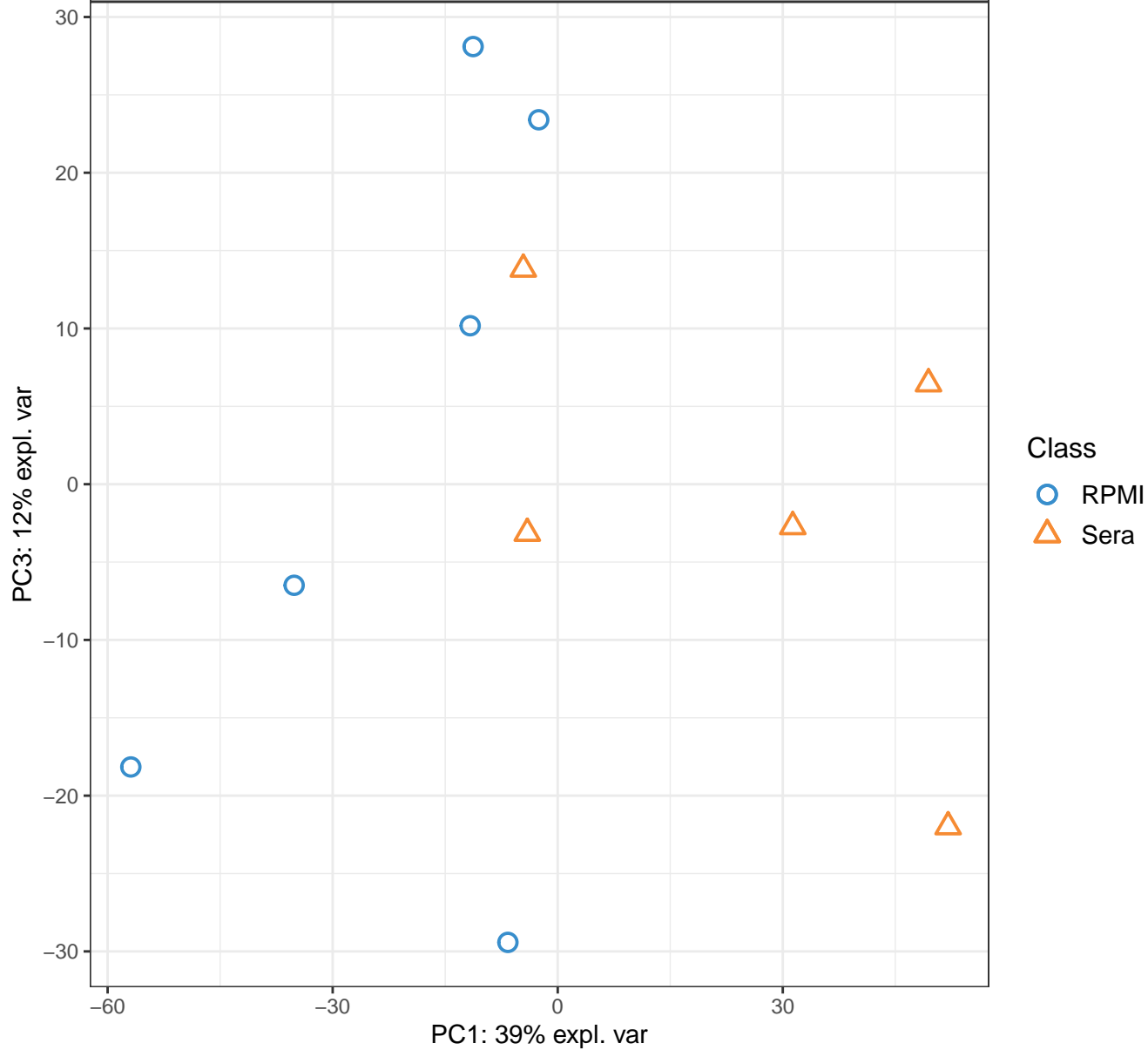
No Impute n_PCs = 10
RNA_Seq PCs (1,2)



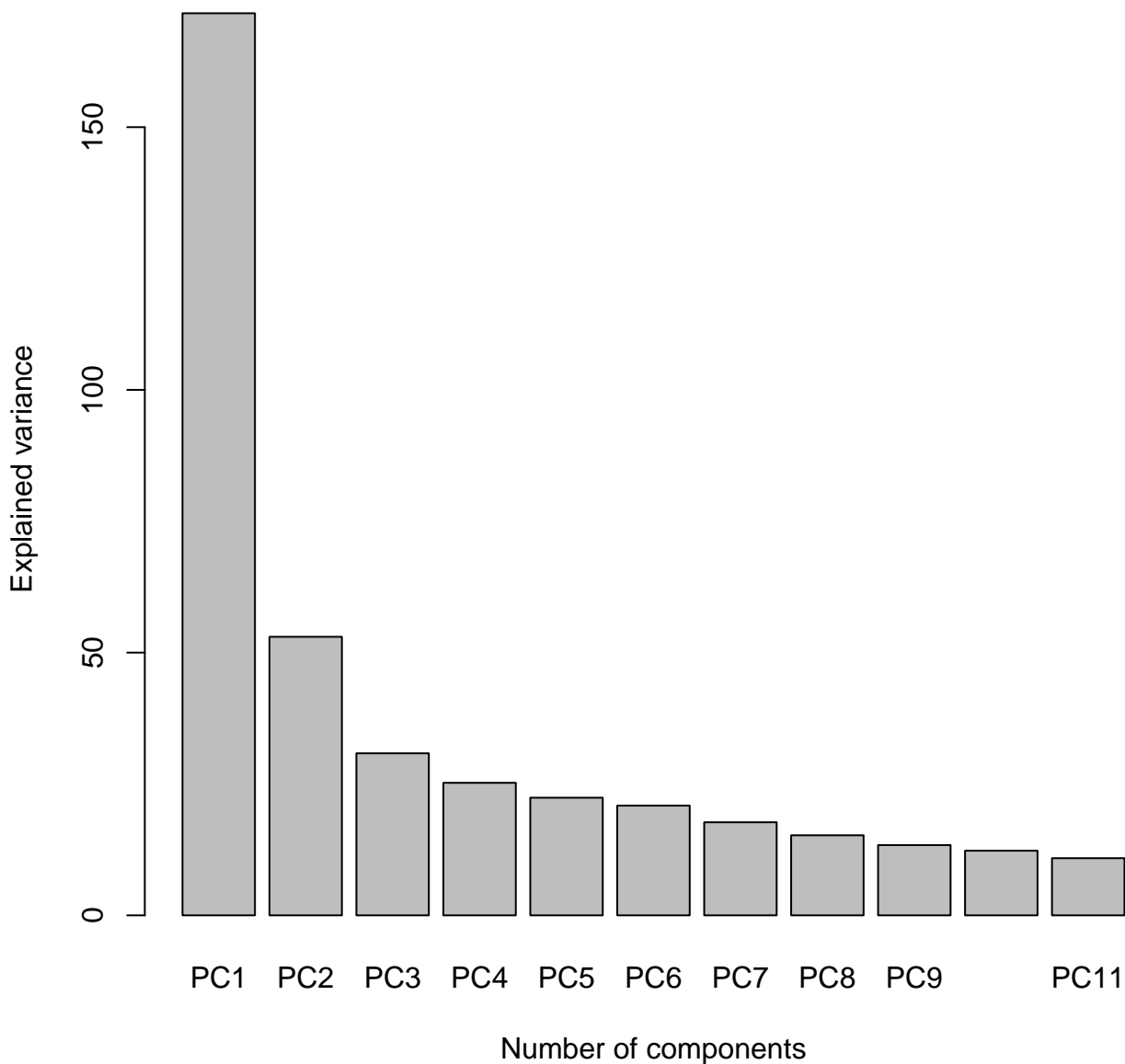
No Impute n_PCs = 10
RNA_Seq PCs (2,3)



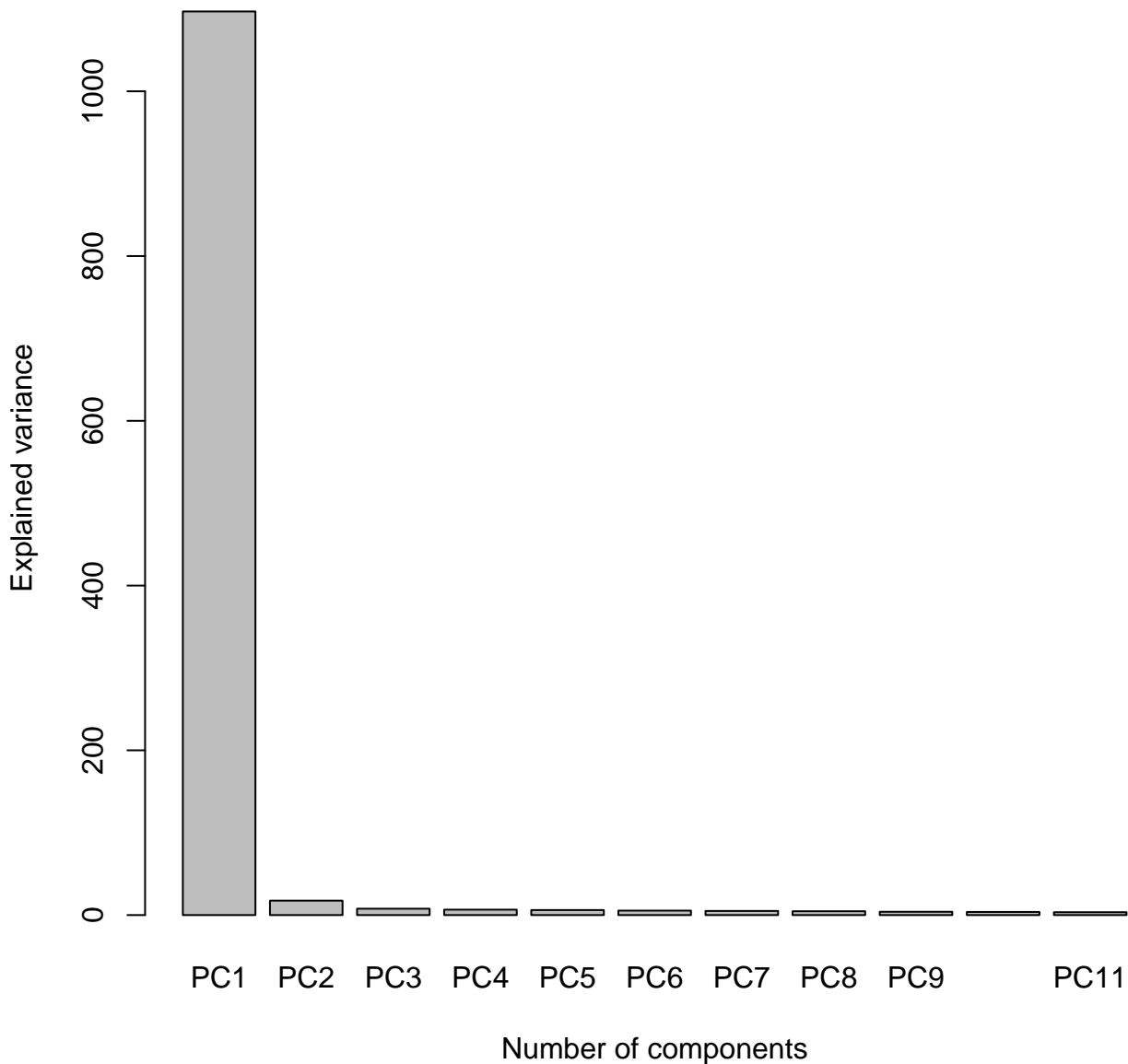
No Impute n_PCs = 10
RNA_Seq PCs (1,3)



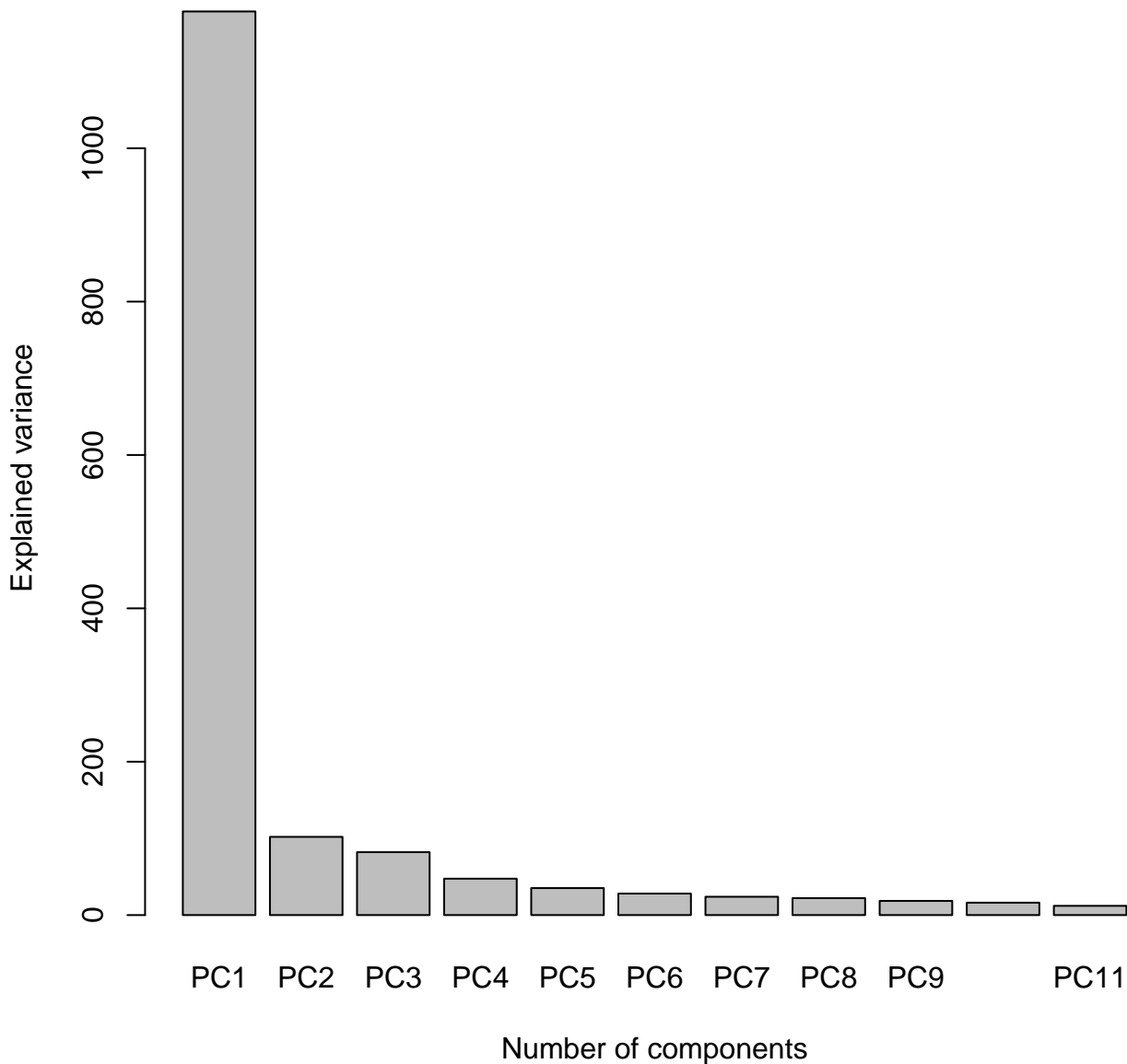
Metabolomics Screeplot (nipals imputed)



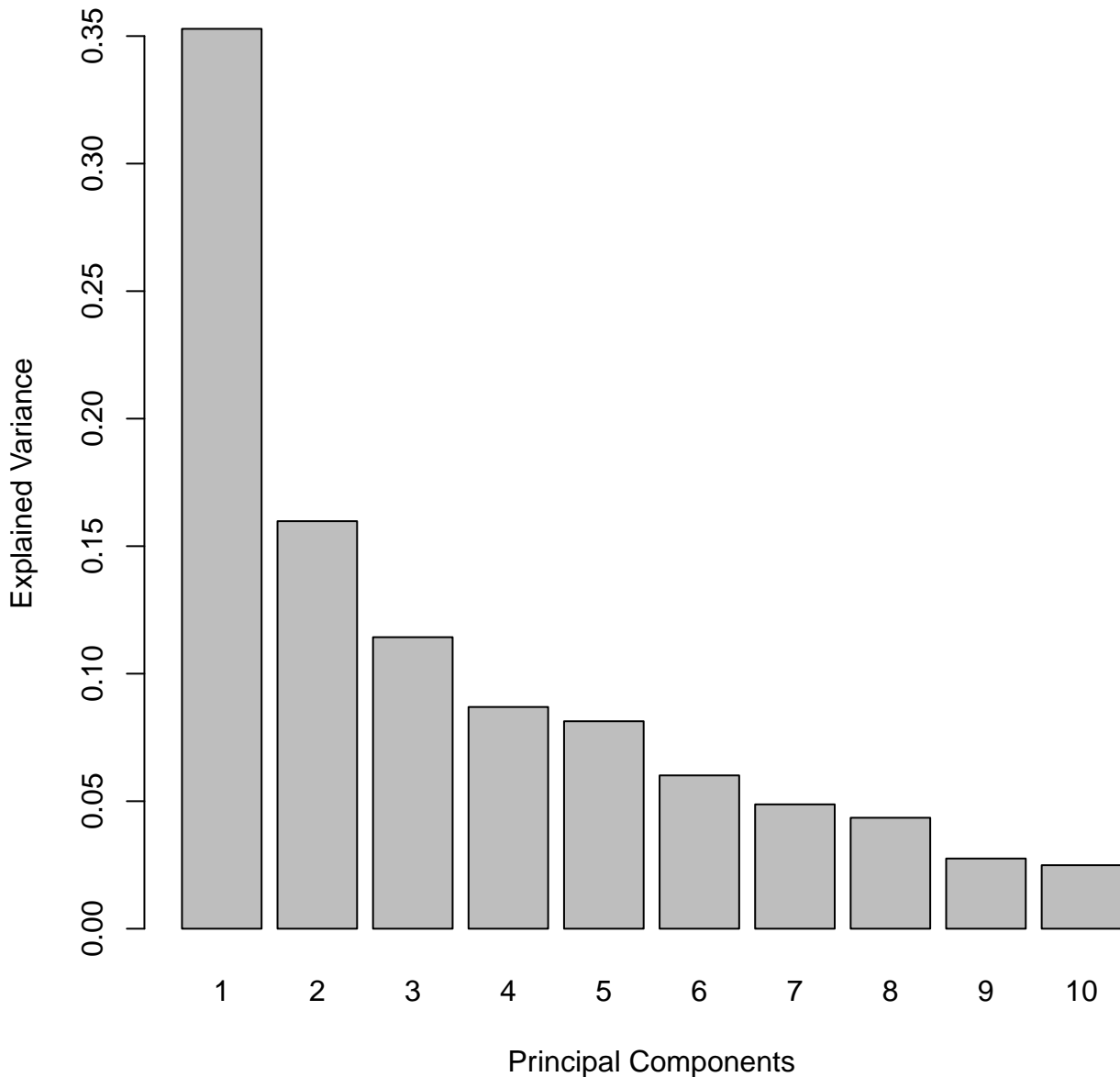
Proteomics Screeplot (nipals imputed)



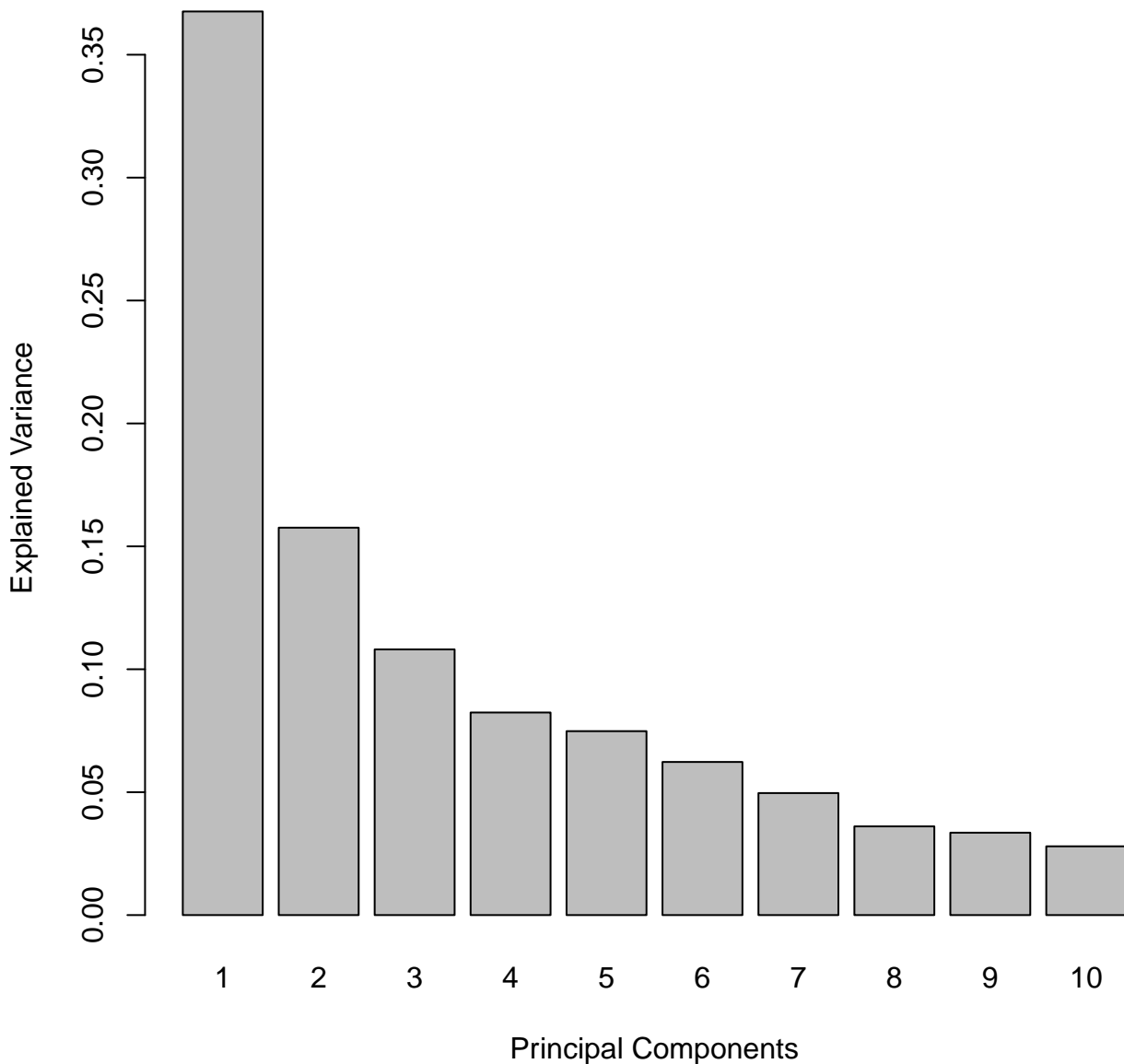
RNA_Seq Screeplot (nipals imputed)



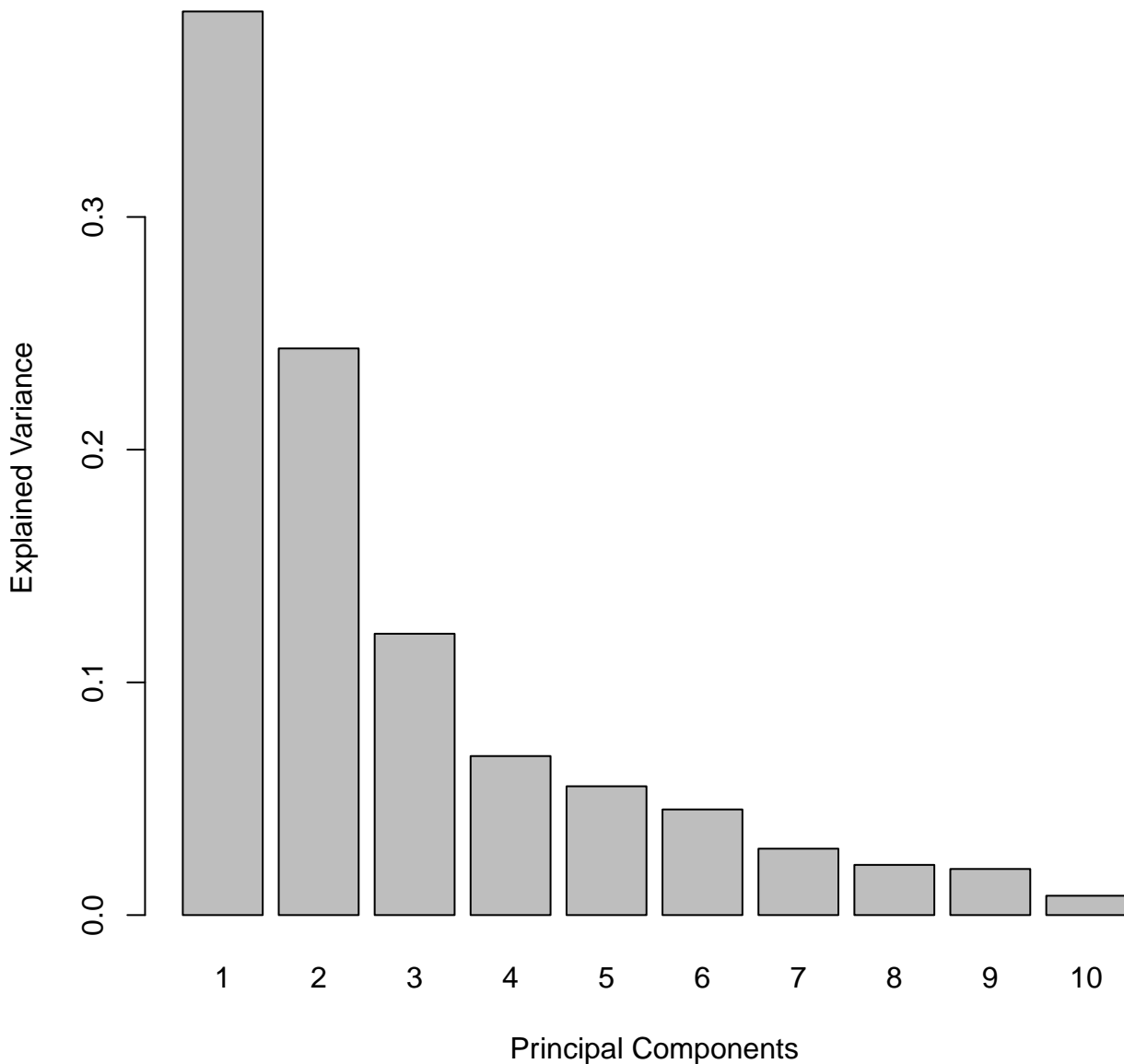
Metabolomics screeplot



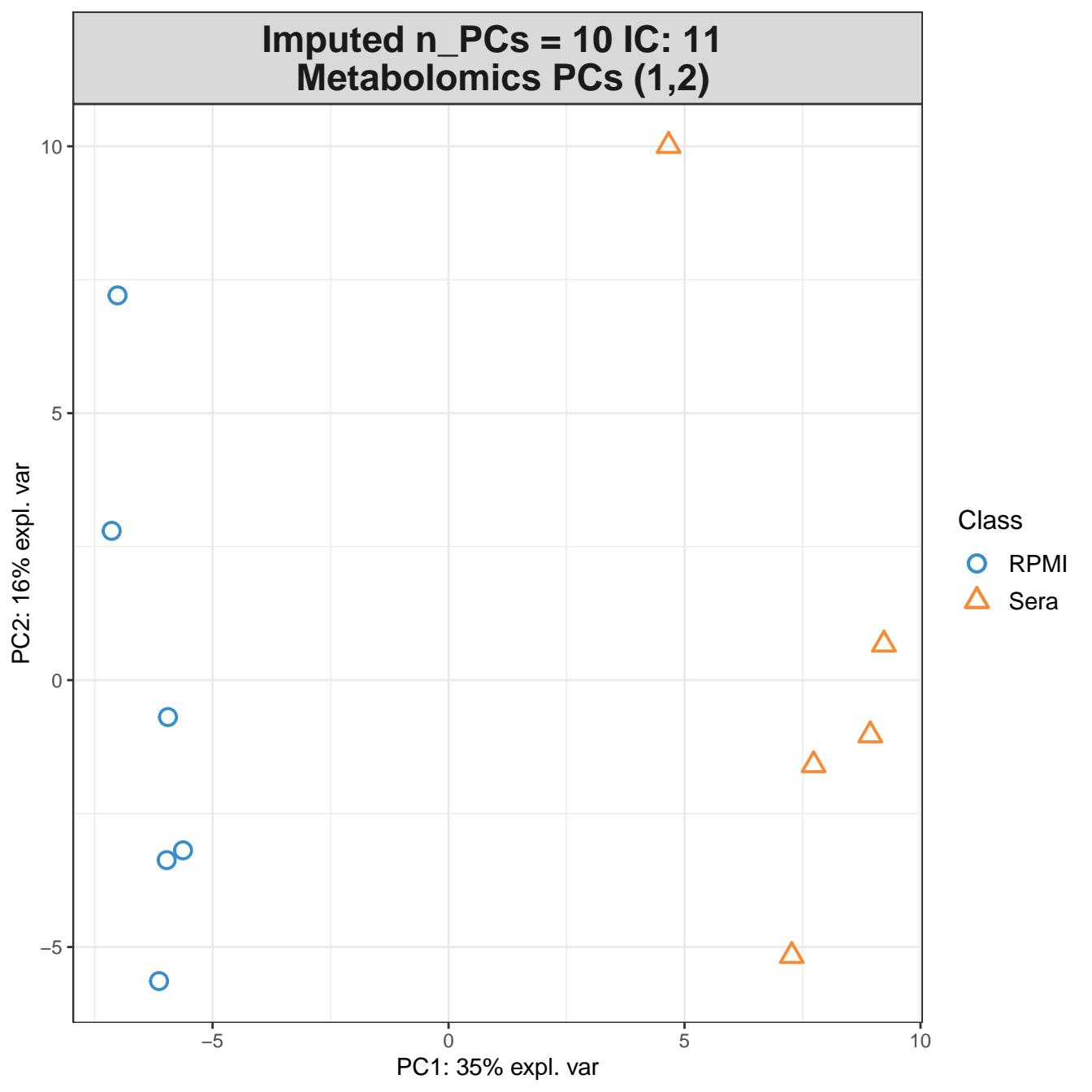
Proteomics screeplot



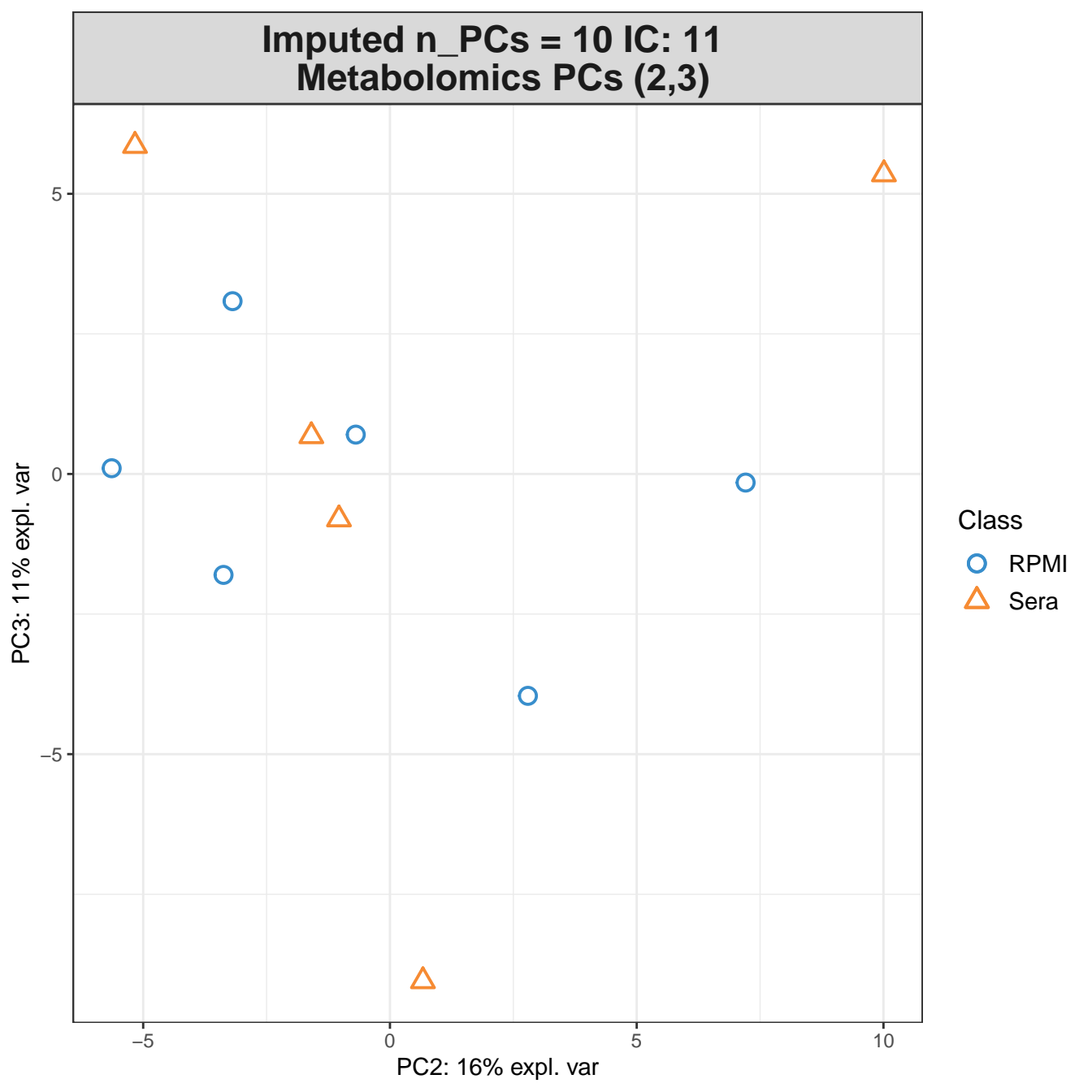
RNA_Seq screeplot



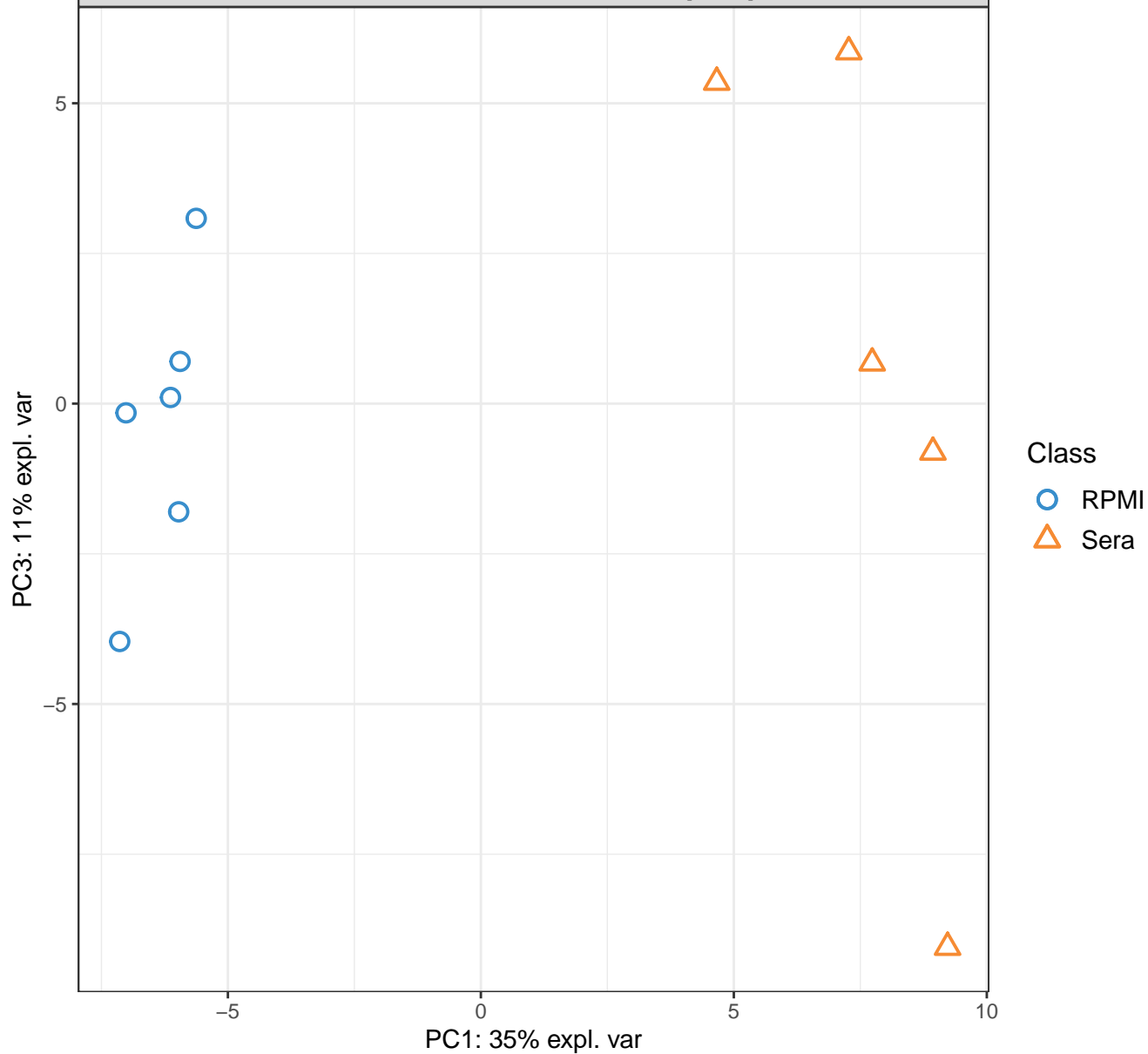
Imputed n_PCs = 10 IC: 11
Metabolomics PCs (1,2)



**Imputed n_PCs = 10 IC: 11
Metabolomics PCs (2,3)**

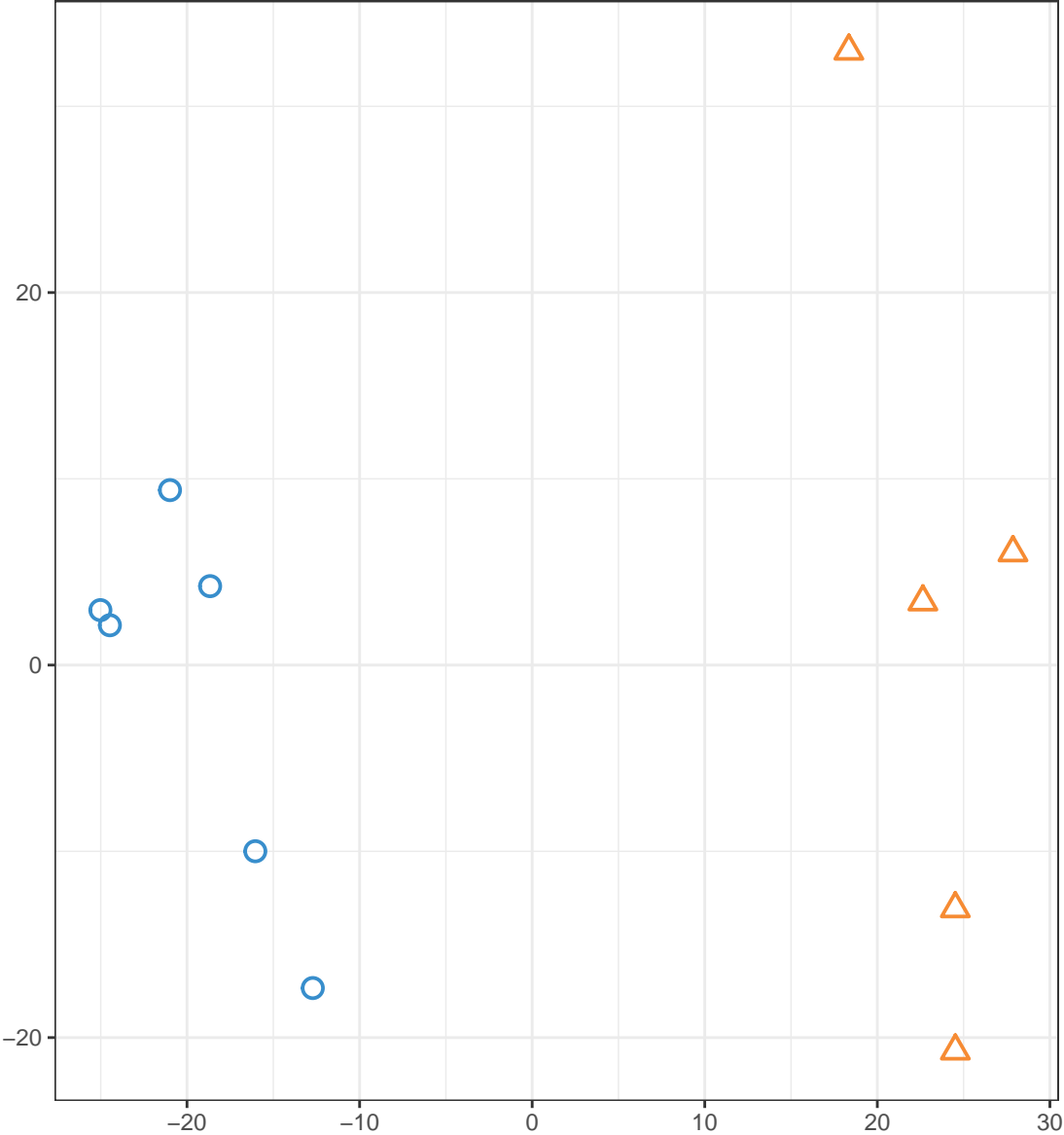


**Imputed n_PCs = 10 IC: 11
Metabolomics PCs (1,3)**



Imputed n_PCs = 10 IC: 11
Proteomics PCs (1,2)

PC2: 16% expl. var

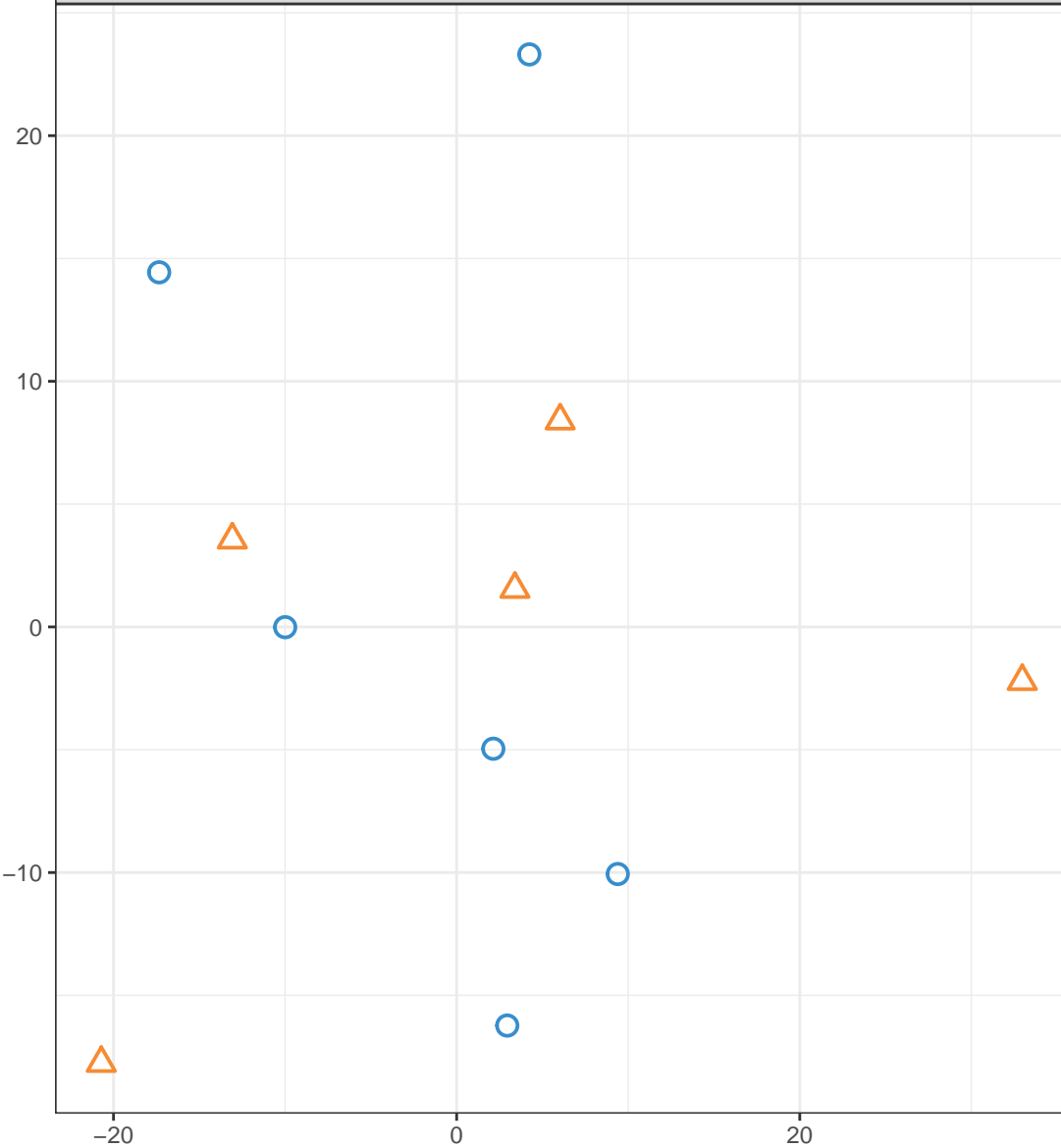


Class

○ RPMI
△ Sera

Imputed n_PCs = 10 IC: 11
Proteomics PCs (2,3)

PC3: 11% expl. var



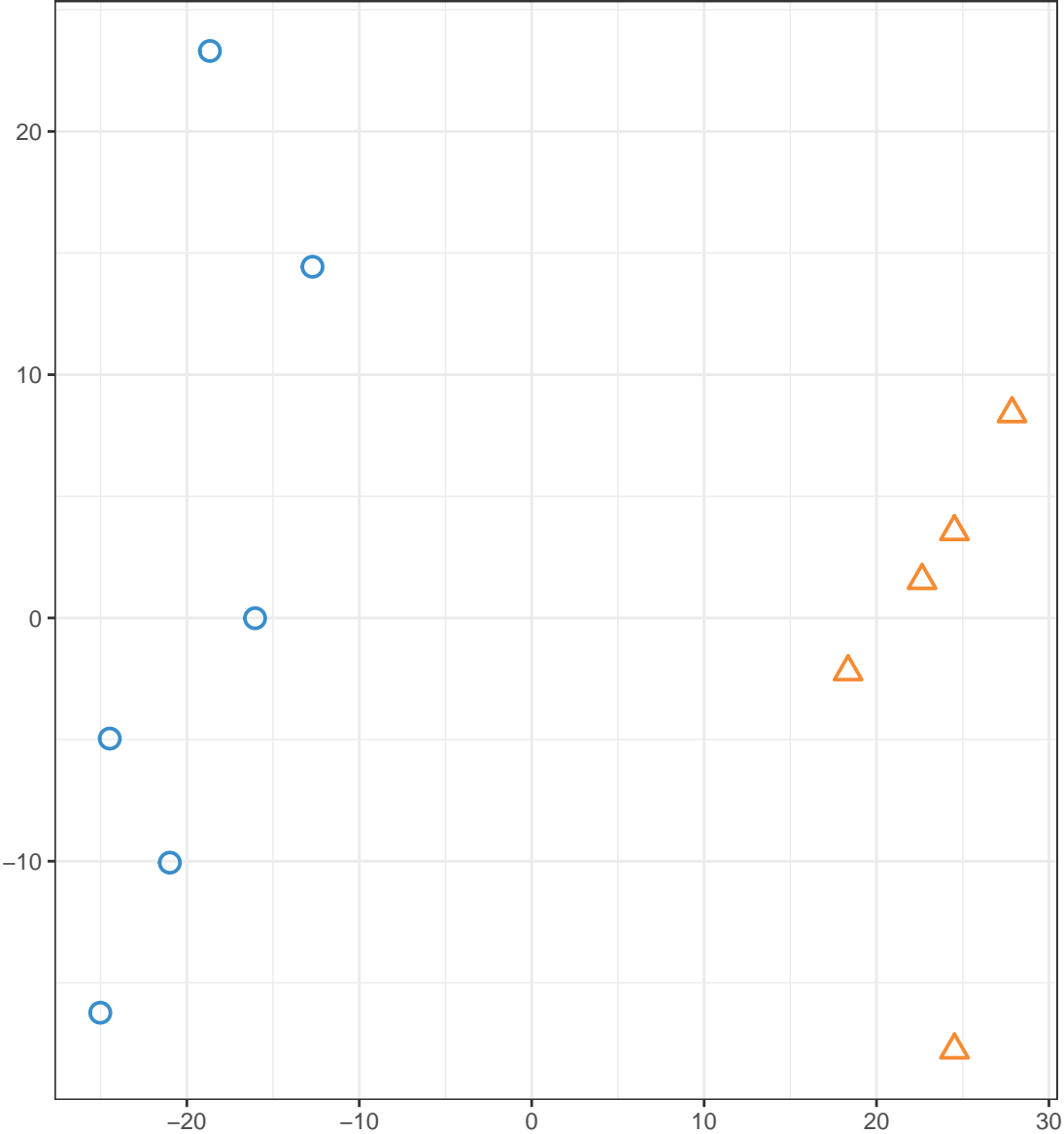
Class

○ RPMI
△ Sera

PC2: 16% expl. var

Imputed n_PCs = 10 IC: 11
Proteomics PCs (1,3)

PC3: 11% expl. var



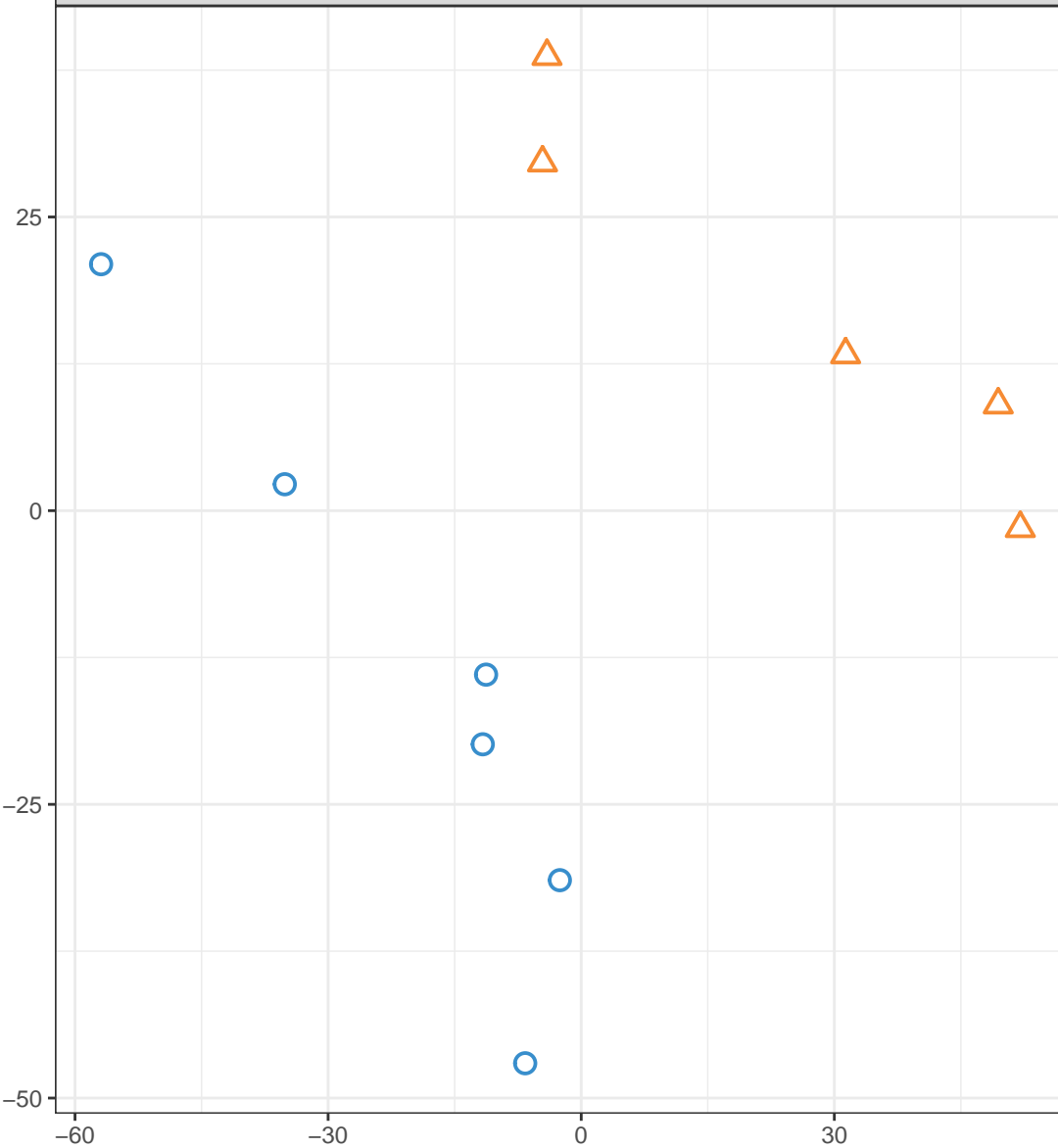
Class

○ RPMI
△ Sera

PC1: 37% expl. var

Imputed n_PCs = 10 IC: 11
RNA_Seq PCs (1,2)

PC2: 24% expl. var

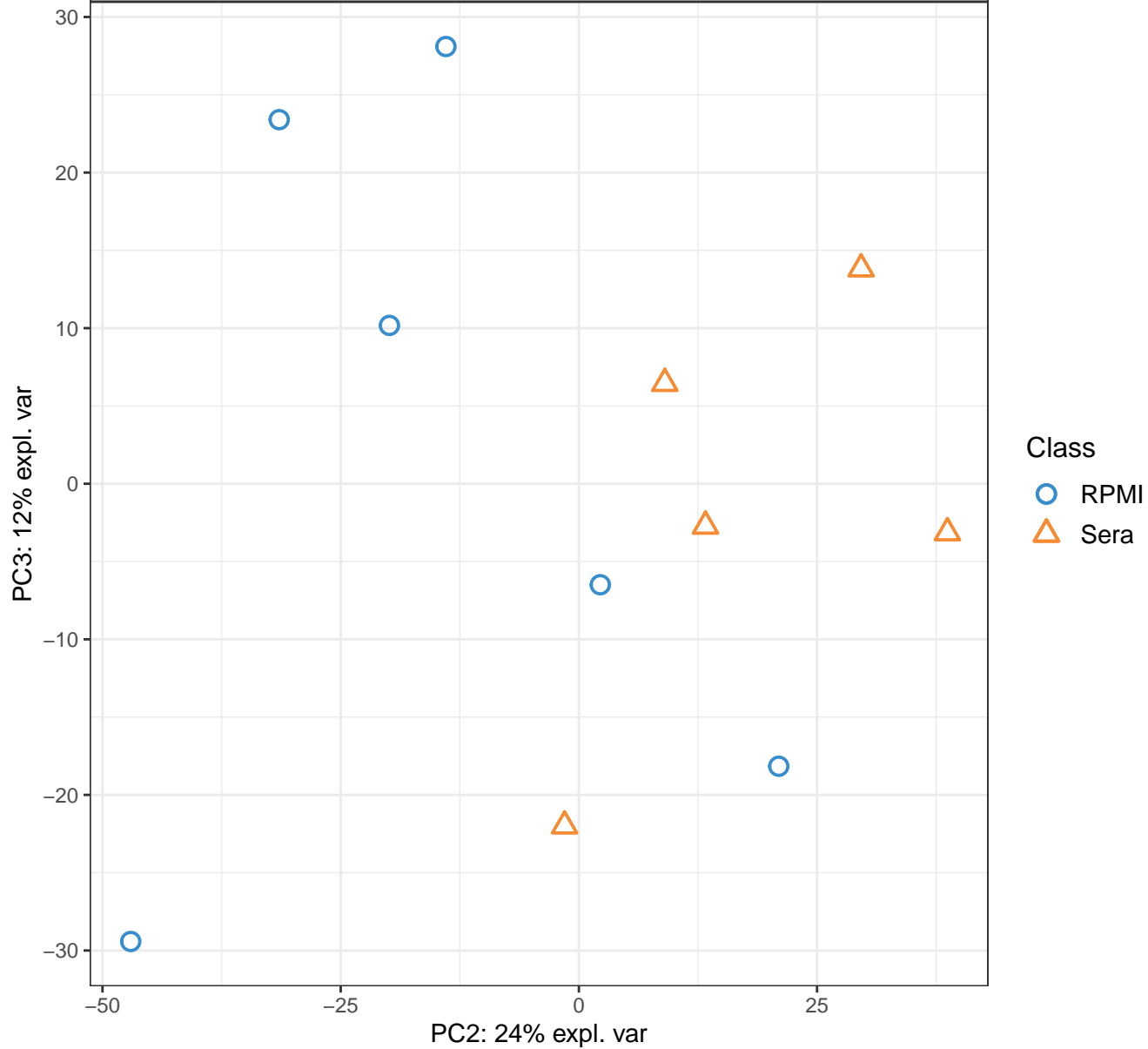


Class

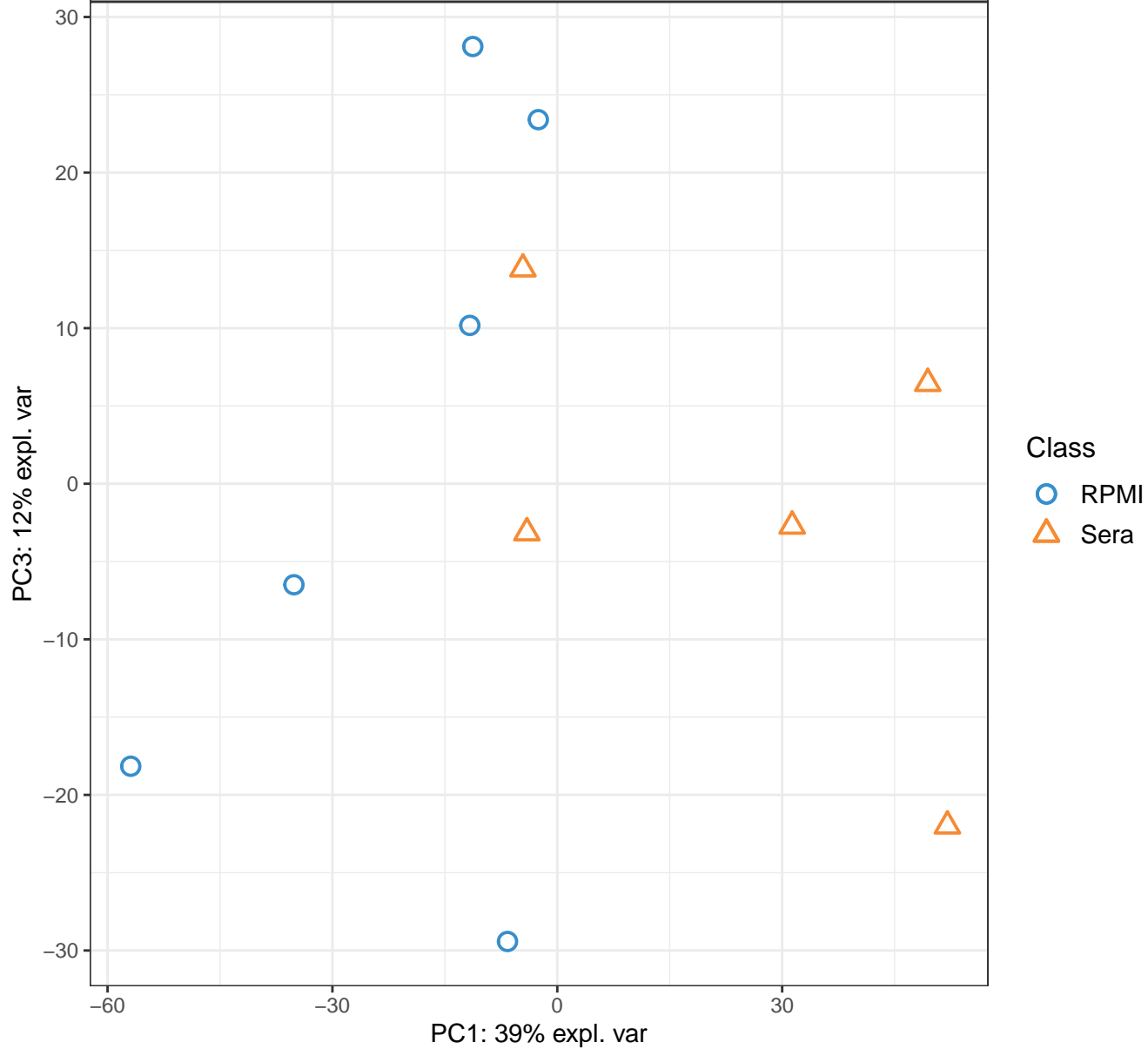
○ RPMI
△ Sera

PC1: 39% expl. var

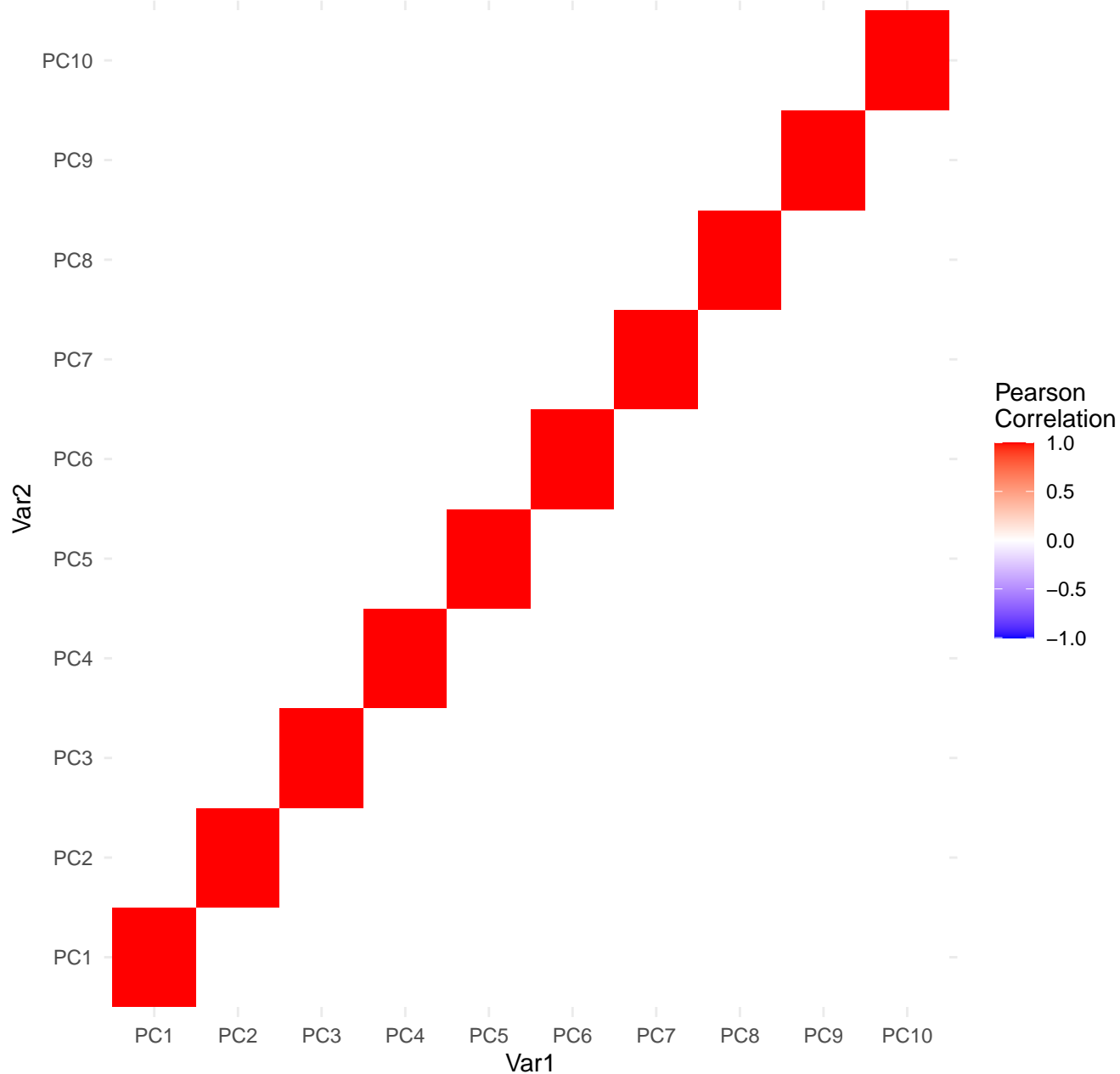
Imputed n_PCs = 10 IC: 11
RNA_Seq PCs (2,3)



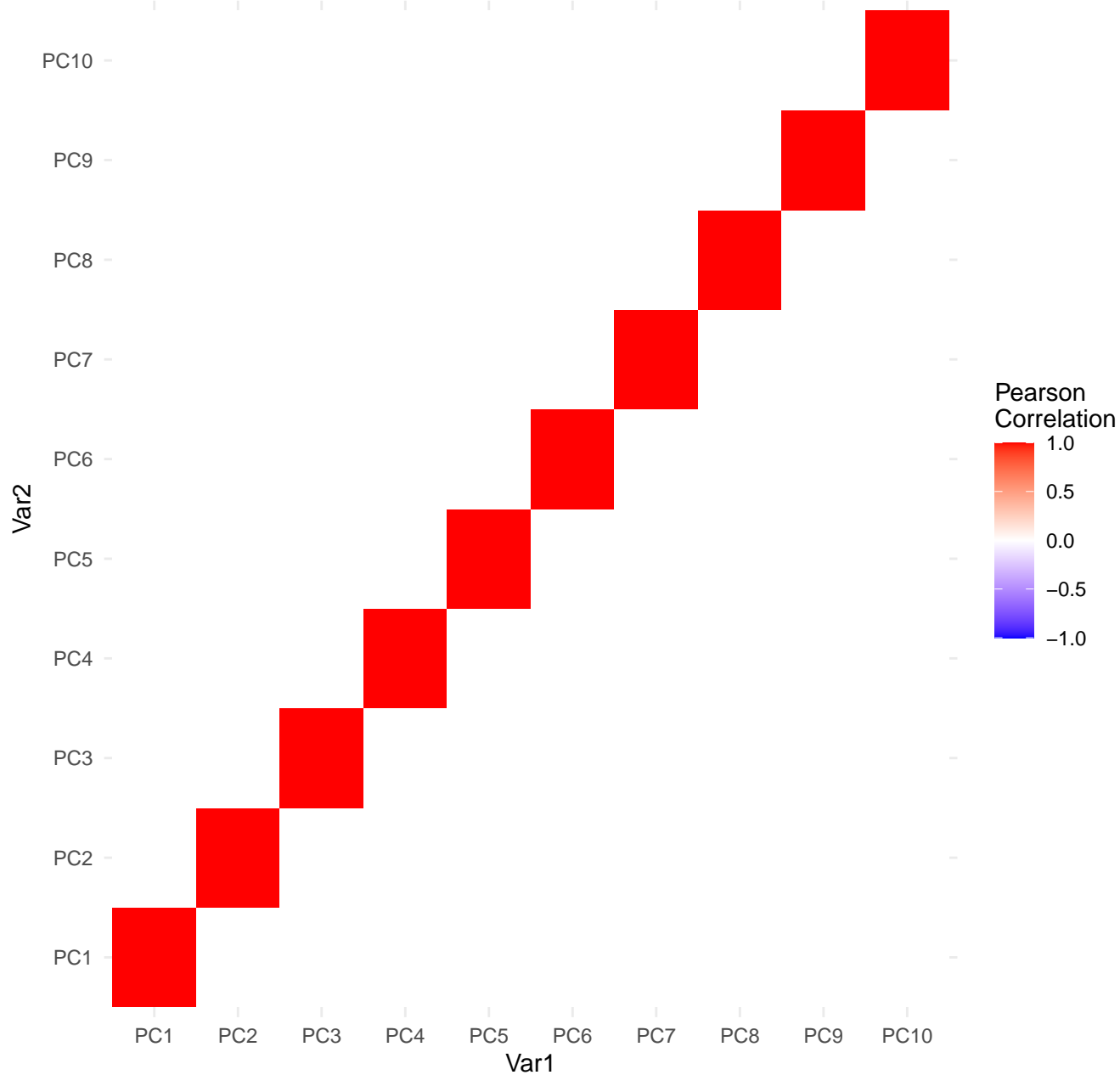
Imputed n_PCs = 10 IC: 11
RNA_Seq PCs (1,3)



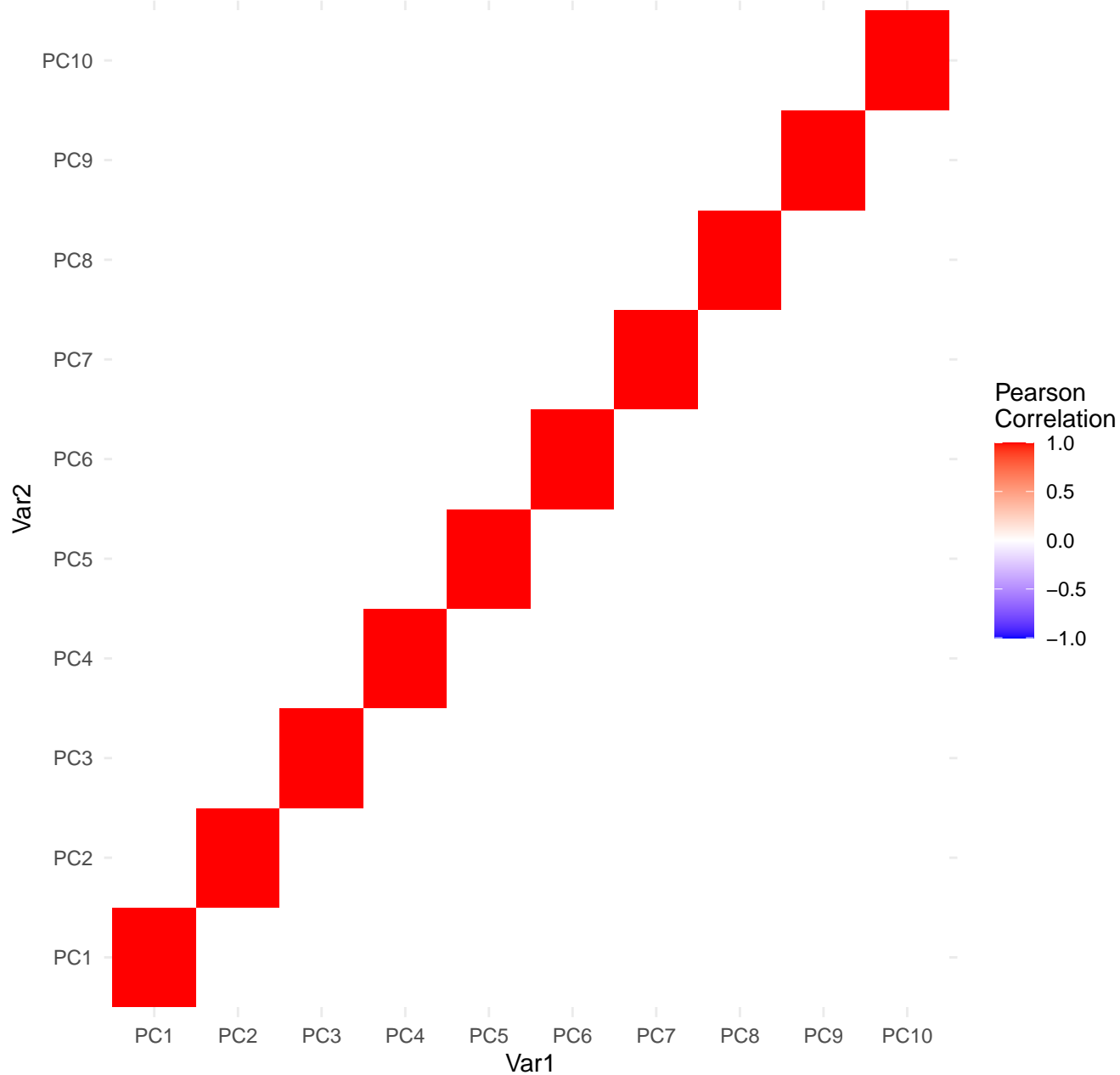
Metabolomics Correlation between imputed and unimputed data



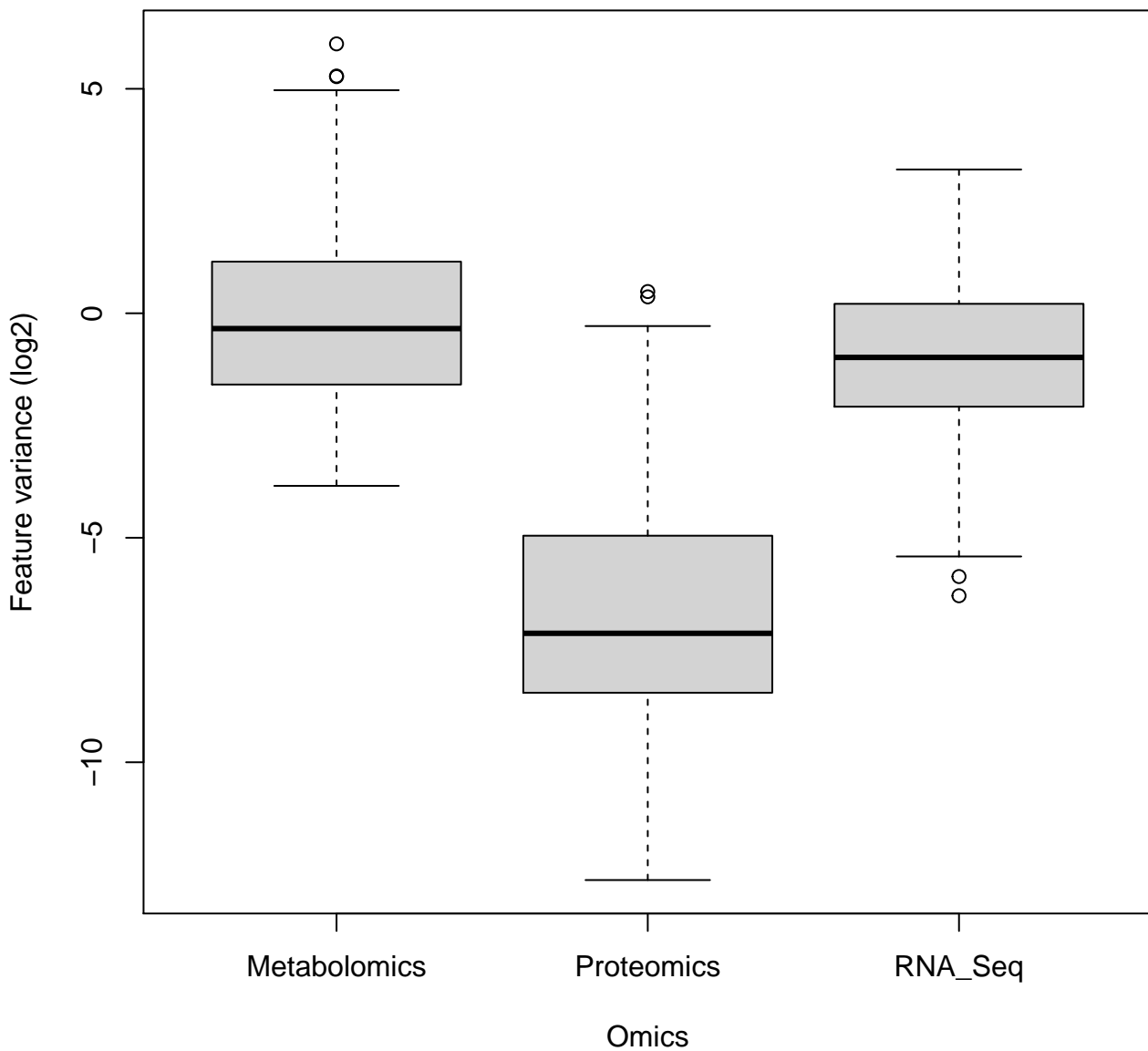
Proteomics Correlation between imputed and unimputed data



RNA_Seq Correlation between imputed and unimputed data

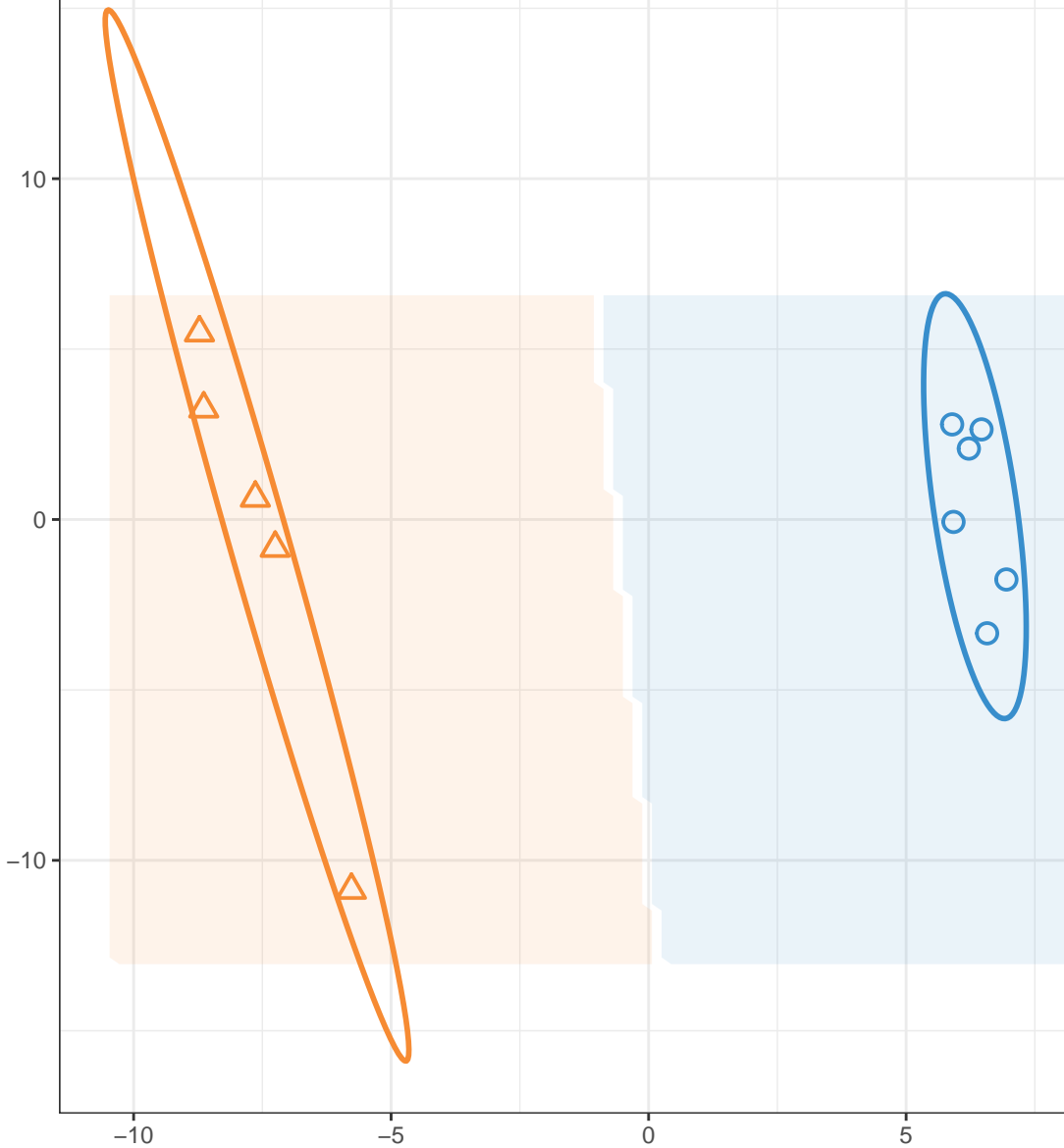


Feature variances (log2) per omics



Metabolomics PLSDA single 1/2

X-variate 2: 14% expl. var



Legend

- RPMI
- △ Sera

Metabolomics PLSDA single 1/2

X-variate 2: 14% expl. var

10
0
-10

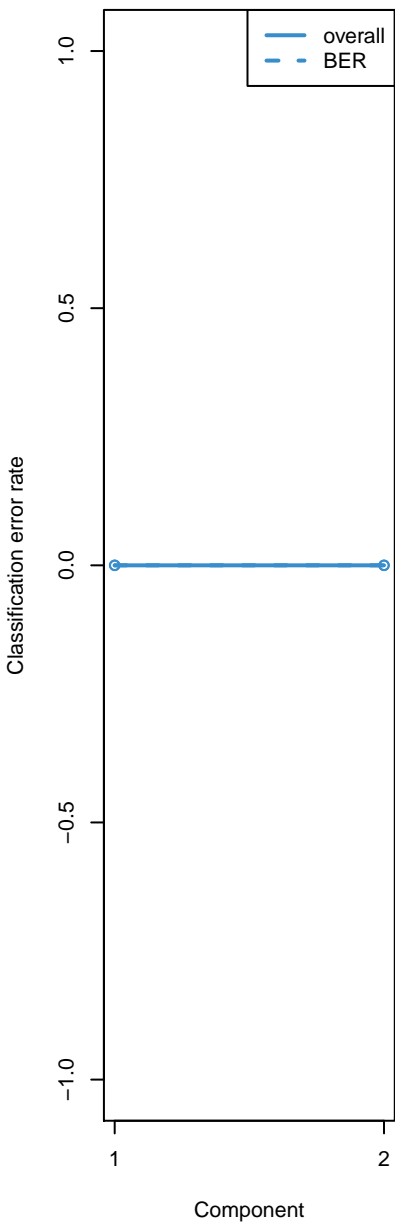
X-variate 1: 35% expl. var

Legend

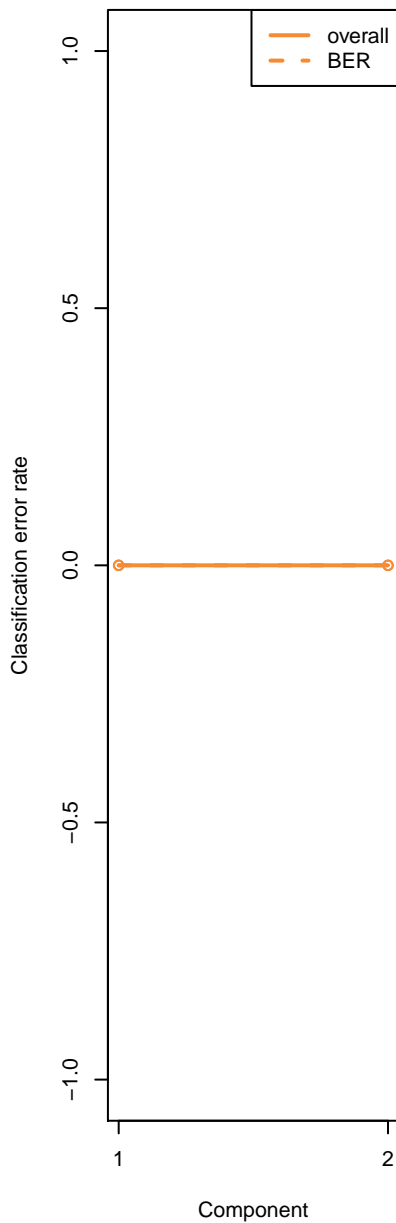
○ RPMI
△ Sera



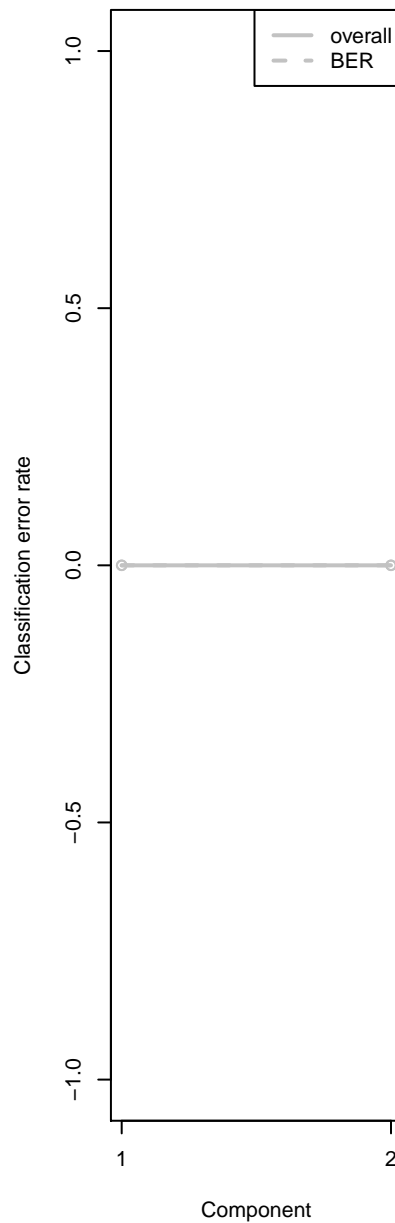
max.dist



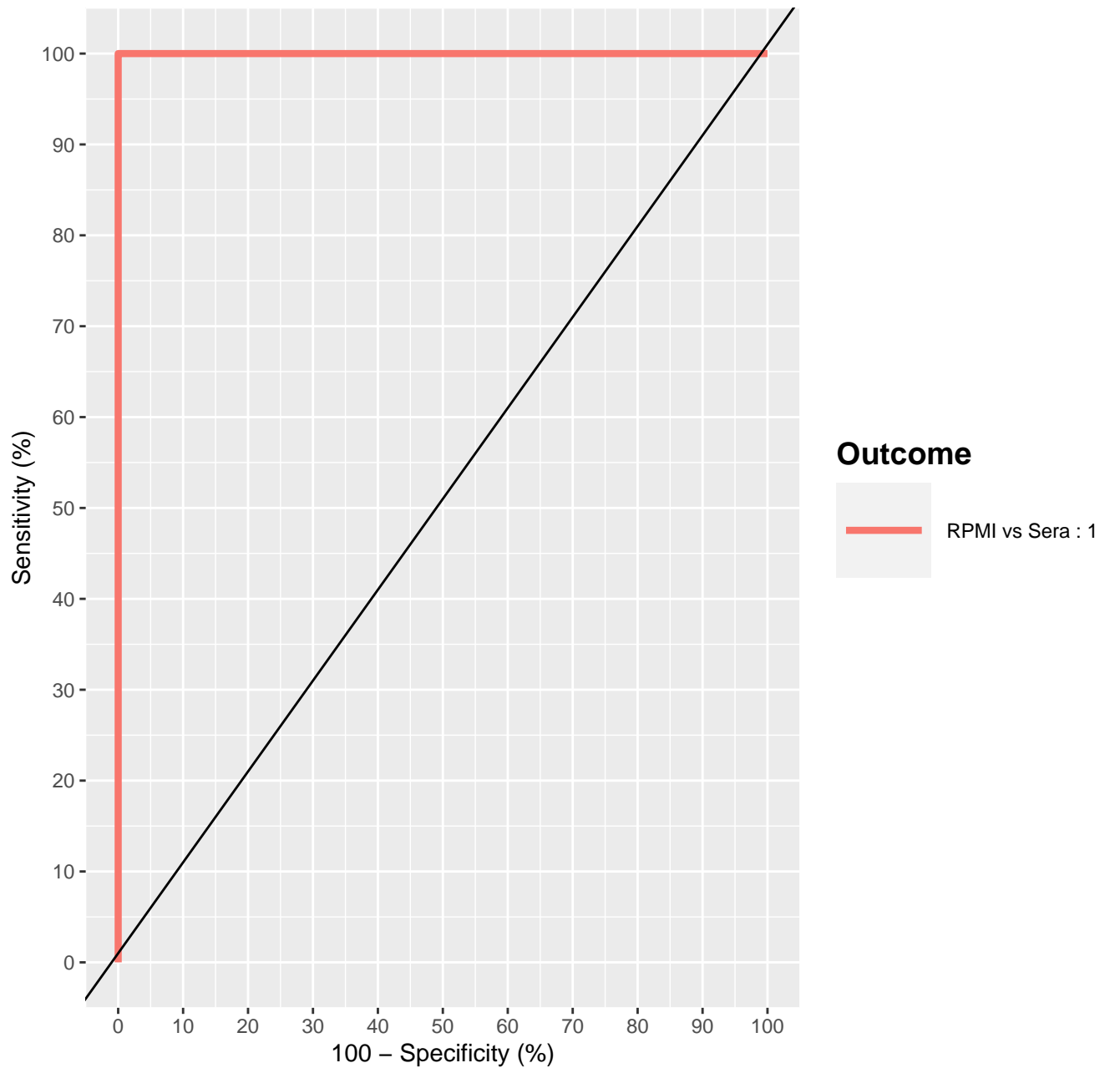
centroids.dist



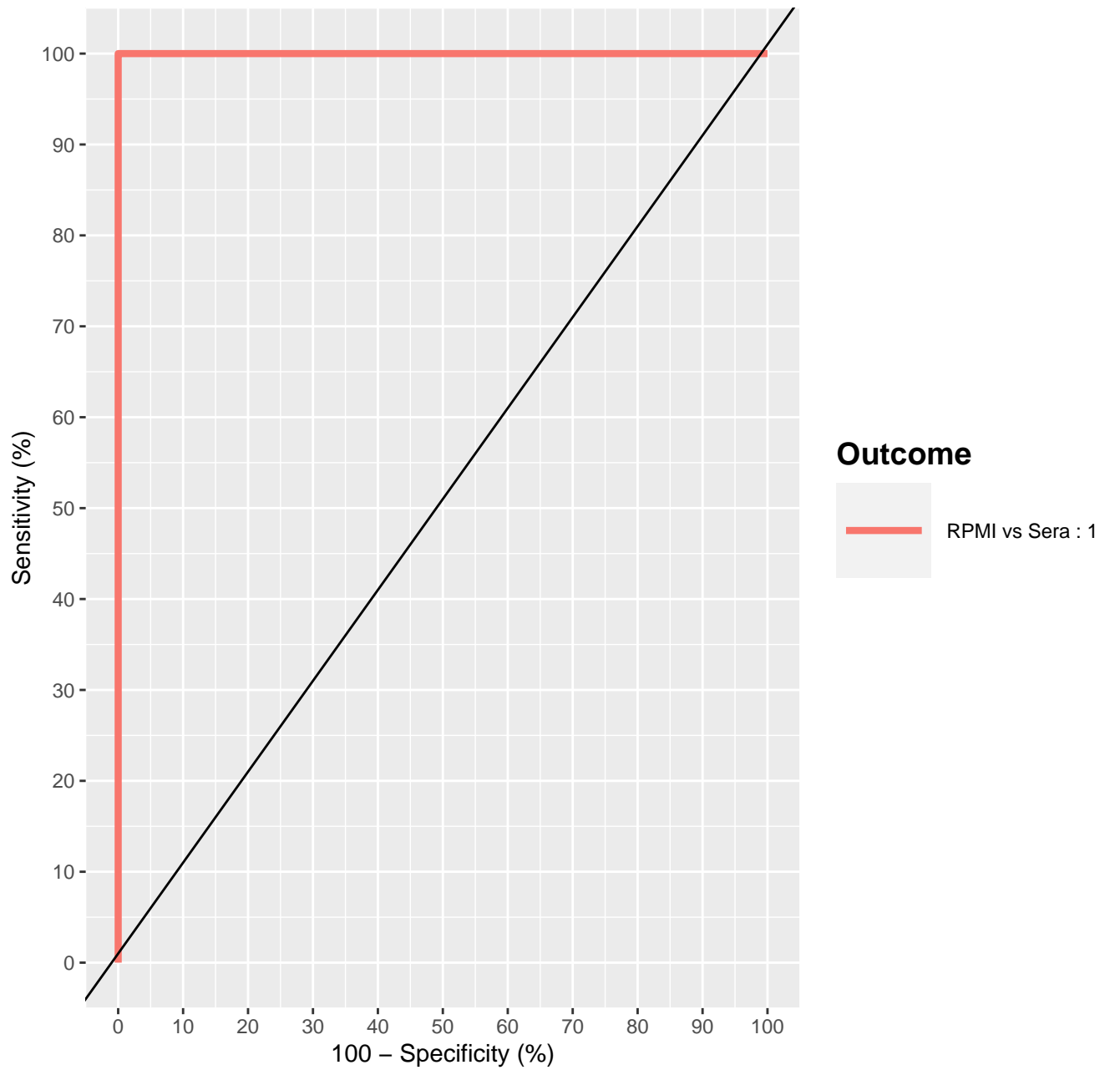
mahalanobis.dist



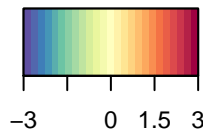
ROC Curve Comp 1



ROC Curve Comp 2



Color key

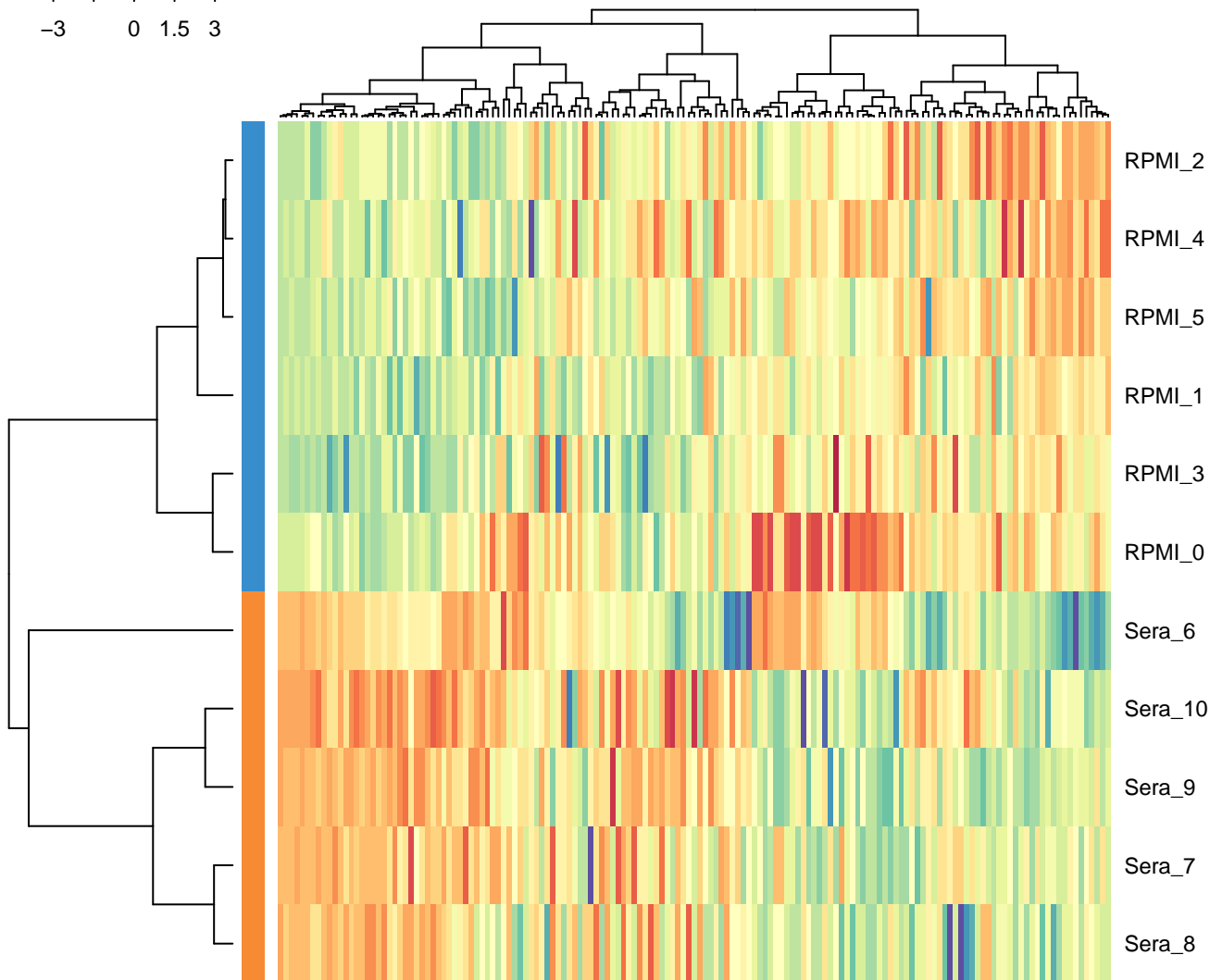


PLSDA

Status

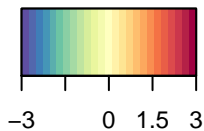
■ RPMI

■ Sera



PLSDA Component 1

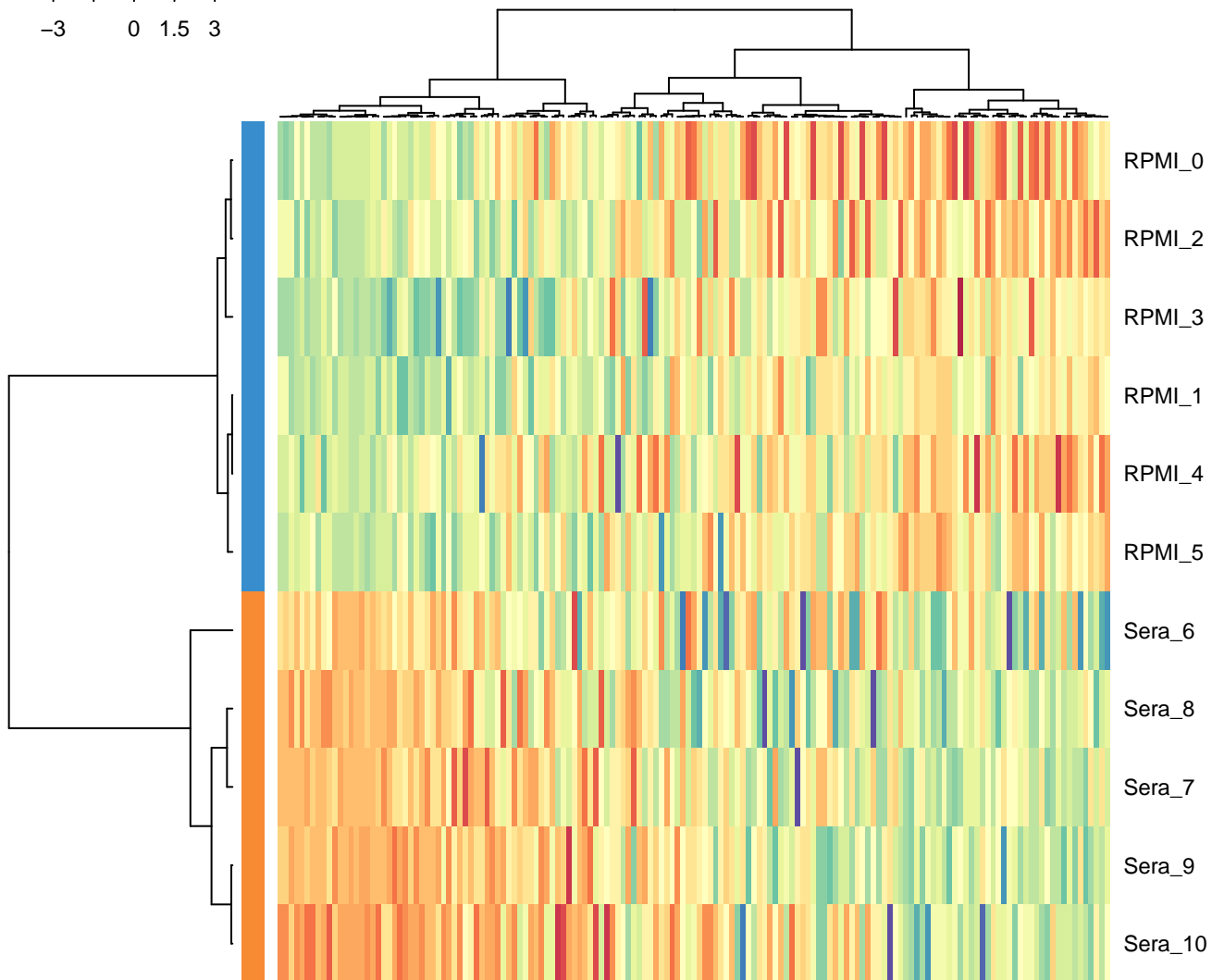
Color key



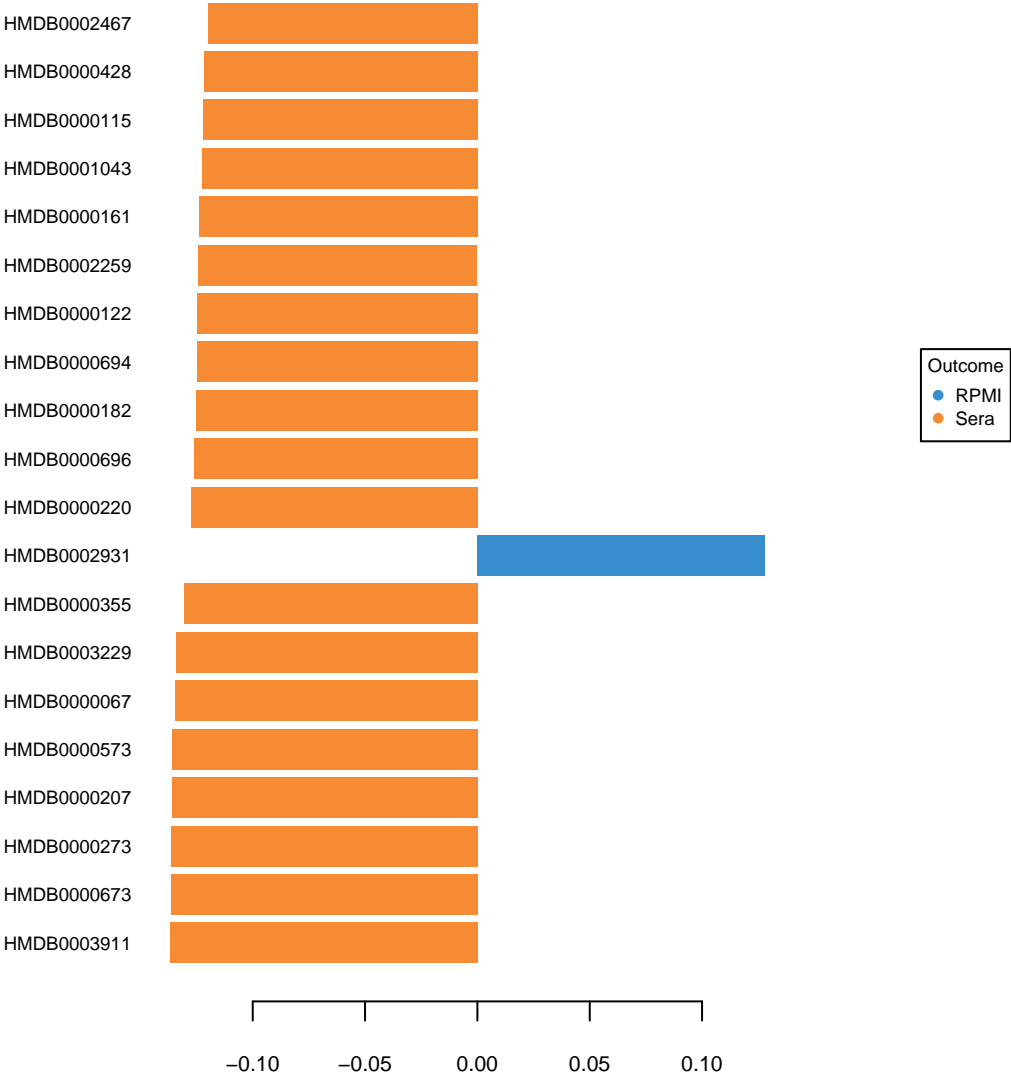
Status

RPMI

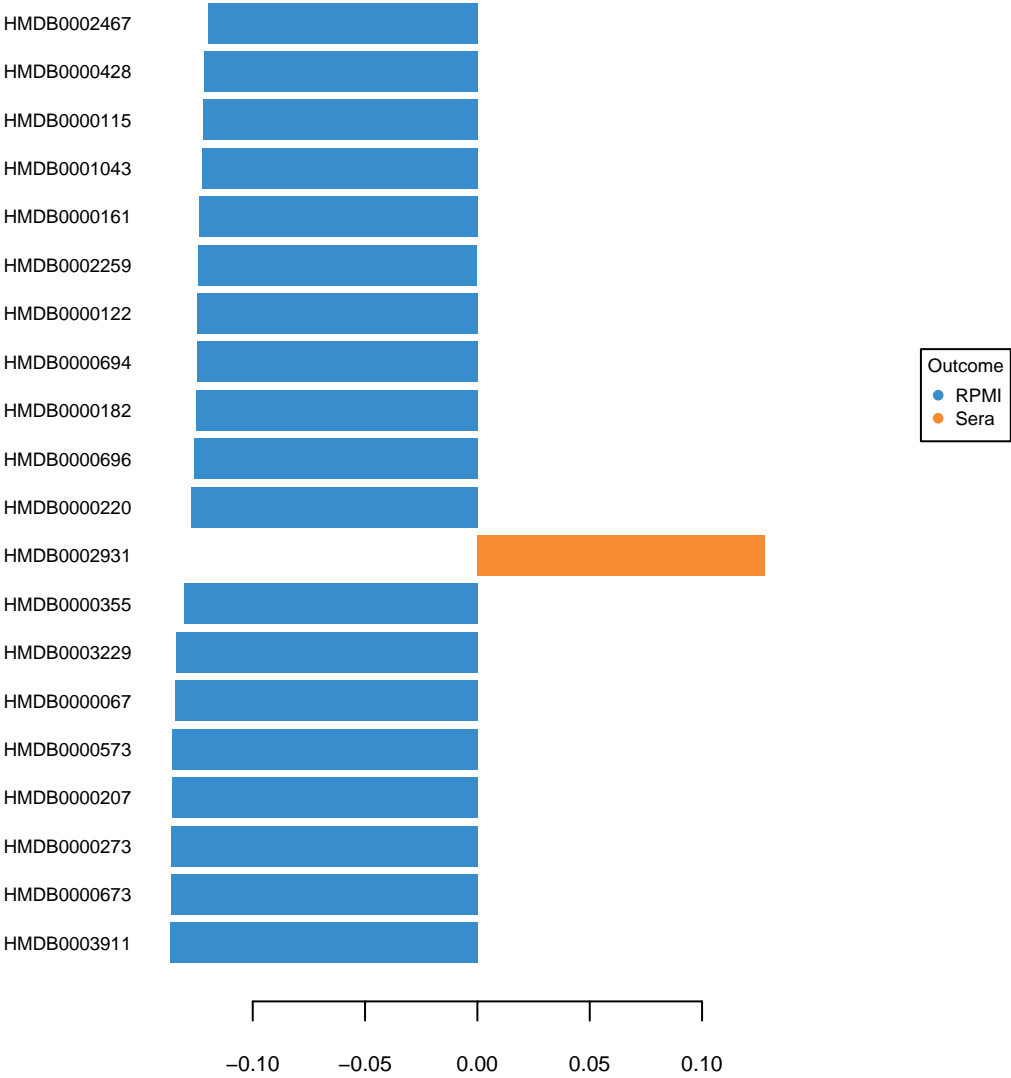
Sera



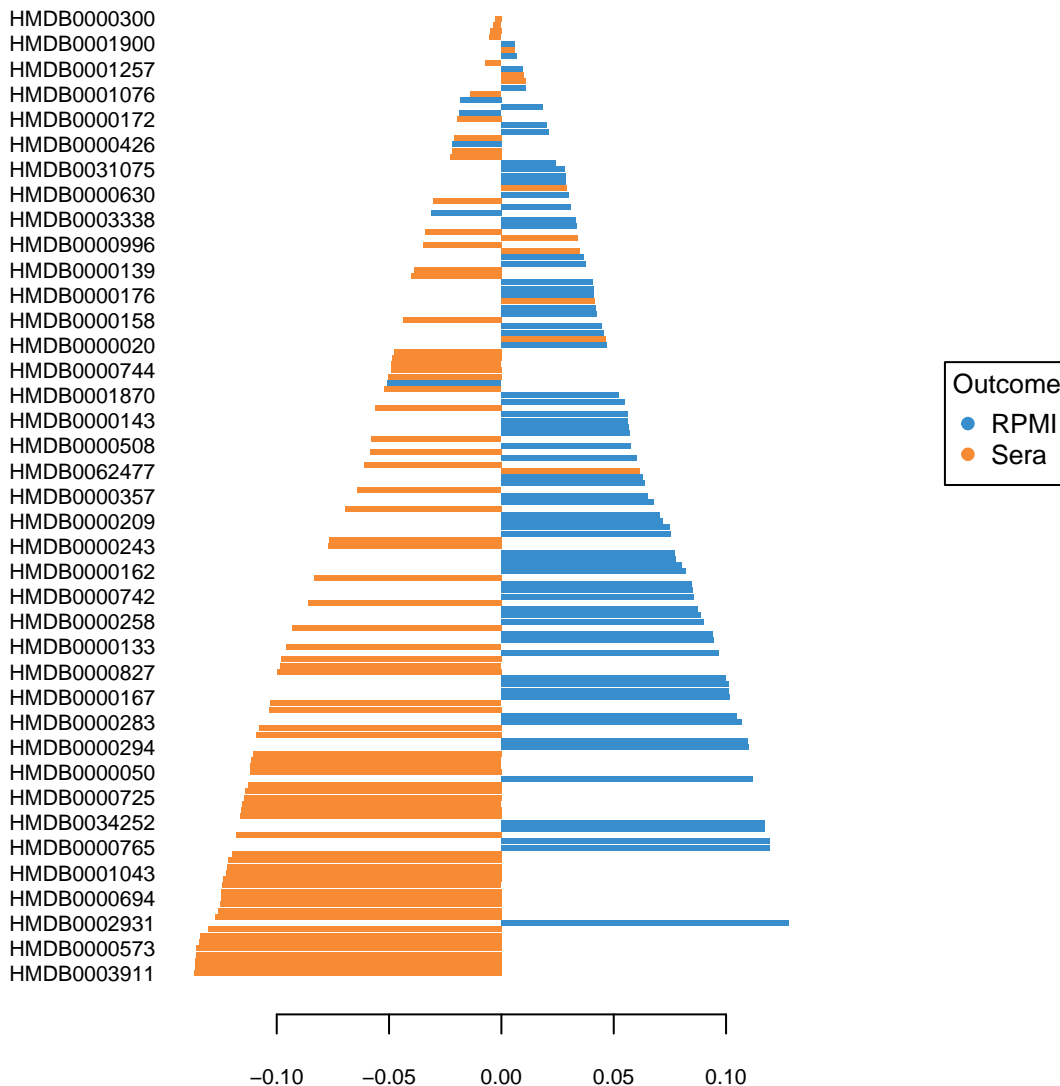
Metabolomics 1 PLSDA max load



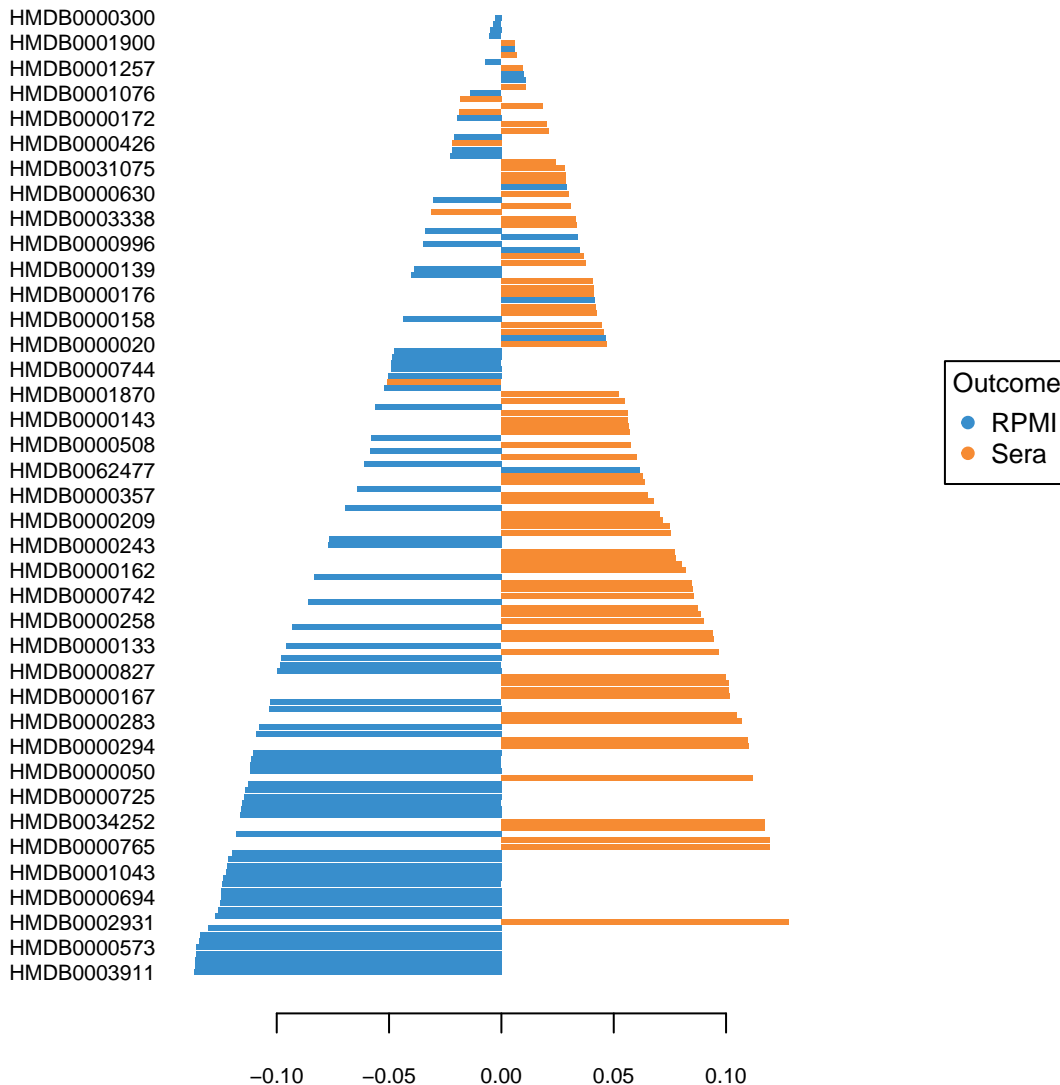
Metabolomics 1 PLSDA min load



Contribution on comp 1

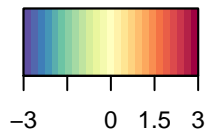


Contribution on comp 1



PLSDA Component 2

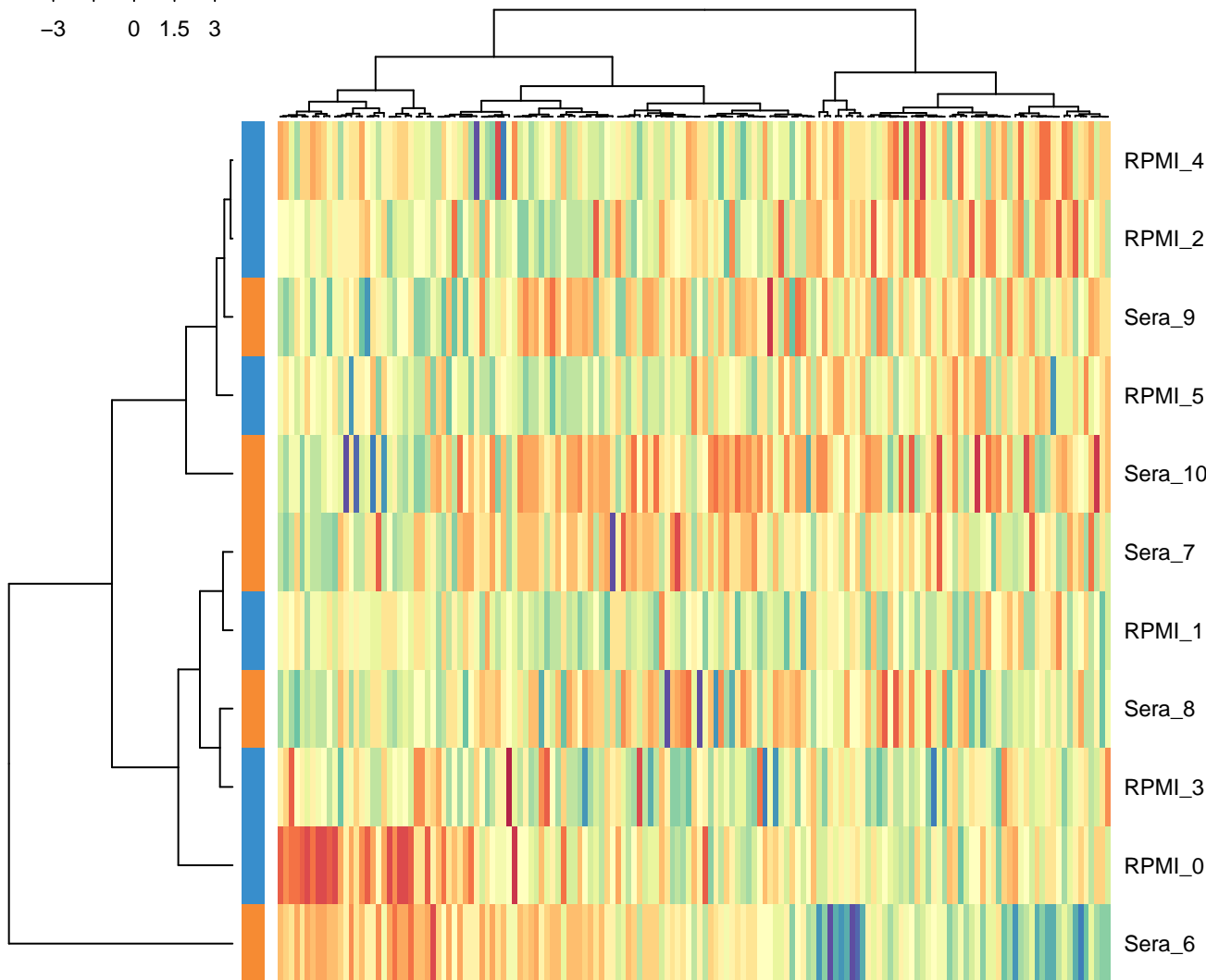
Color key



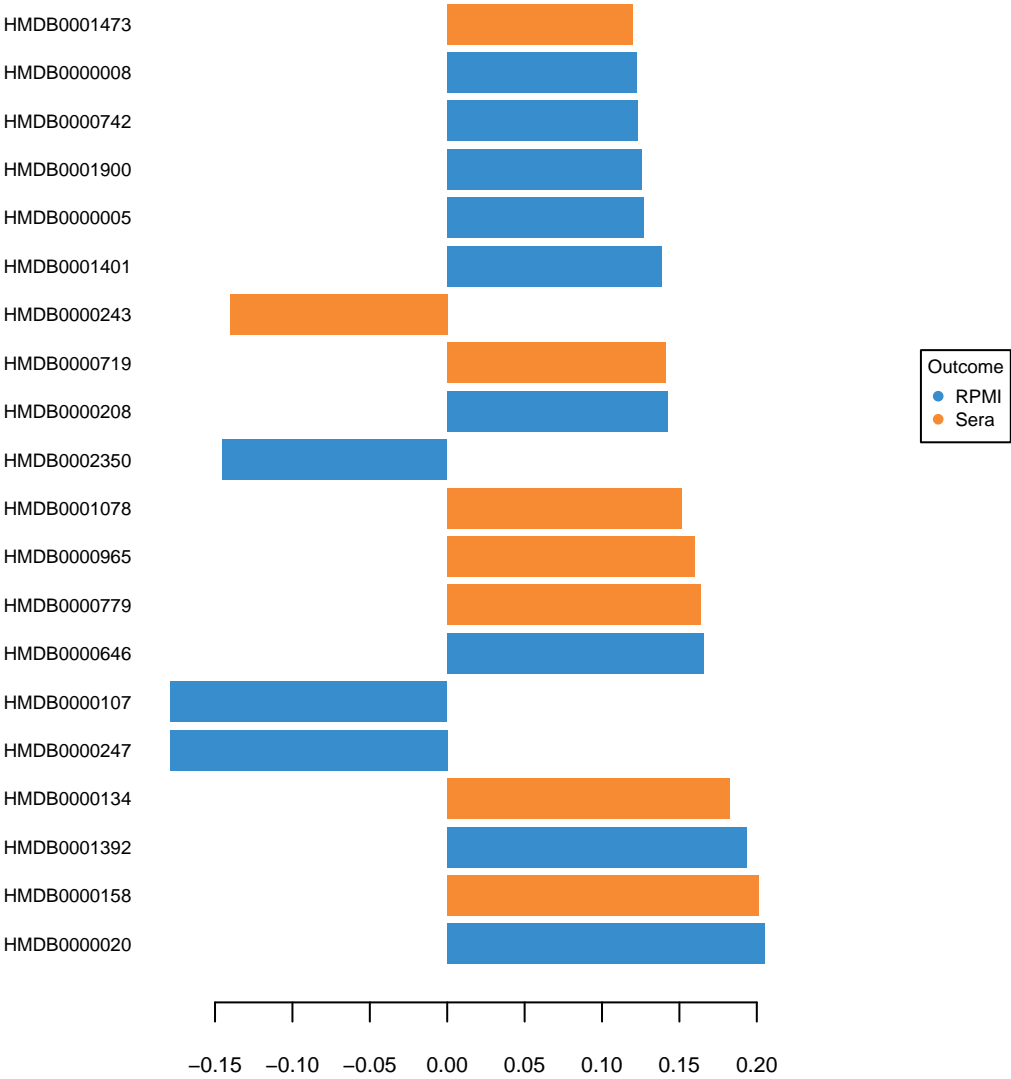
Status

RPMI

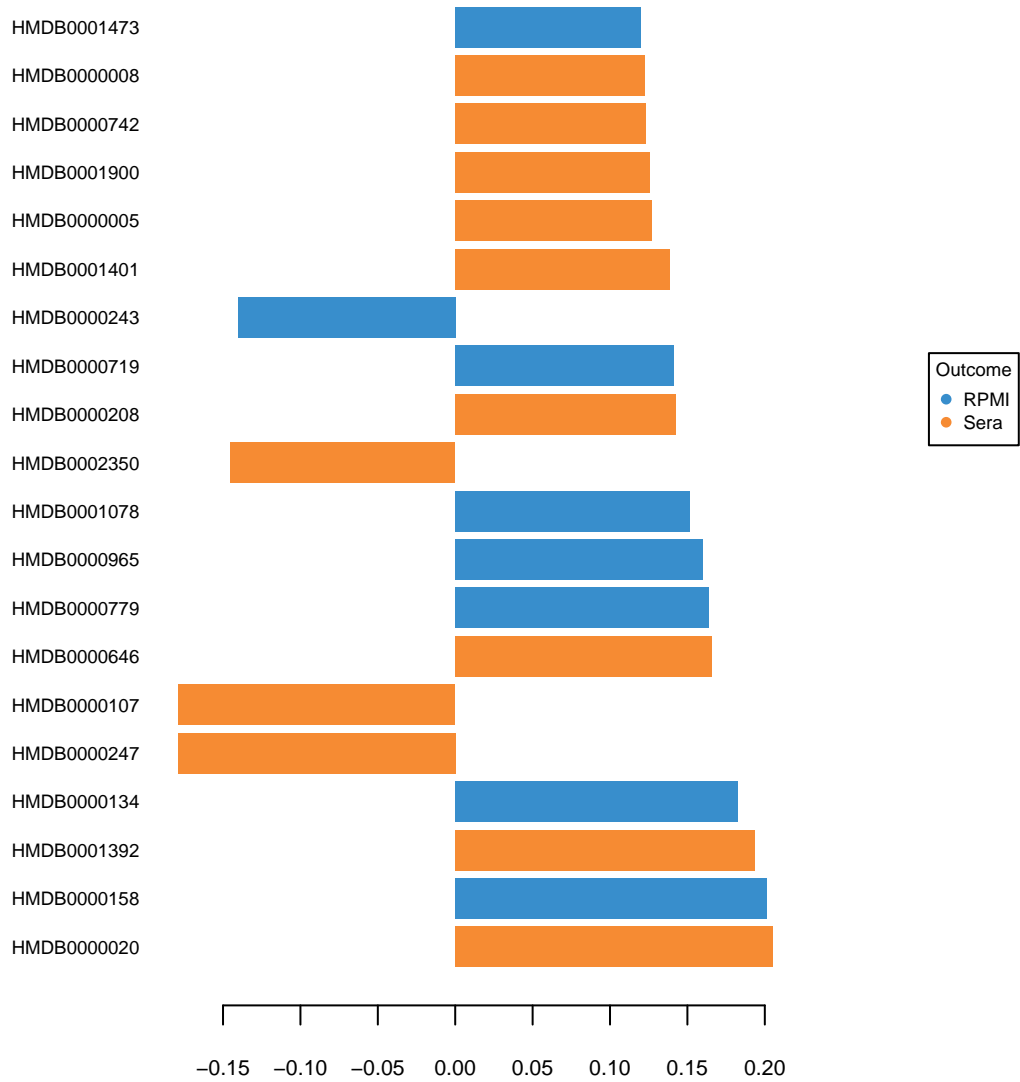
Sera



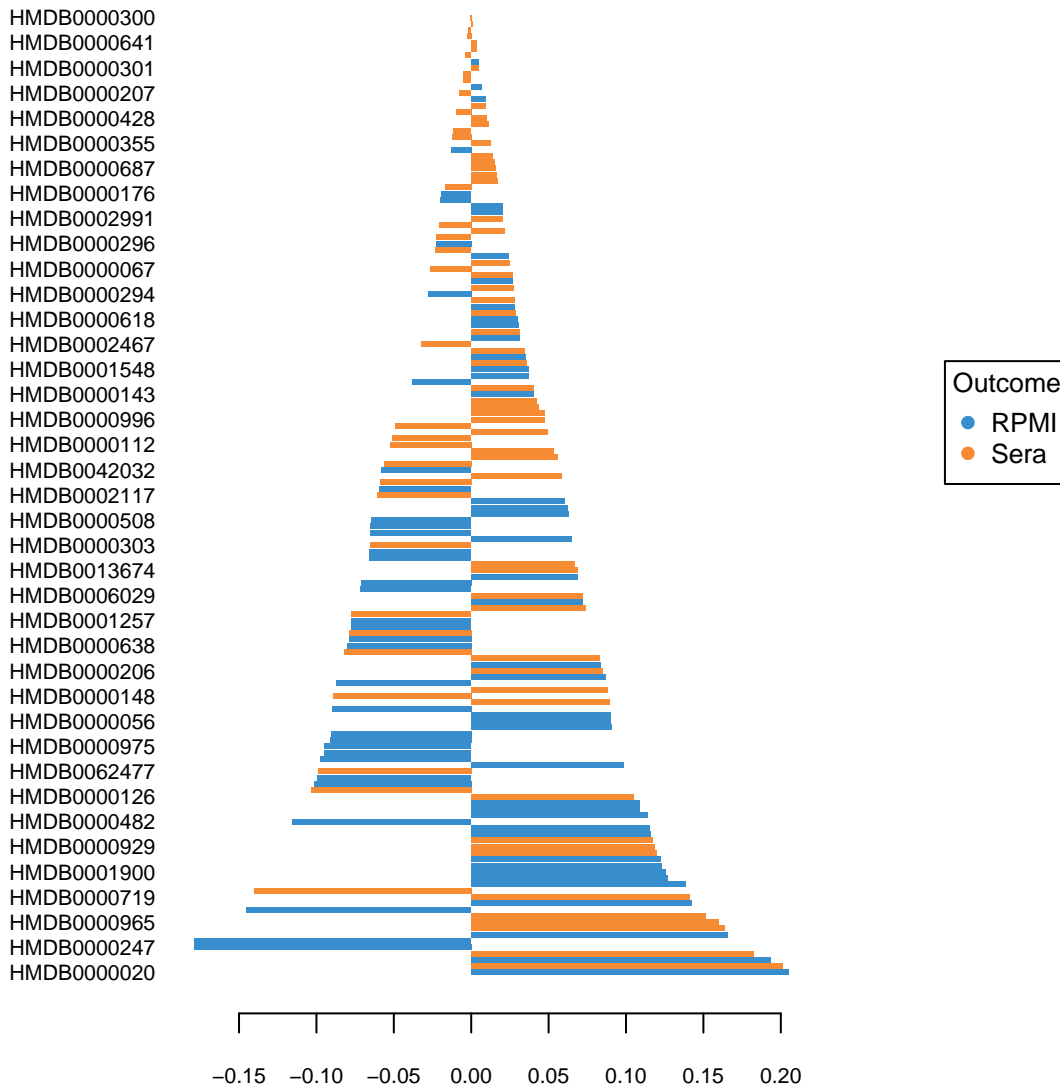
Metabolomics 2 PLSDA max load



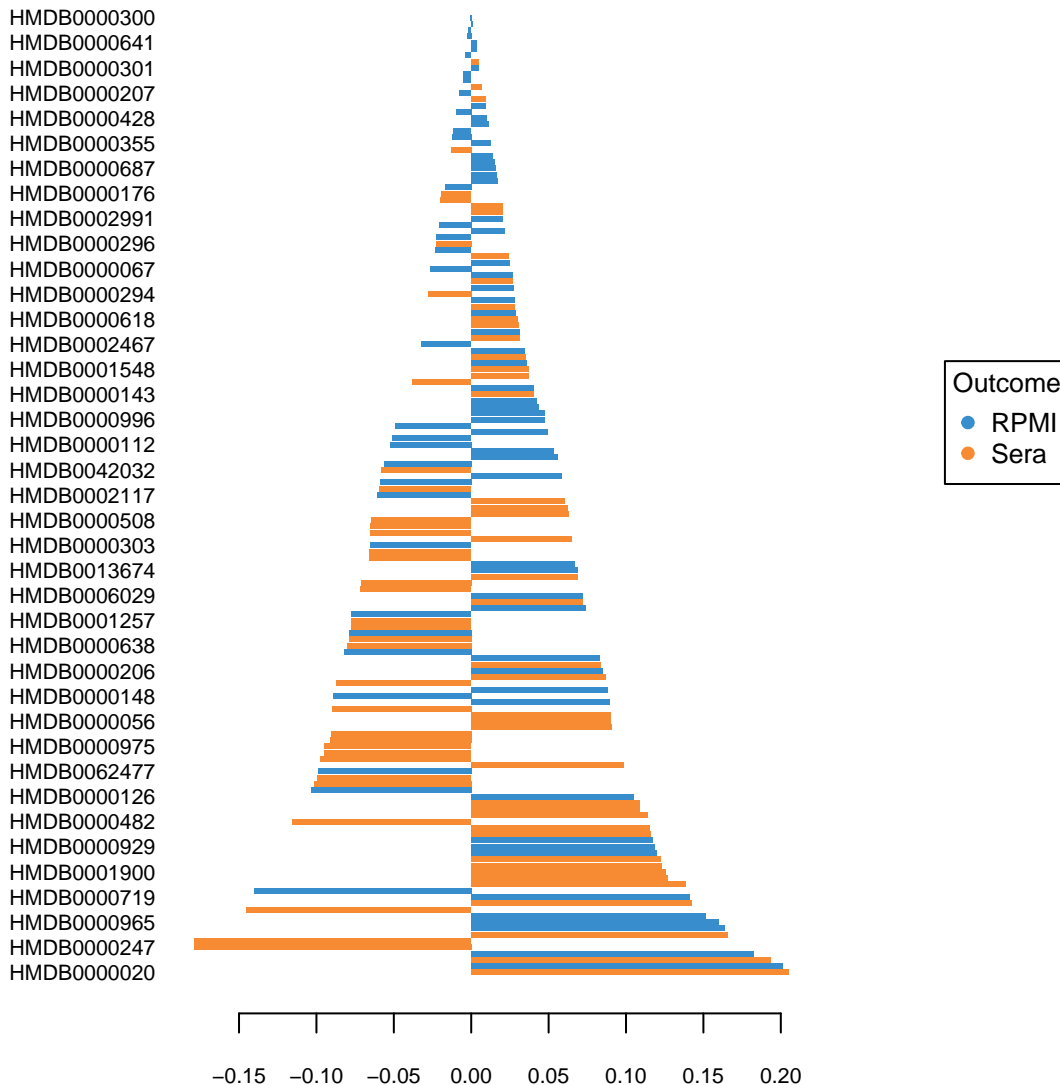
Metabolomics 2 PLSDA min load



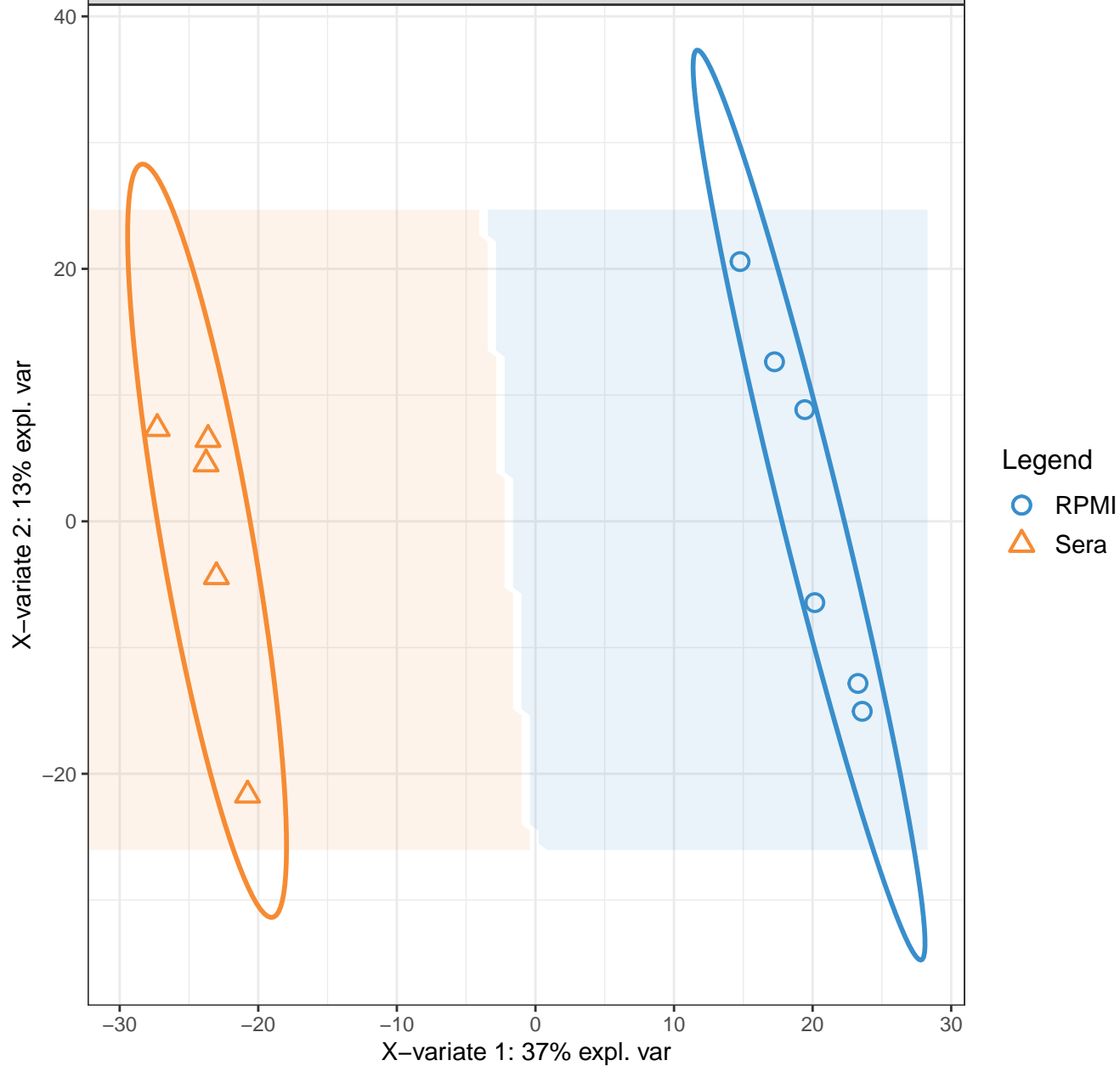
Contribution on comp 2



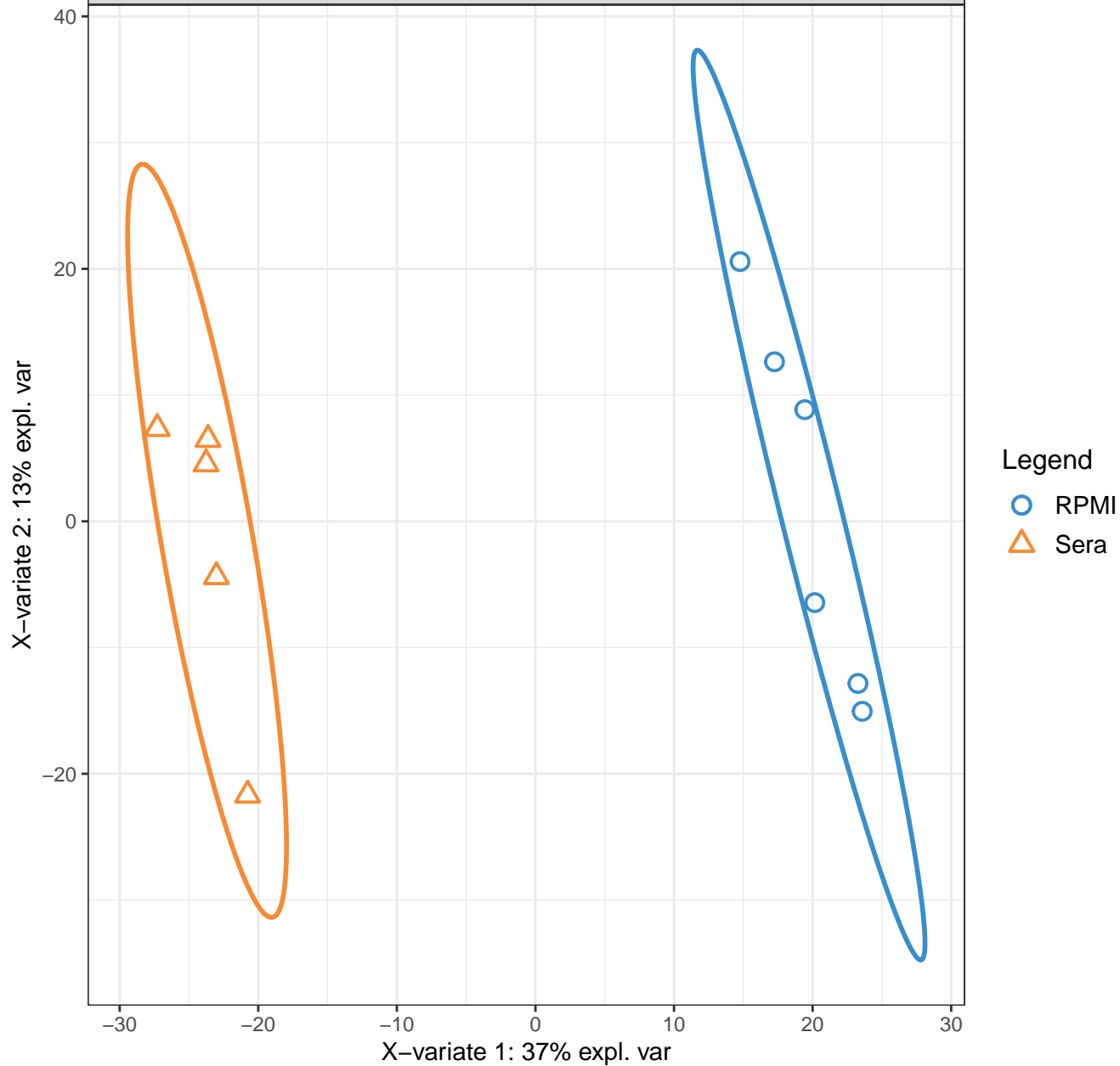
Contribution on comp 2



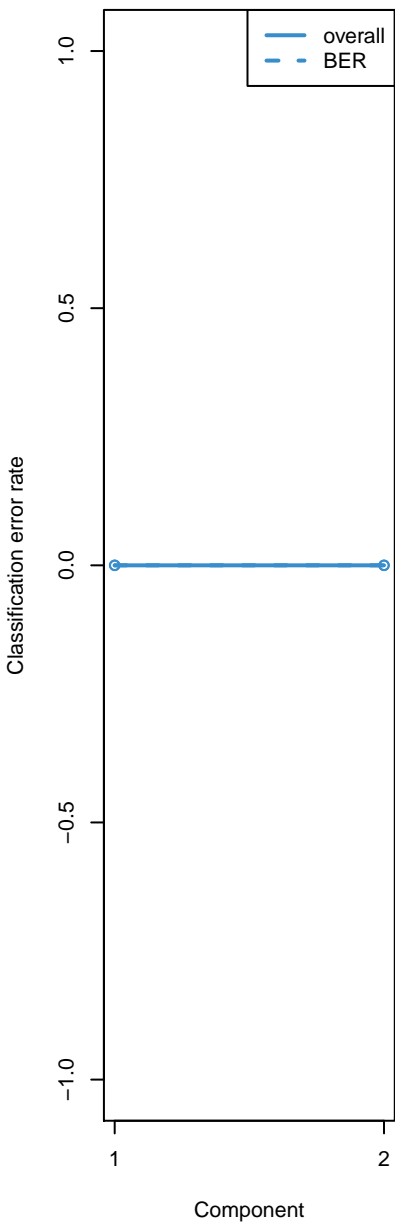
Proteomics PLSDA single 1/2



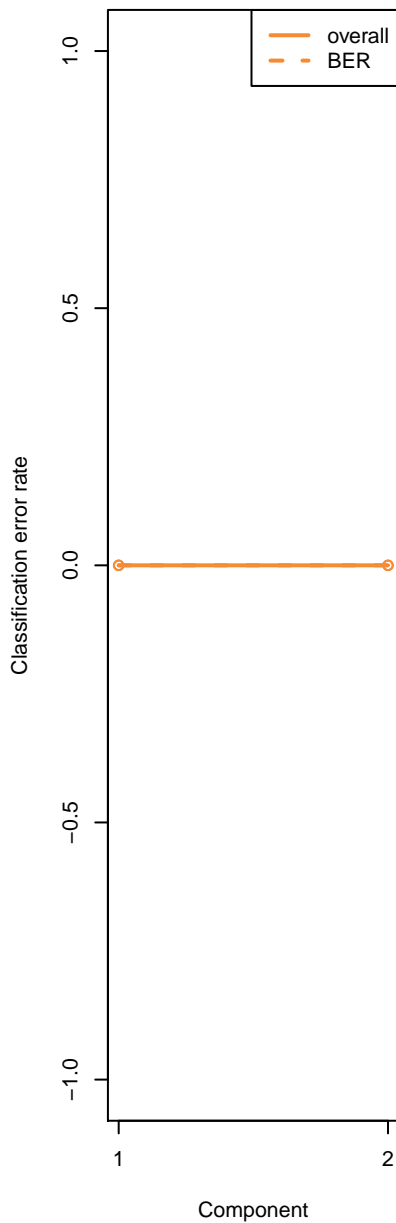
Proteomics PLSDA single 1/2



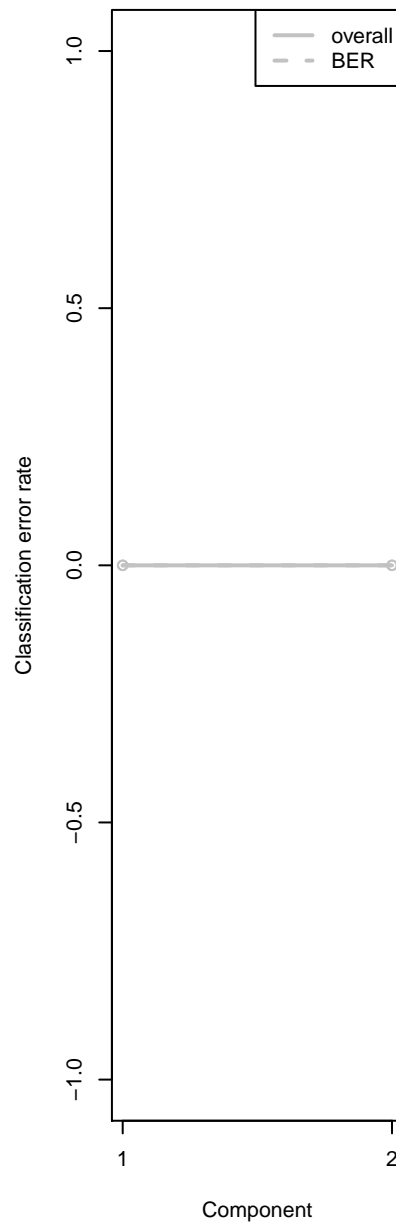
max.dist



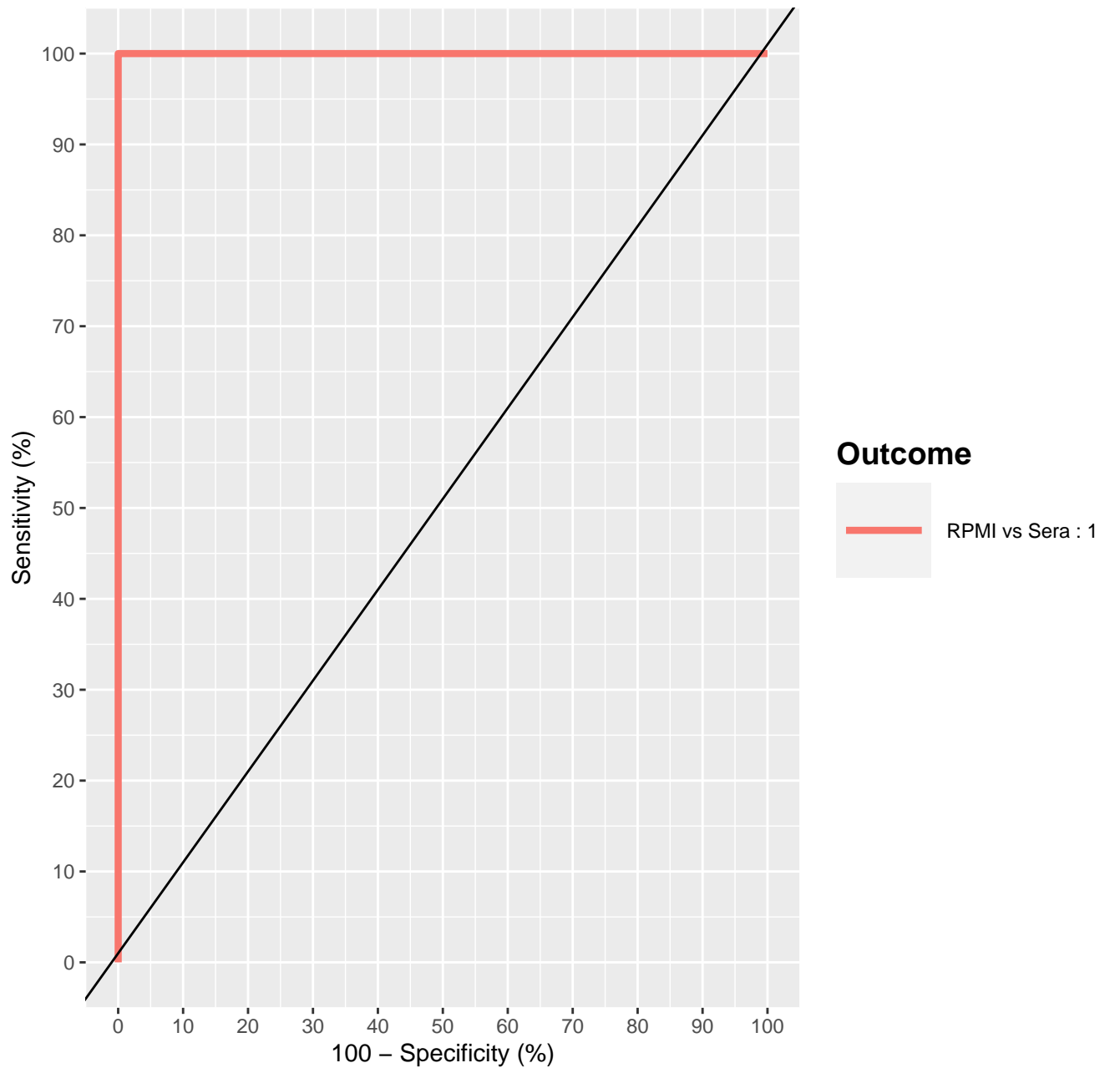
centroids.dist



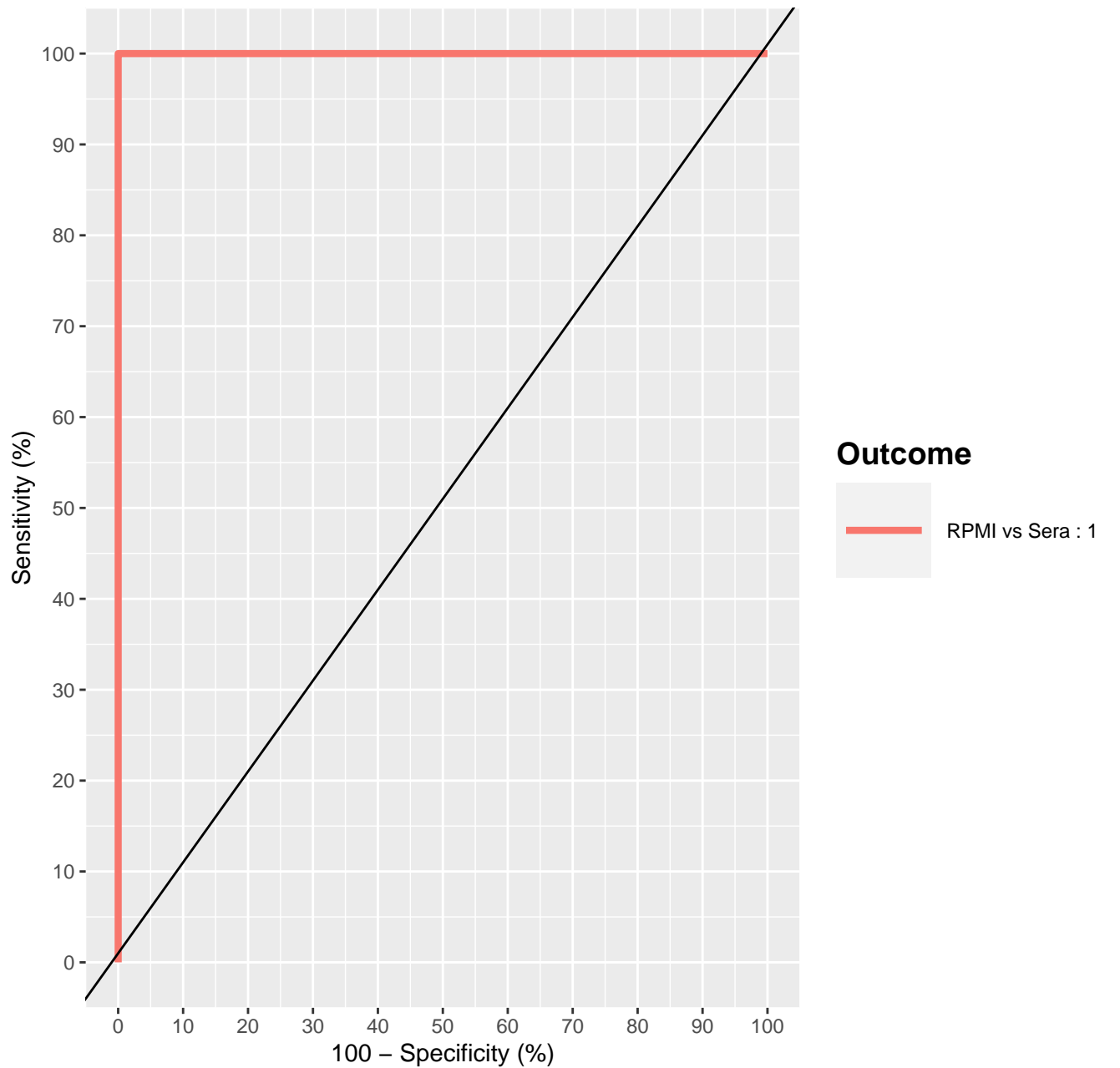
mahalanobis.dist



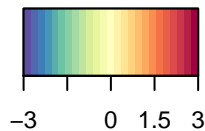
ROC Curve Comp 1



ROC Curve Comp 2



Color key

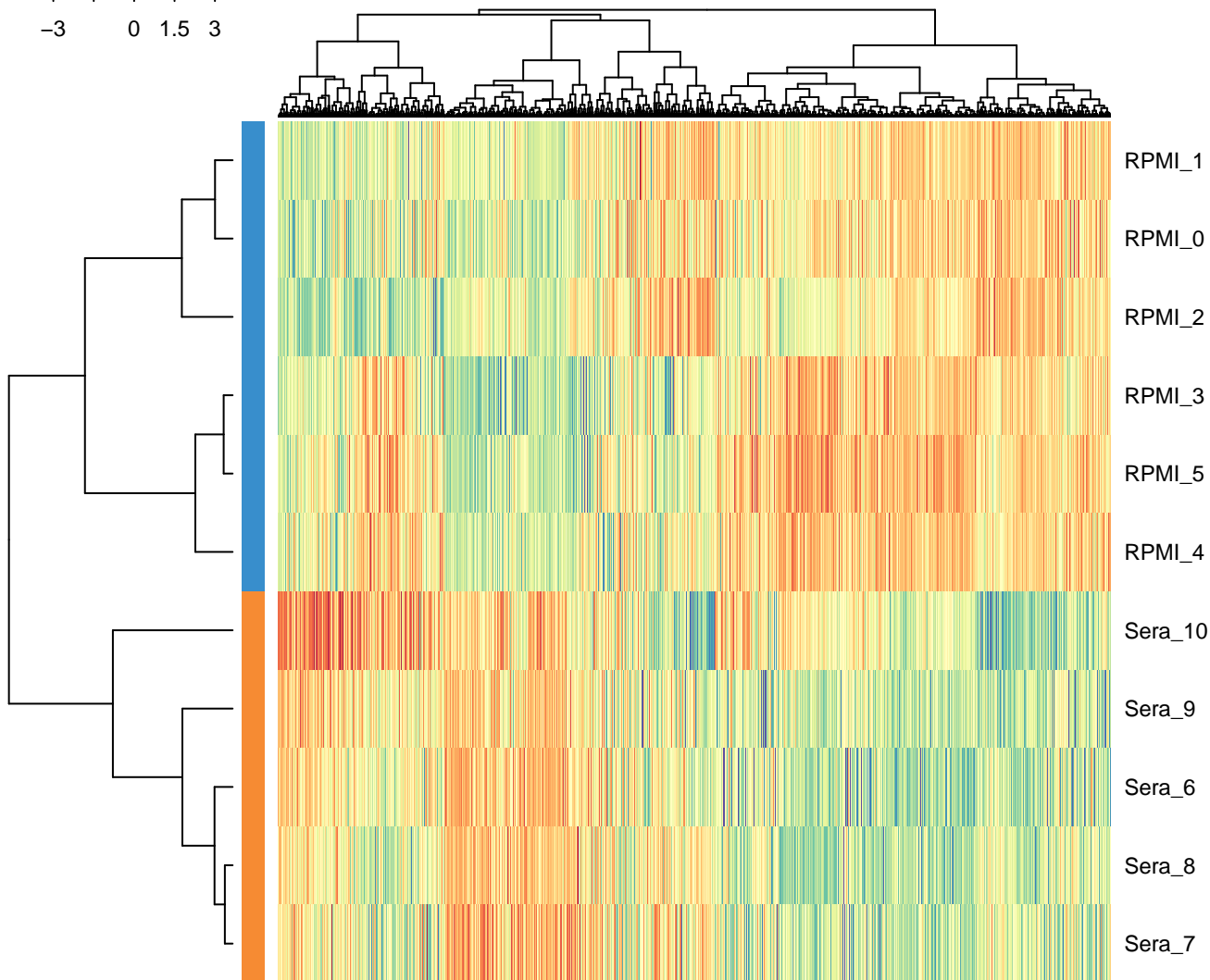


PLSDA

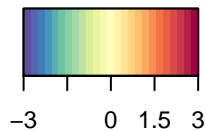
Status

■ RPMI

■ Sera



Color key

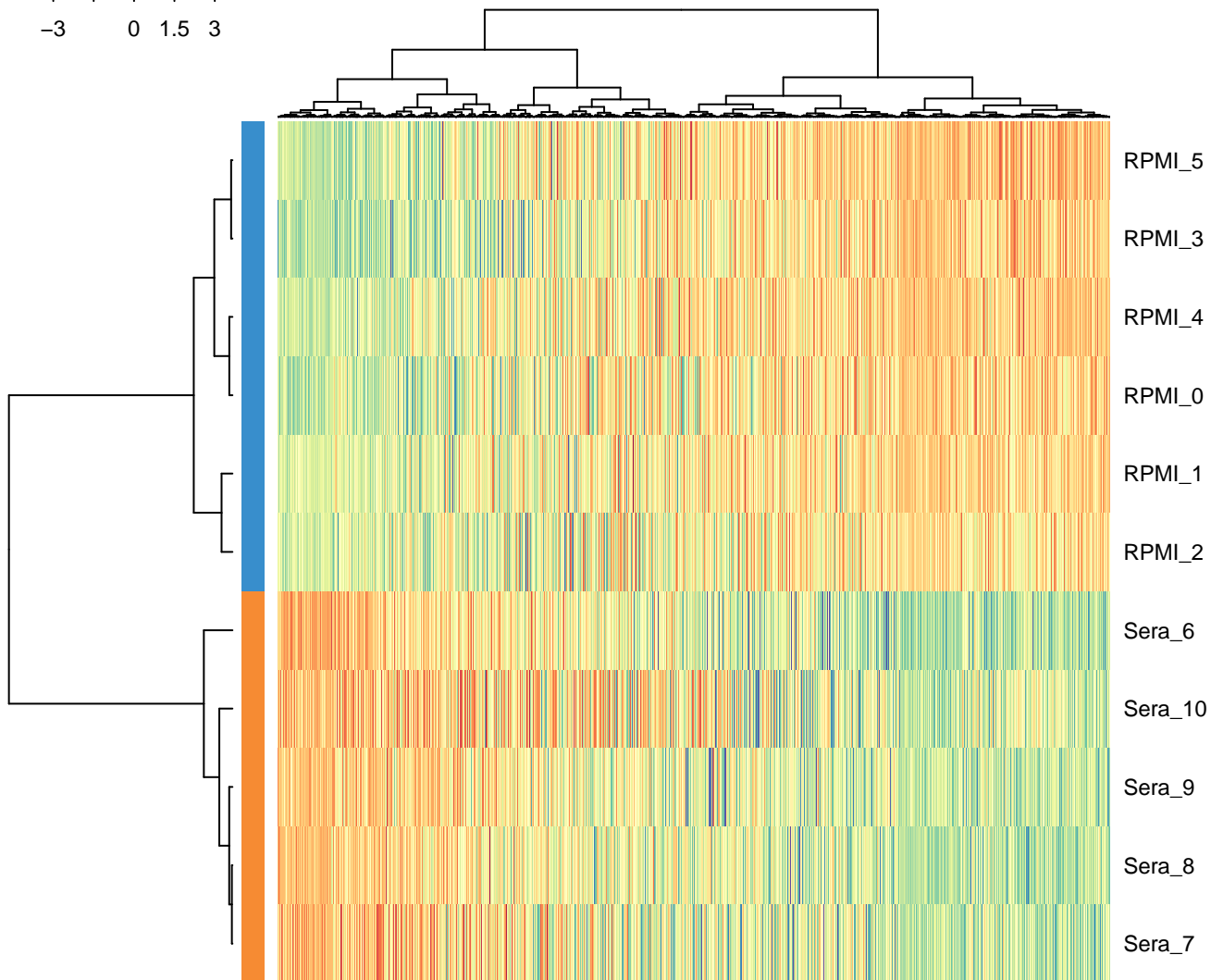


PLSDA Component 1

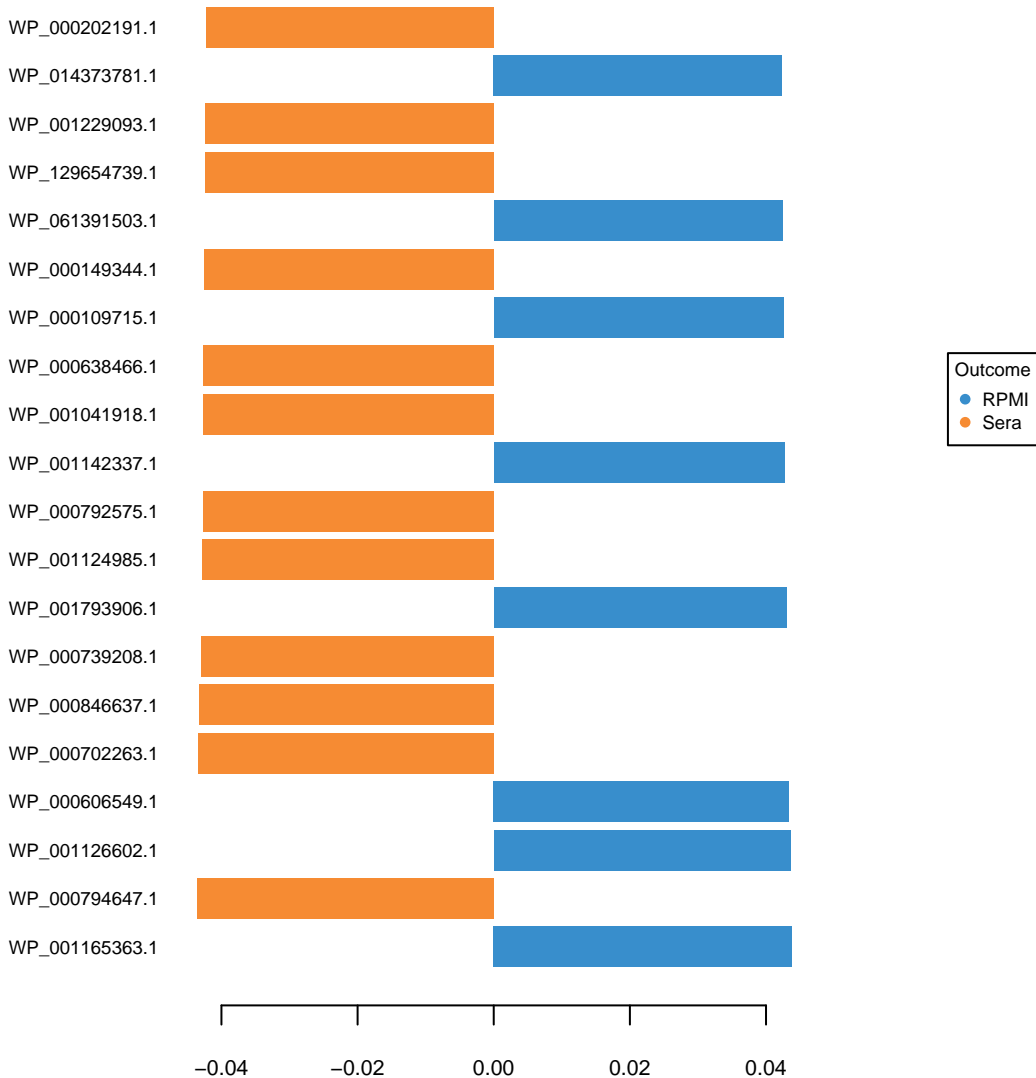
Status

RPMI

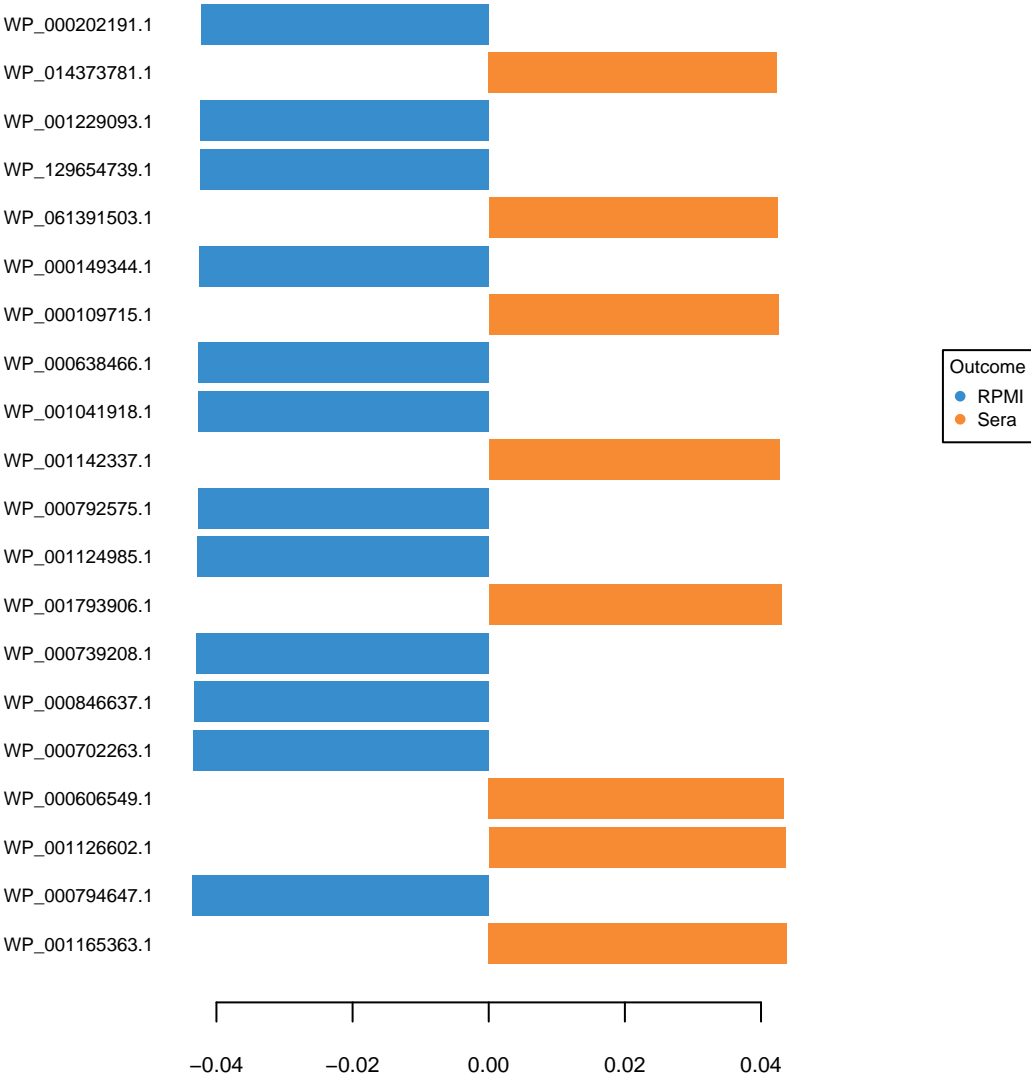
Sera



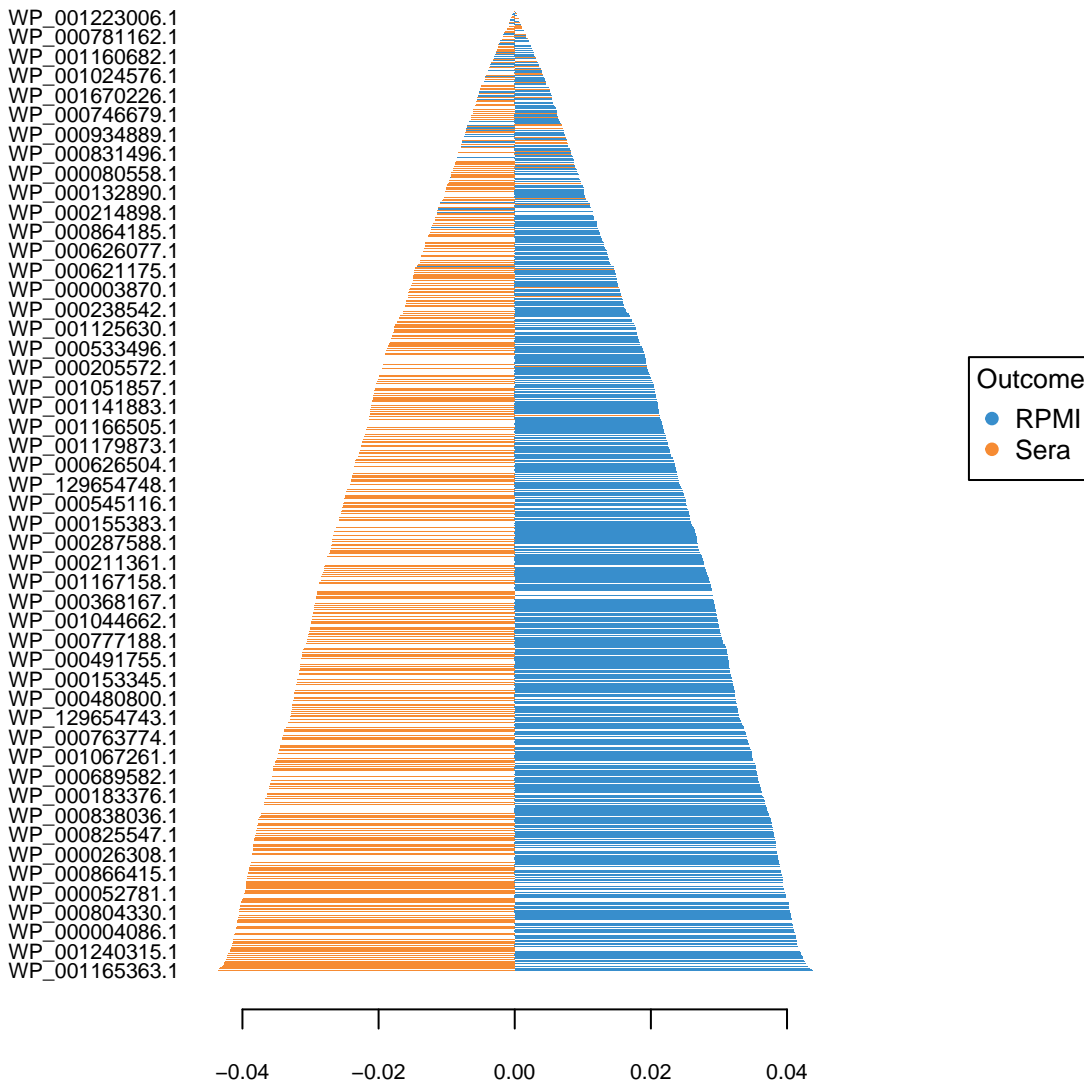
Proteomics 1 PLSDA max loadings



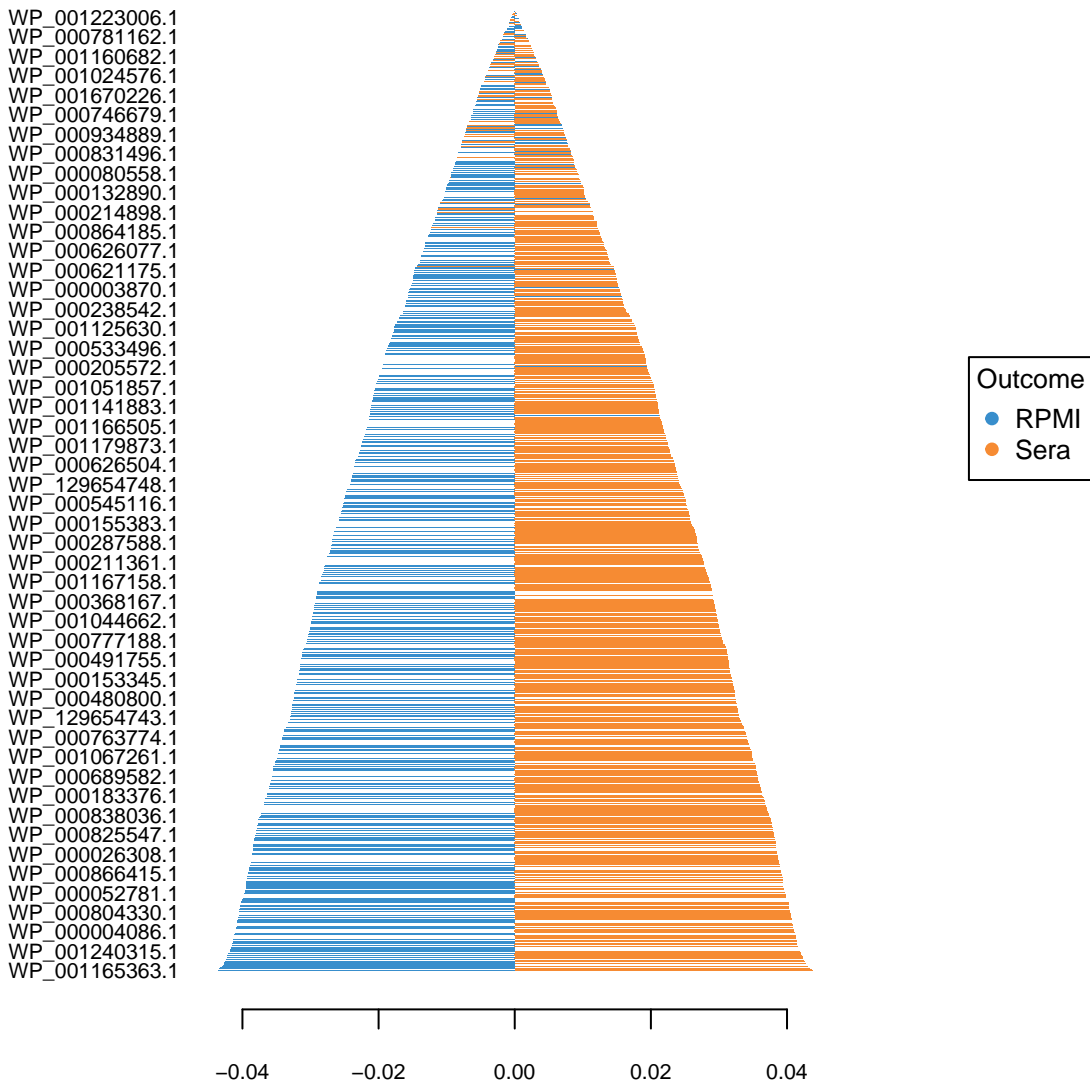
Proteomics 1 PLSDA min load



Contribution on comp 1



Contribution on comp 1



Color key

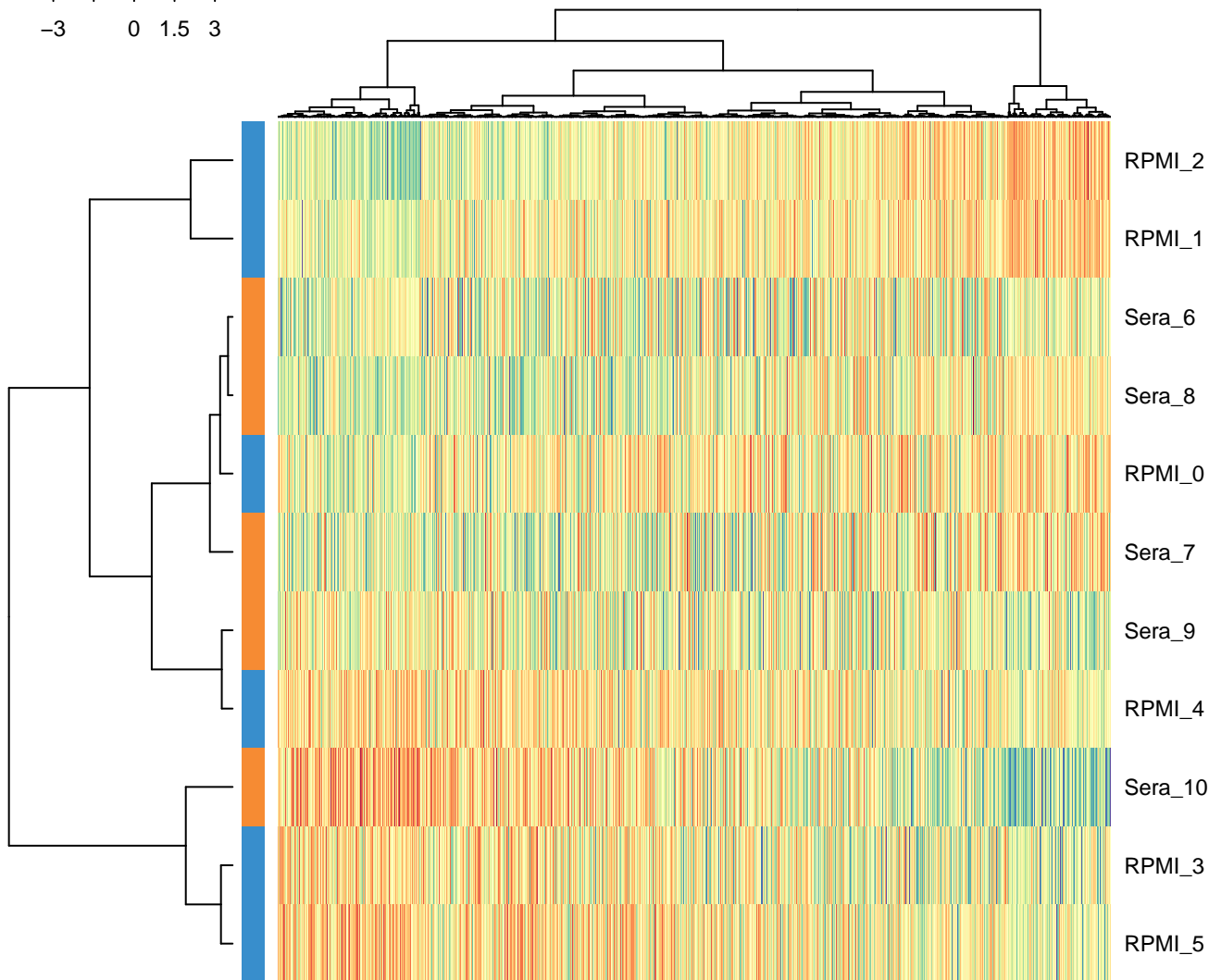
PLSDA Component 2

Status

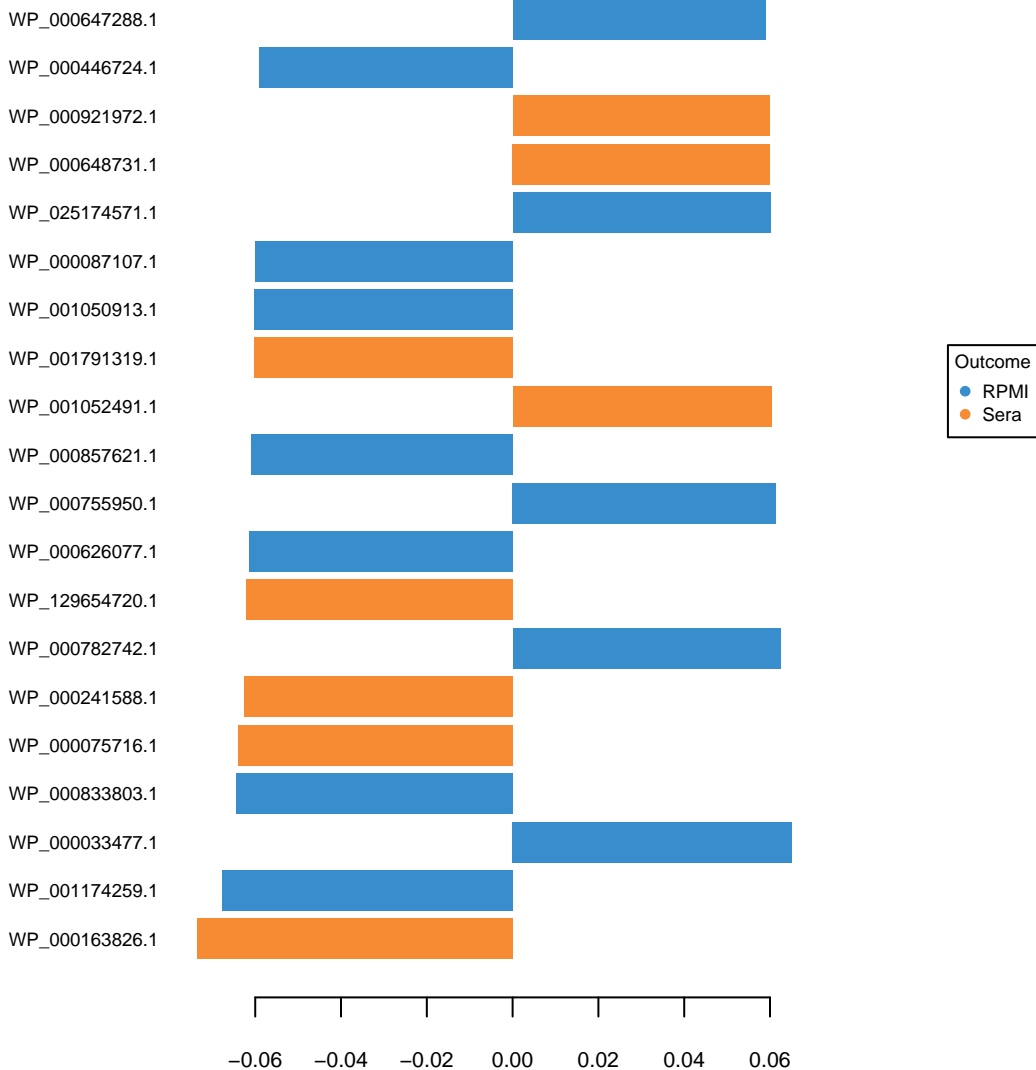
RPMI

Sera

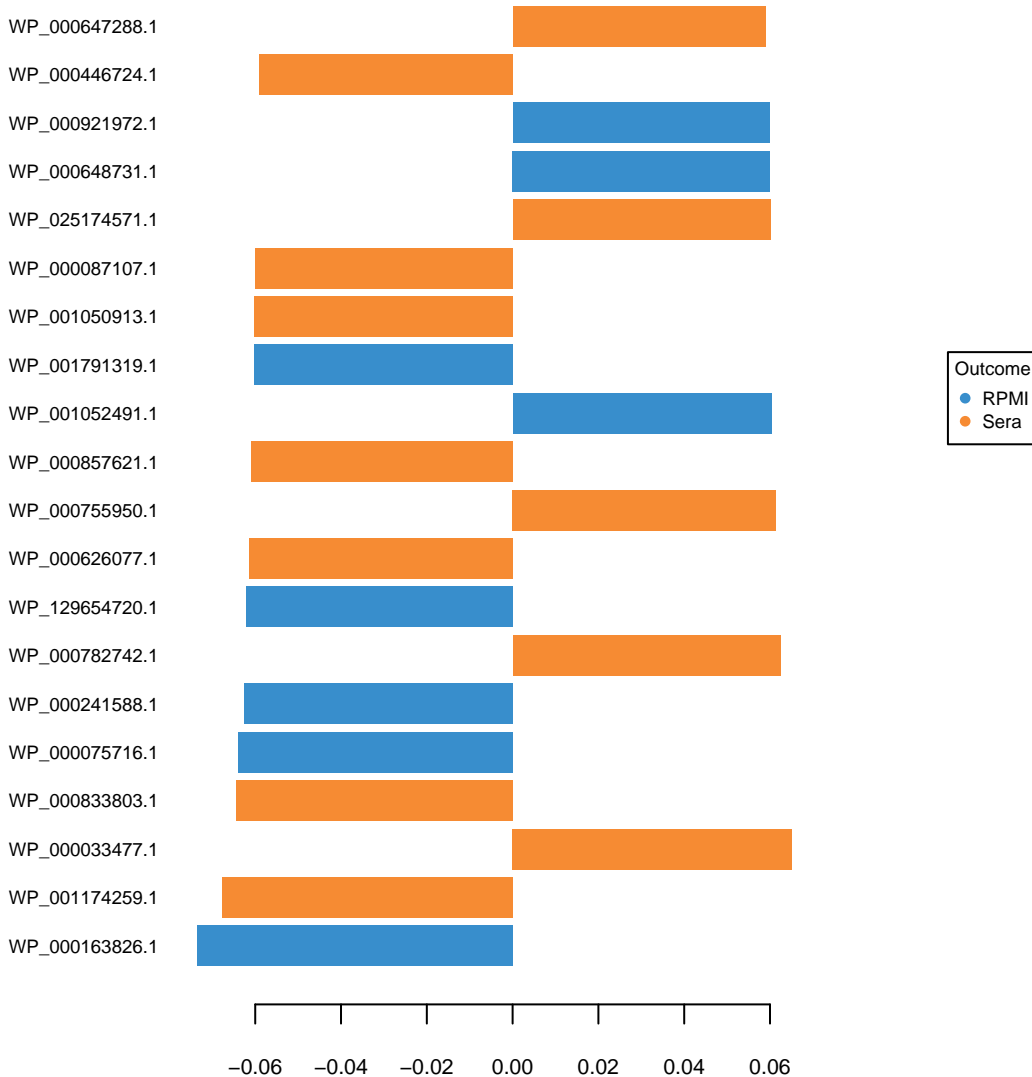
-3 0 1.5 3



Proteomics 2 PLSDA max loadings

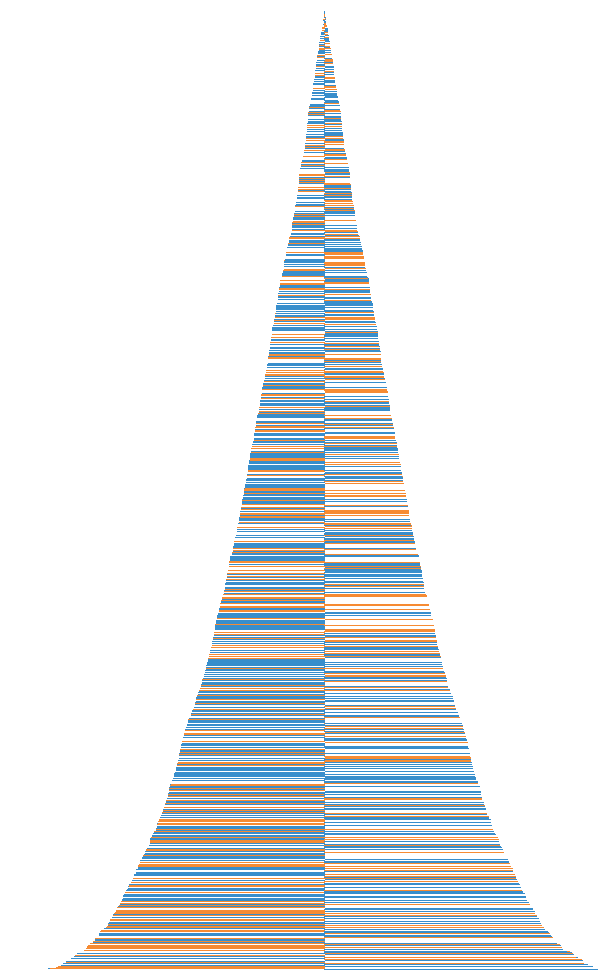


Proteomics 2 PLSDA min load



Contribution on comp 2

WP_000220938.1
WP_129654728.1
WP_001222133.1
WP_000862728.1
WP_000479573.1
WP_000547687.1
WP_000435071.1
WP_000251253.1
WP_000608837.1
WP_001126602.1
WP_000062417.1
WP_000616864.1
WP_000154918.1
WP_000024827.1
WP_000731878.1
WP_000514373.1
WP_001250329.1
WP_001670298.1
WP_000611469.1
WP_000902175.1
WP_000024119.1
WP_001789170.1
WP_000775173.1
WP_001167828.1
WP_001221857.1
WP_000708692.1
WP_000922316.1
WP_031922431.1
WP_000960863.1
WP_000566670.1
WP_001103743.1
WP_000340119.1
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WP_000524902.1
WP_000198598.1
WP_000035320.1
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WP_000514288.1
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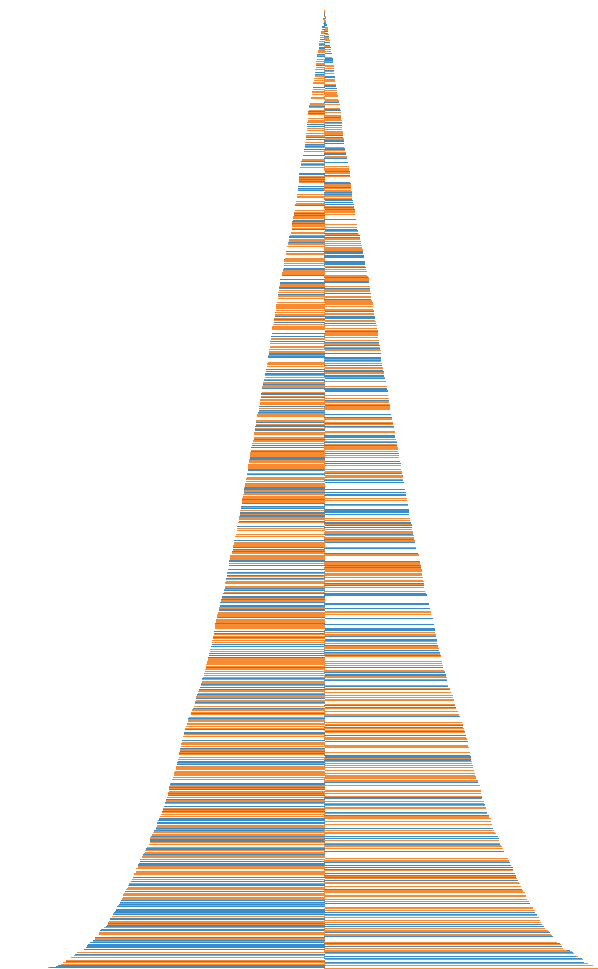
Outcome

- RPMI
- Sera

-0.06 -0.04 -0.02 0.00 0.02 0.04 0.06

Contribution on comp 2

WP_000220938.1
WP_129654728.1
WP_001222133.1
WP_000862728.1
WP_000479573.1
WP_000547687.1
WP_000435071.1
WP_000251253.1
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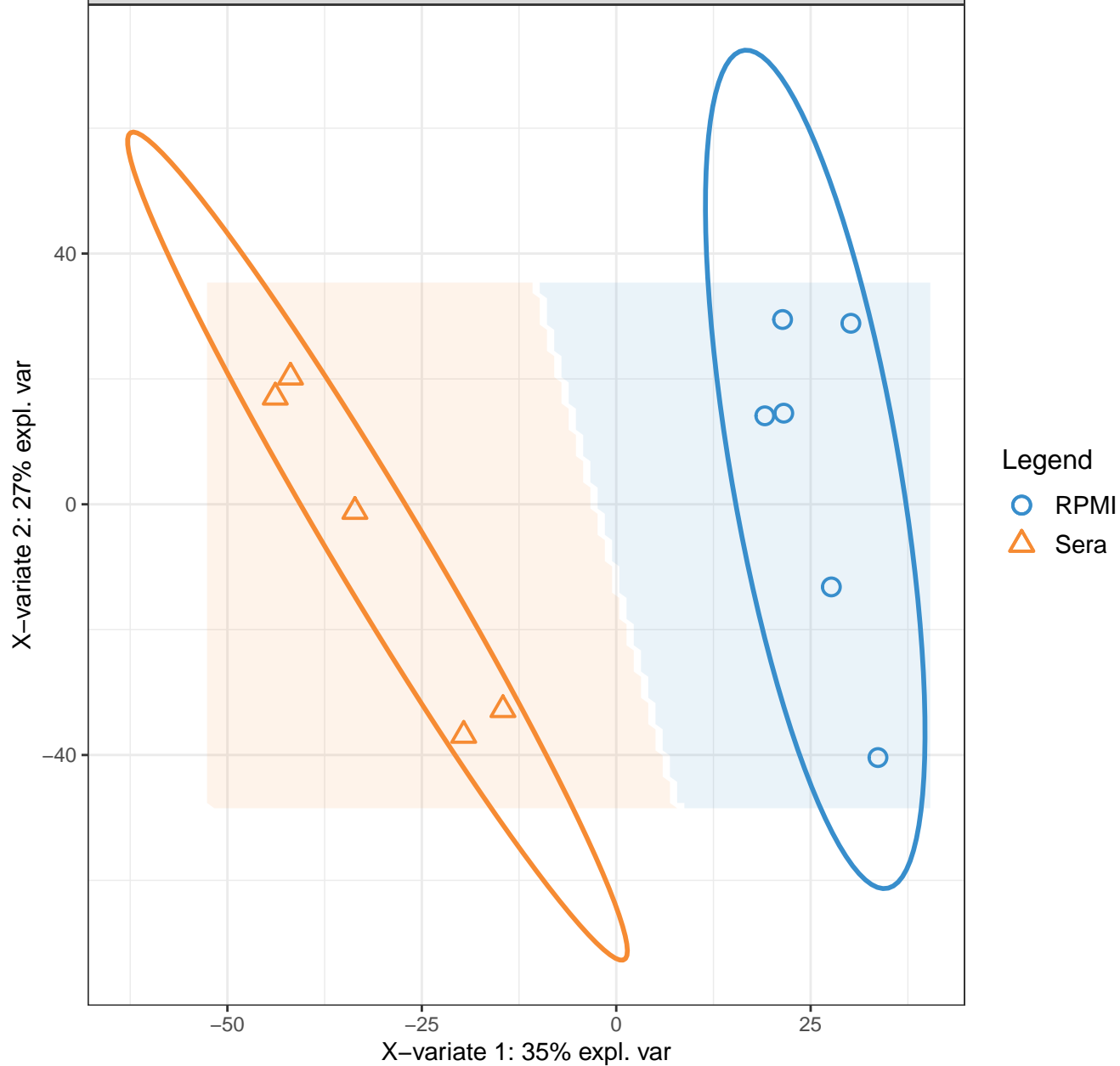


Outcome

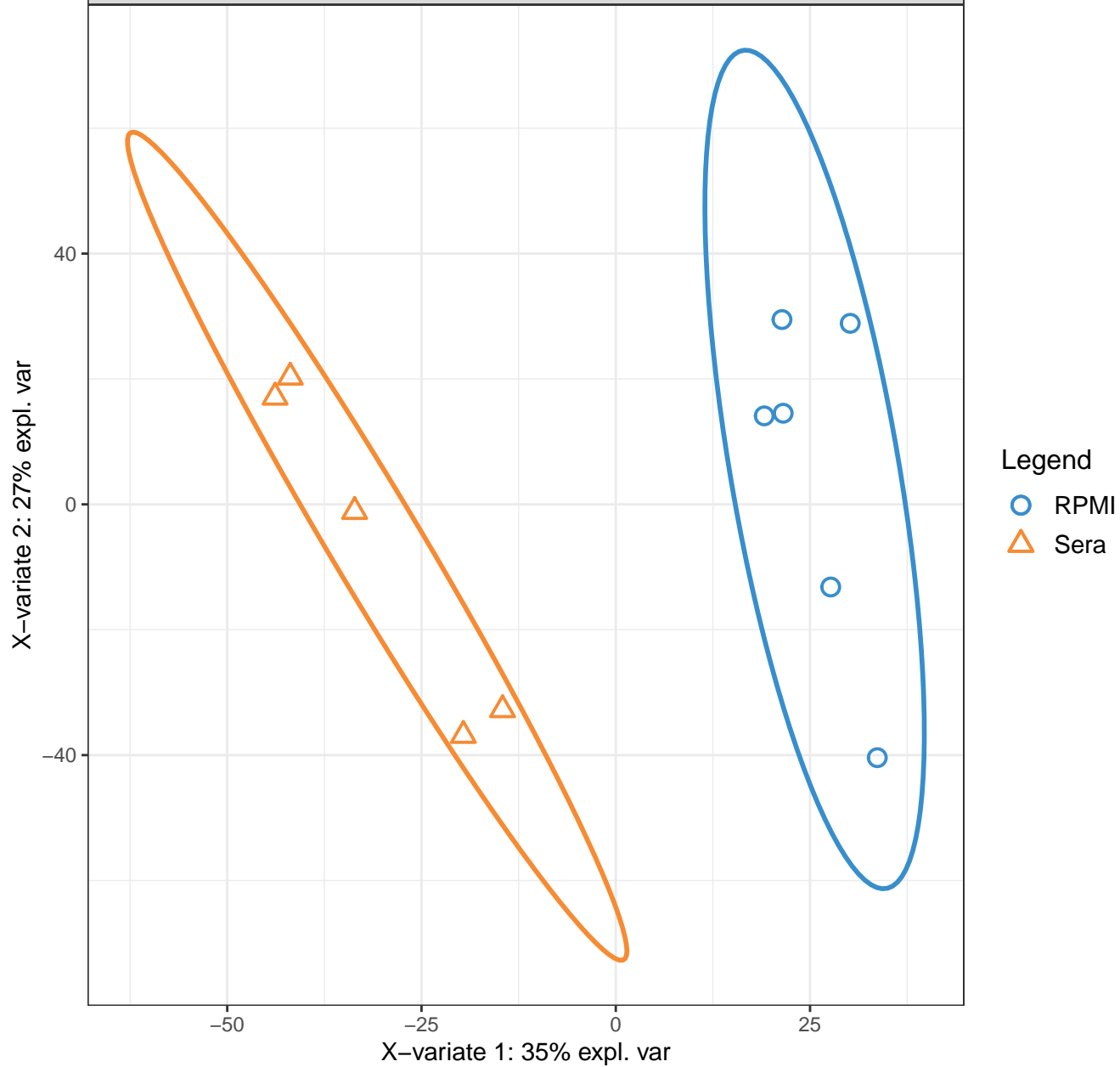
- RPMI
- Sera

-0.06 -0.04 -0.02 0.00 0.02 0.04 0.06

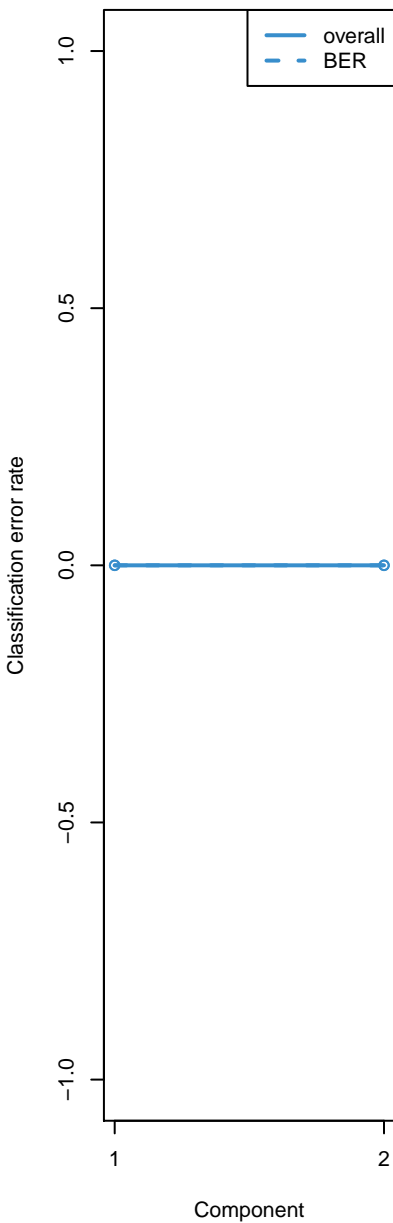
RNA_Seq PLSDA single 1/2



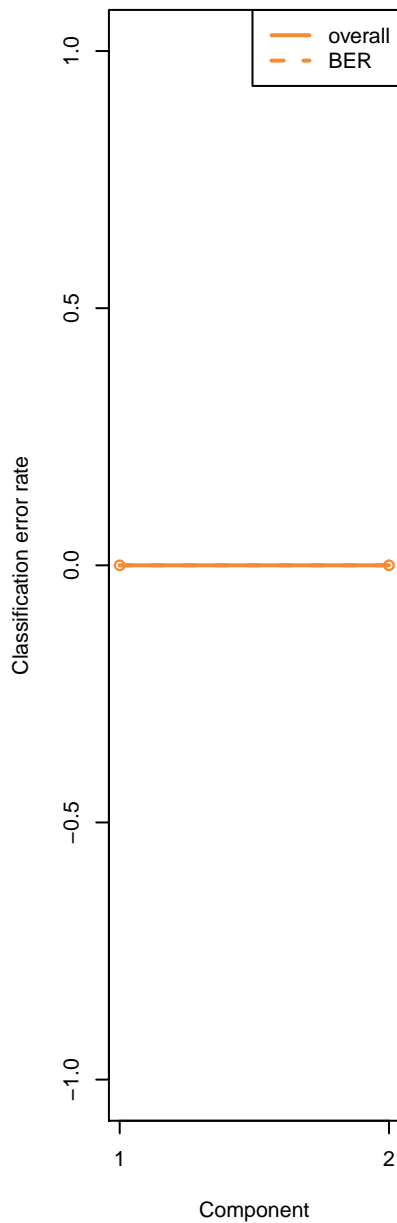
RNA_Seq PLSDA single 1/2



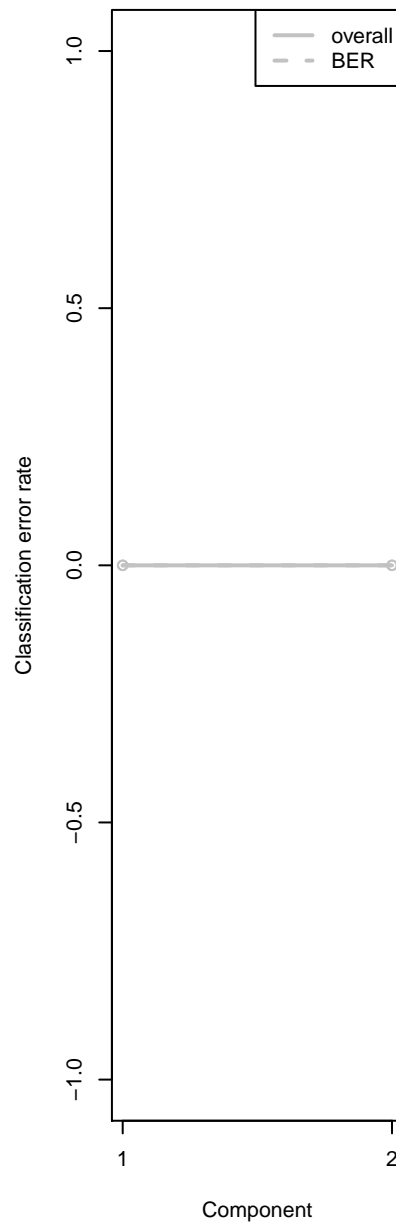
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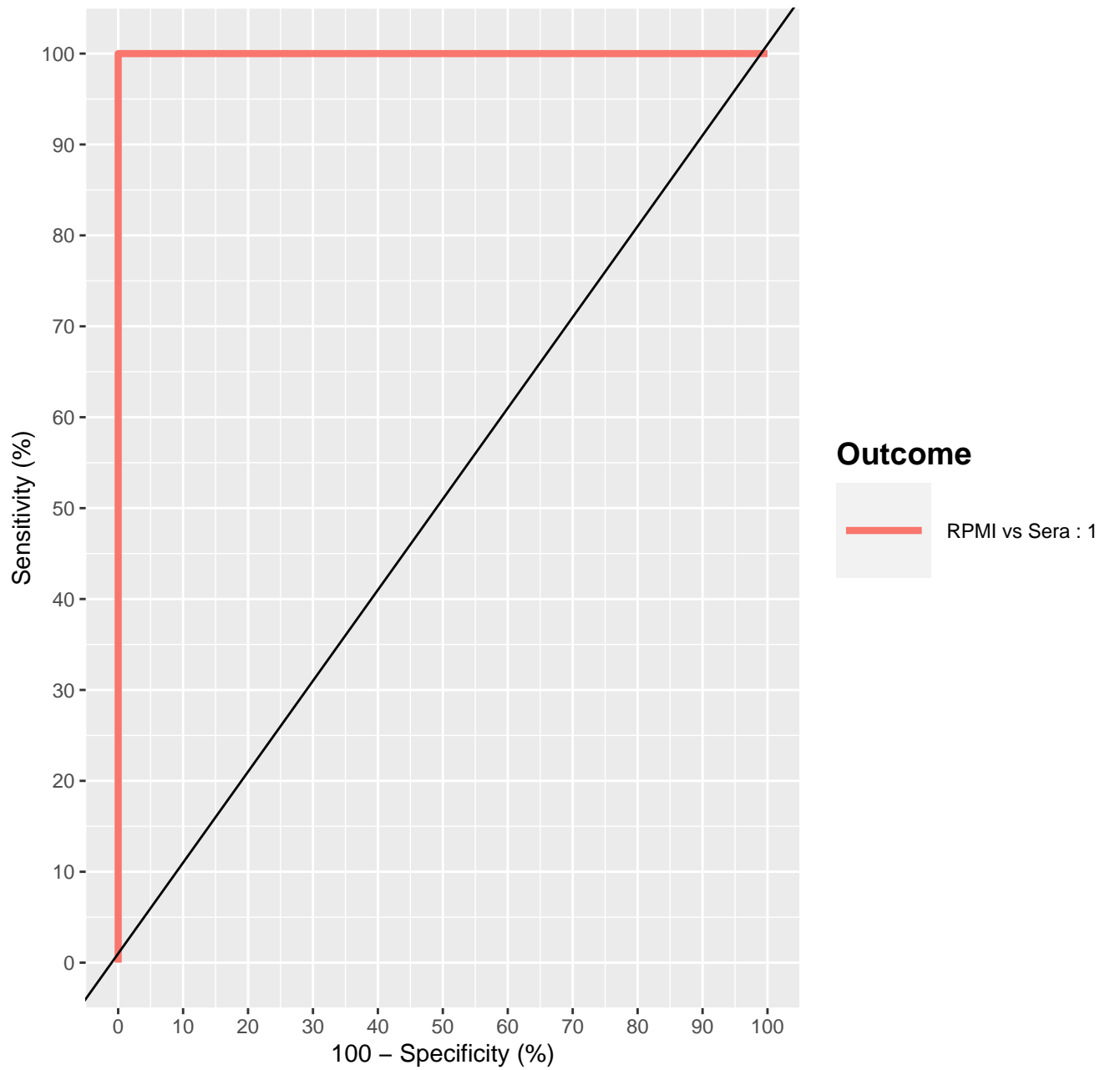
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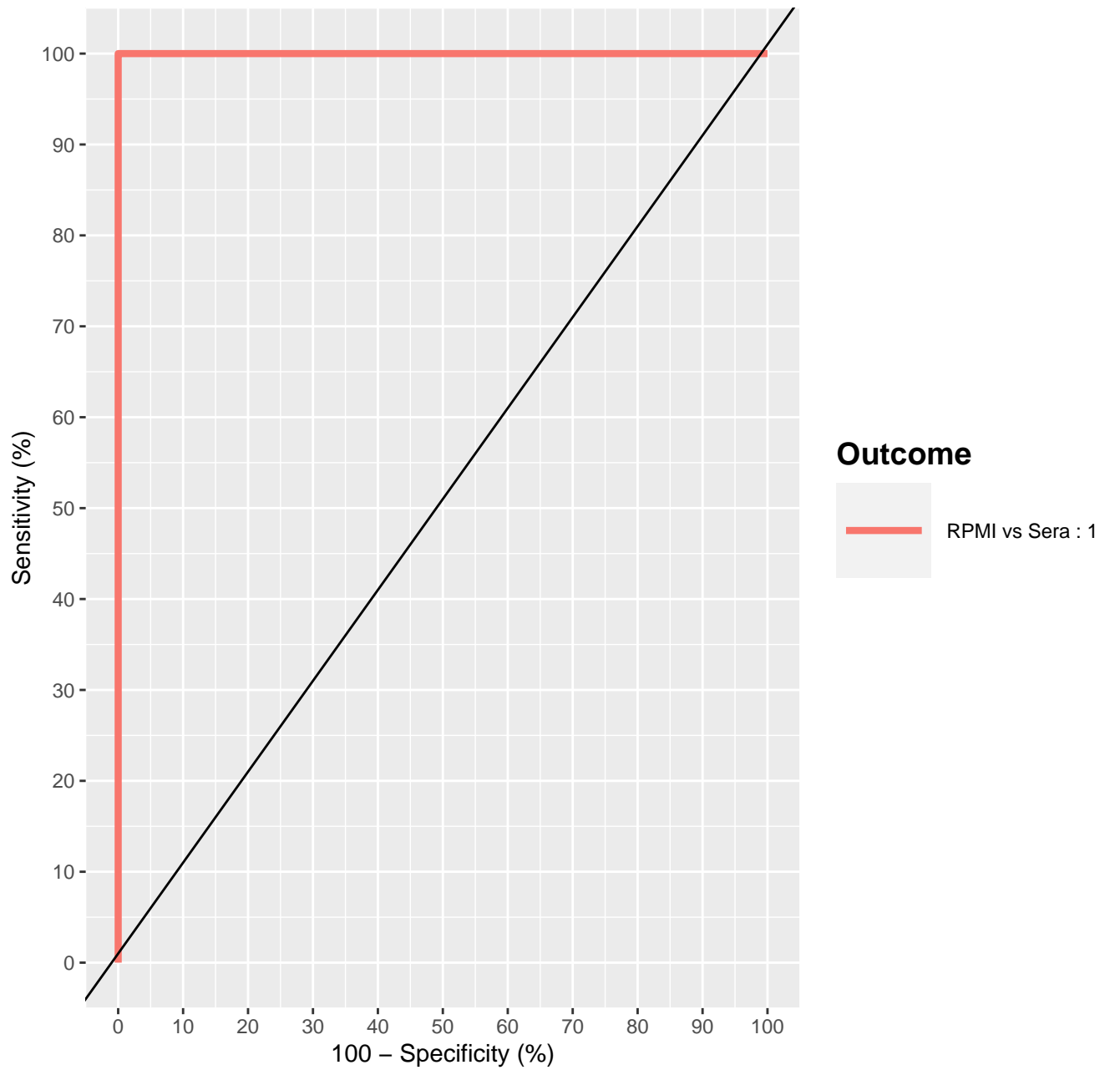
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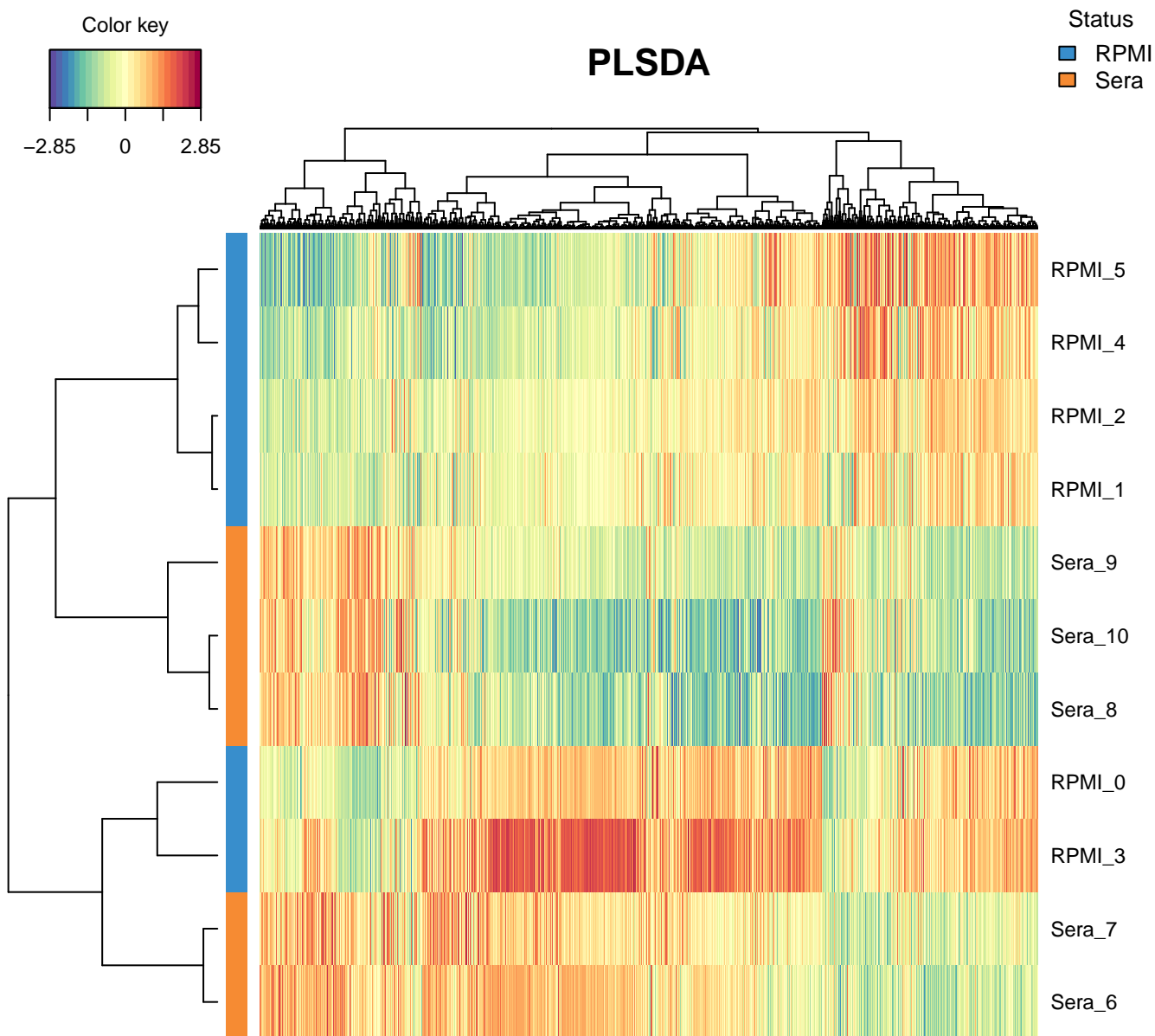


ROC Curve Comp 1

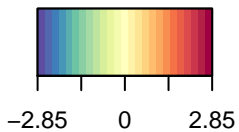


ROC Curve Comp 2





Color key

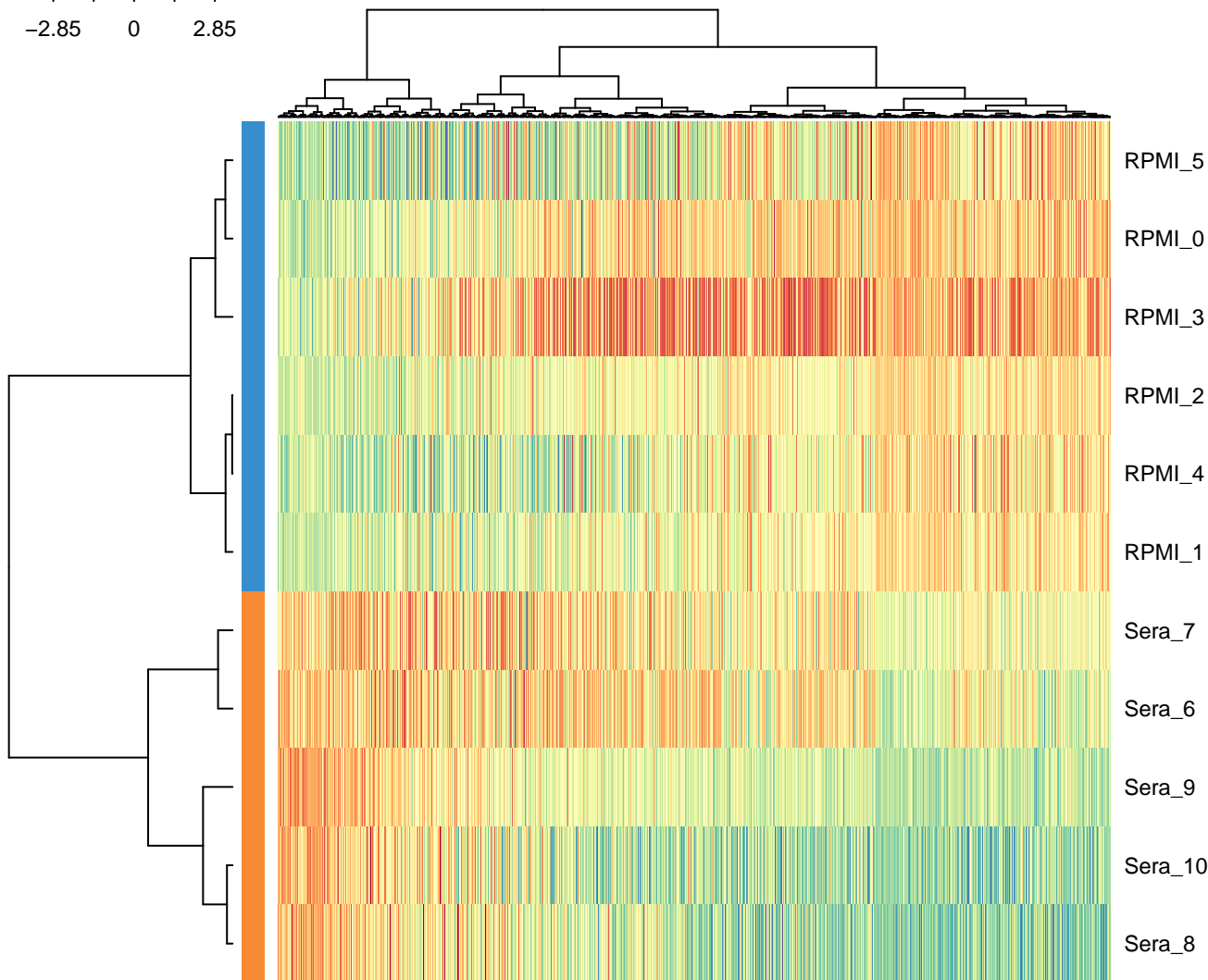


PLSDA Component 1

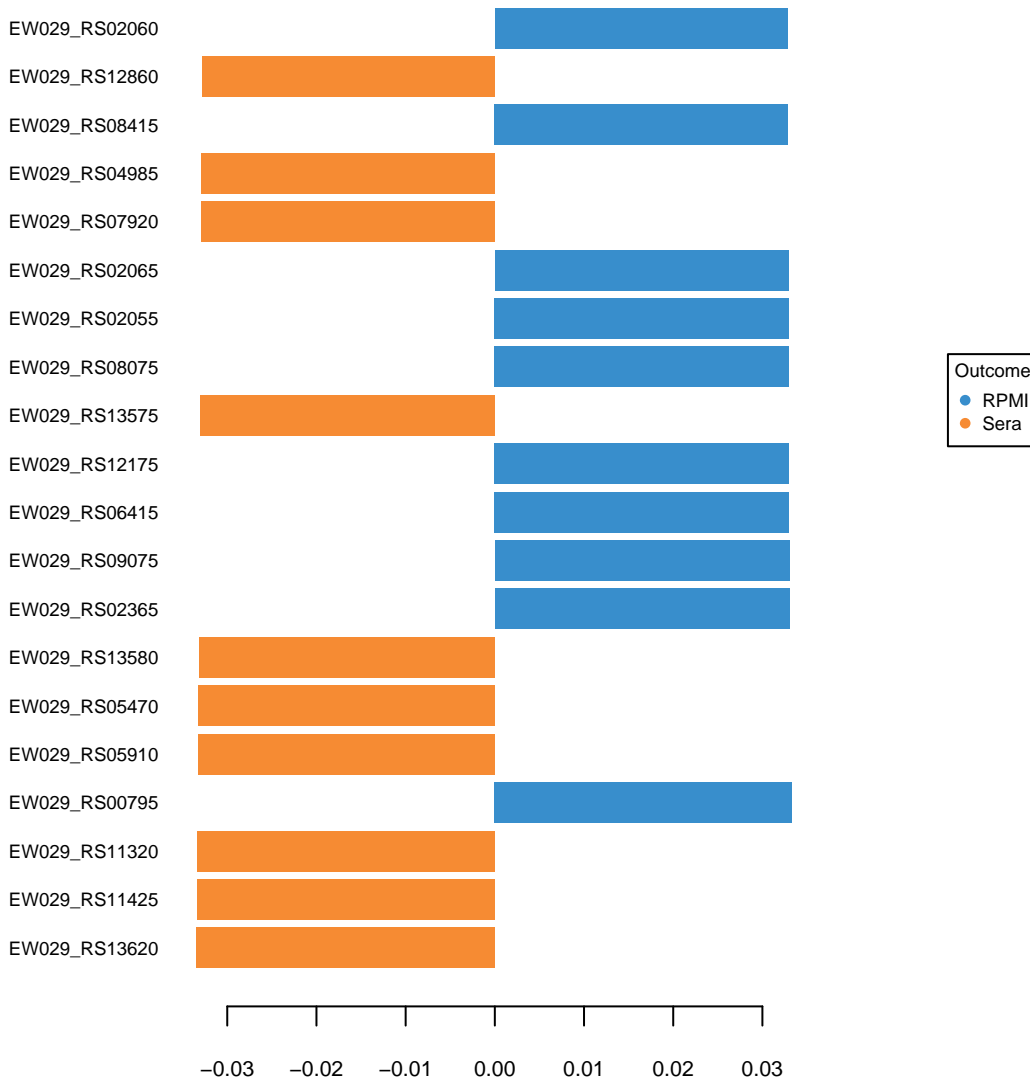
Status

RPMI

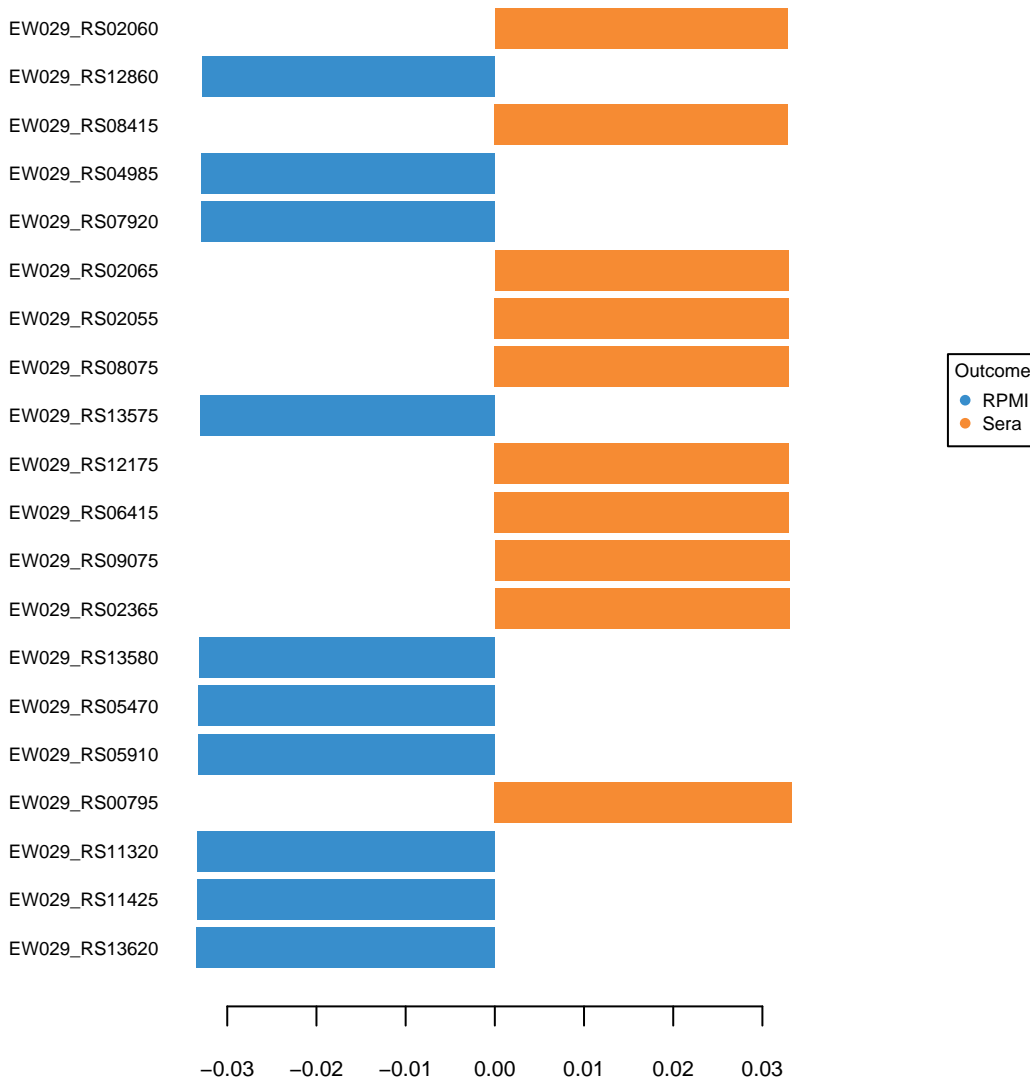
Sera



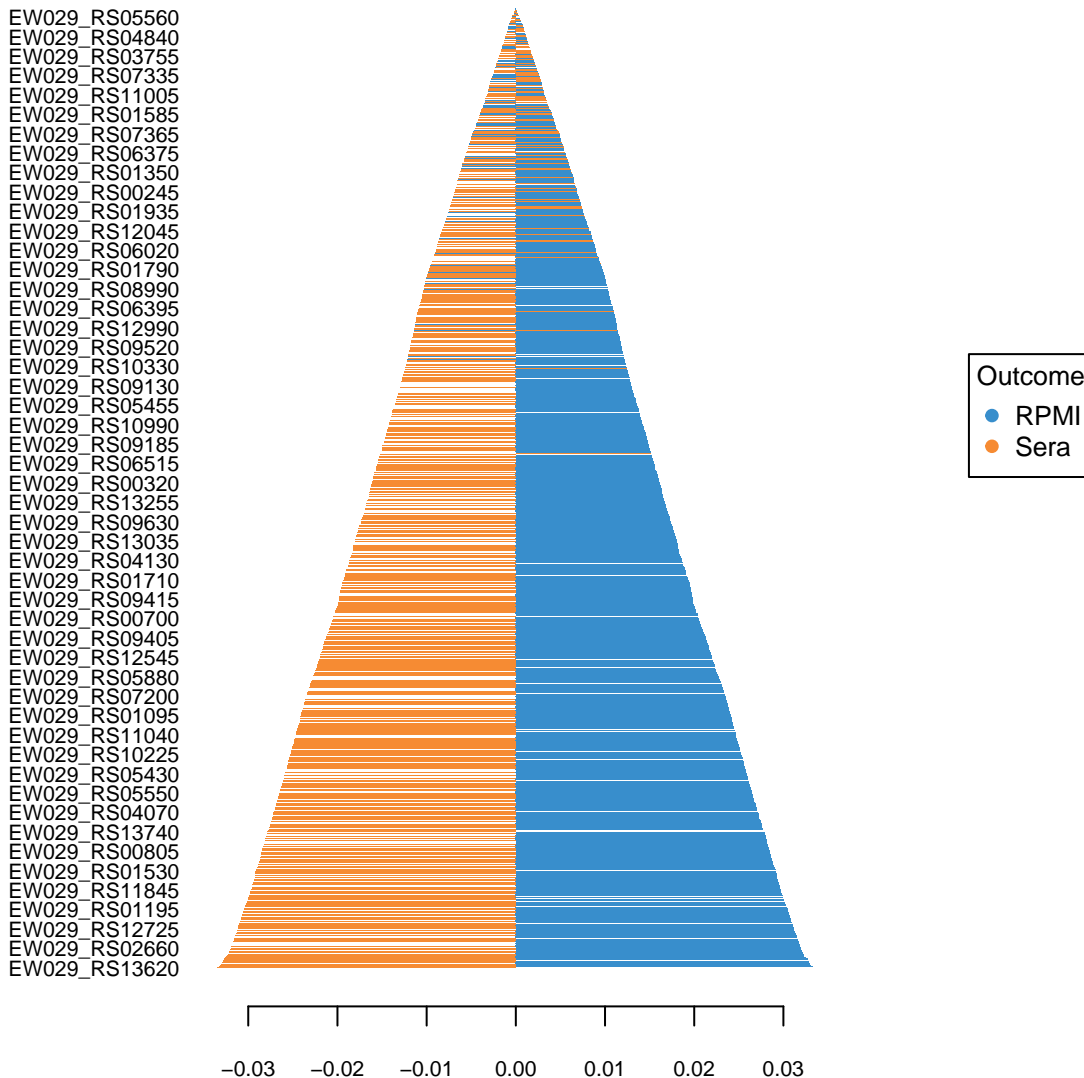
RNA_Seq 1 PLSDA max loadir



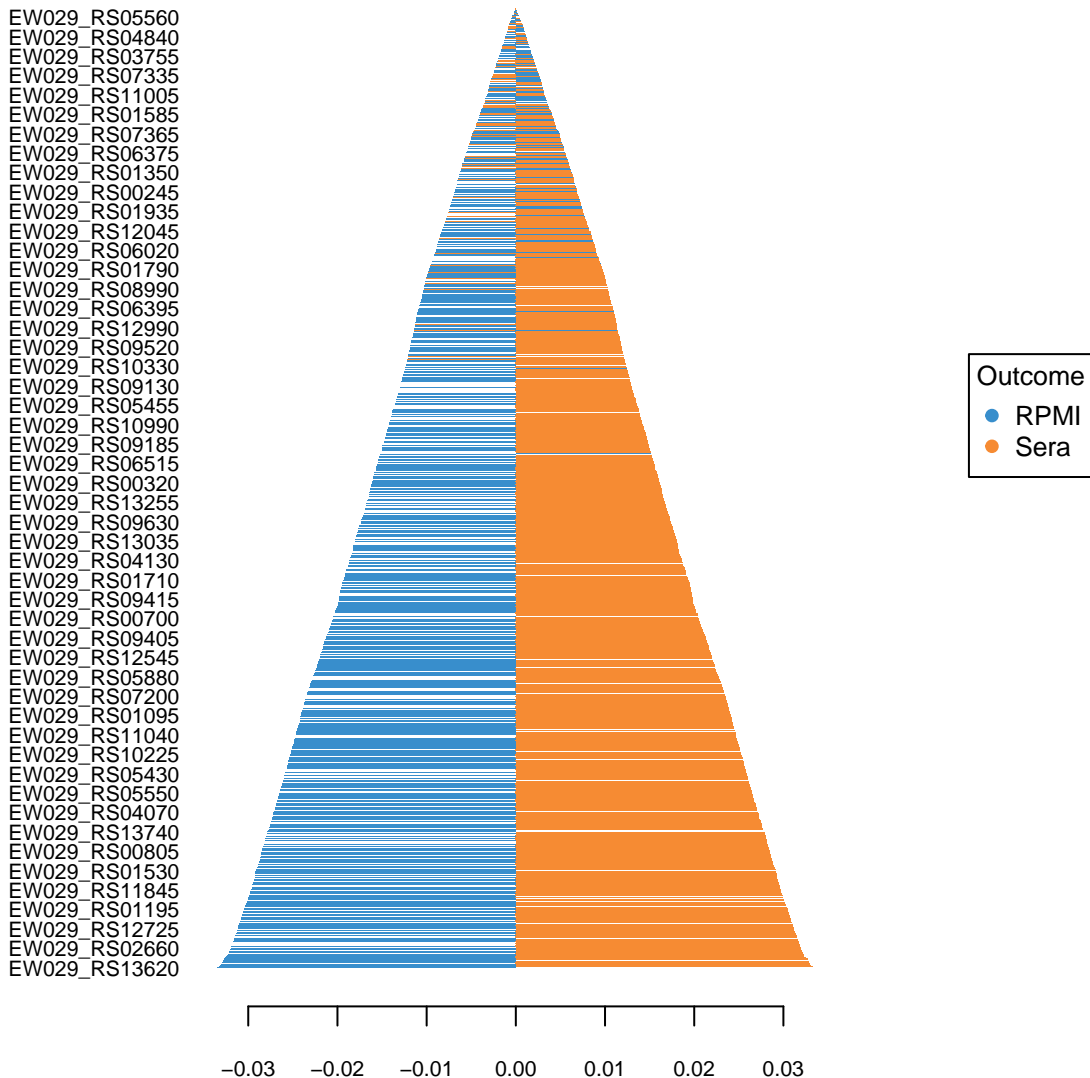
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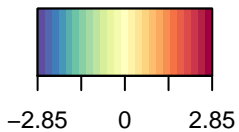
Contribution on comp 1



Contribution on comp 1



Color key

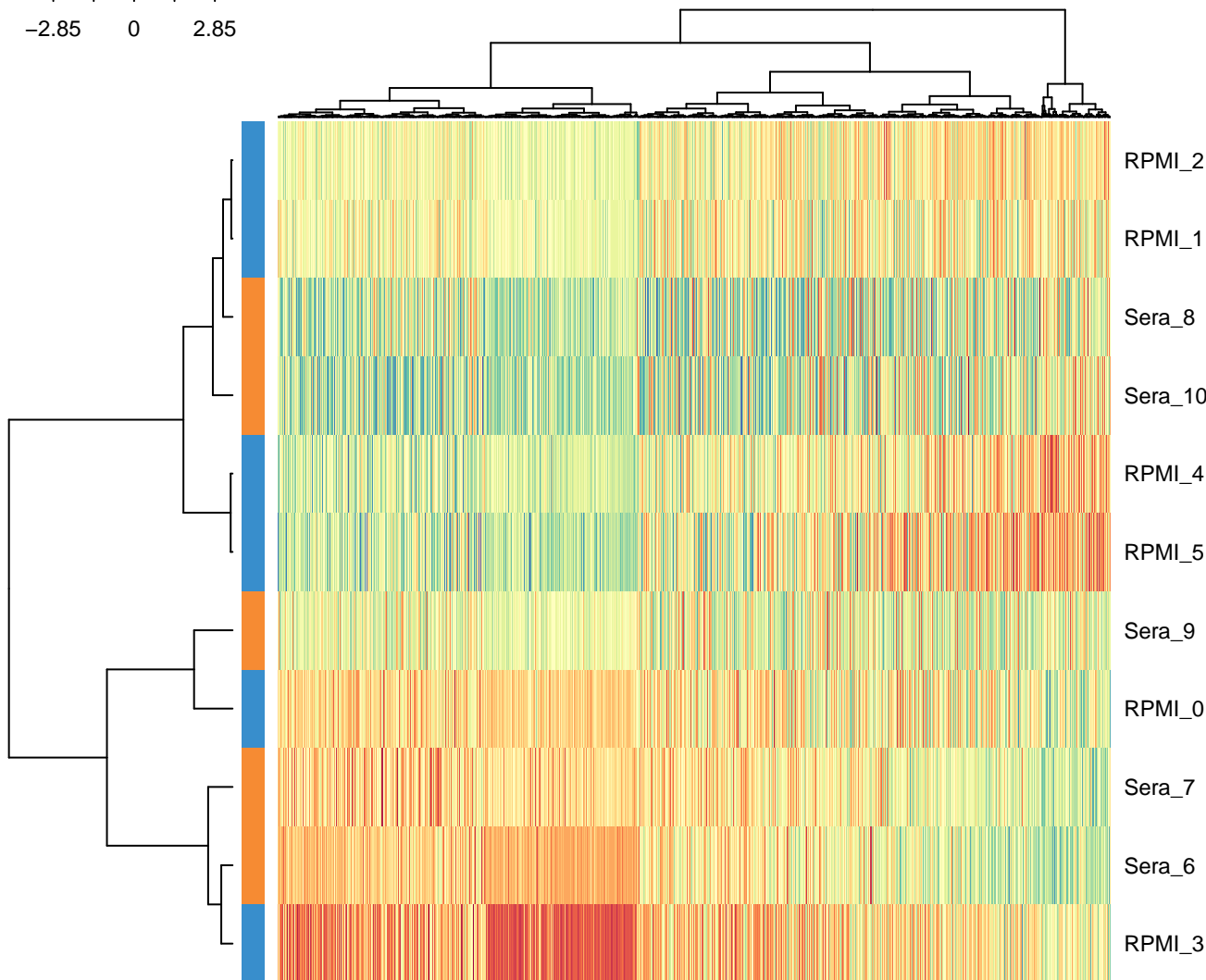


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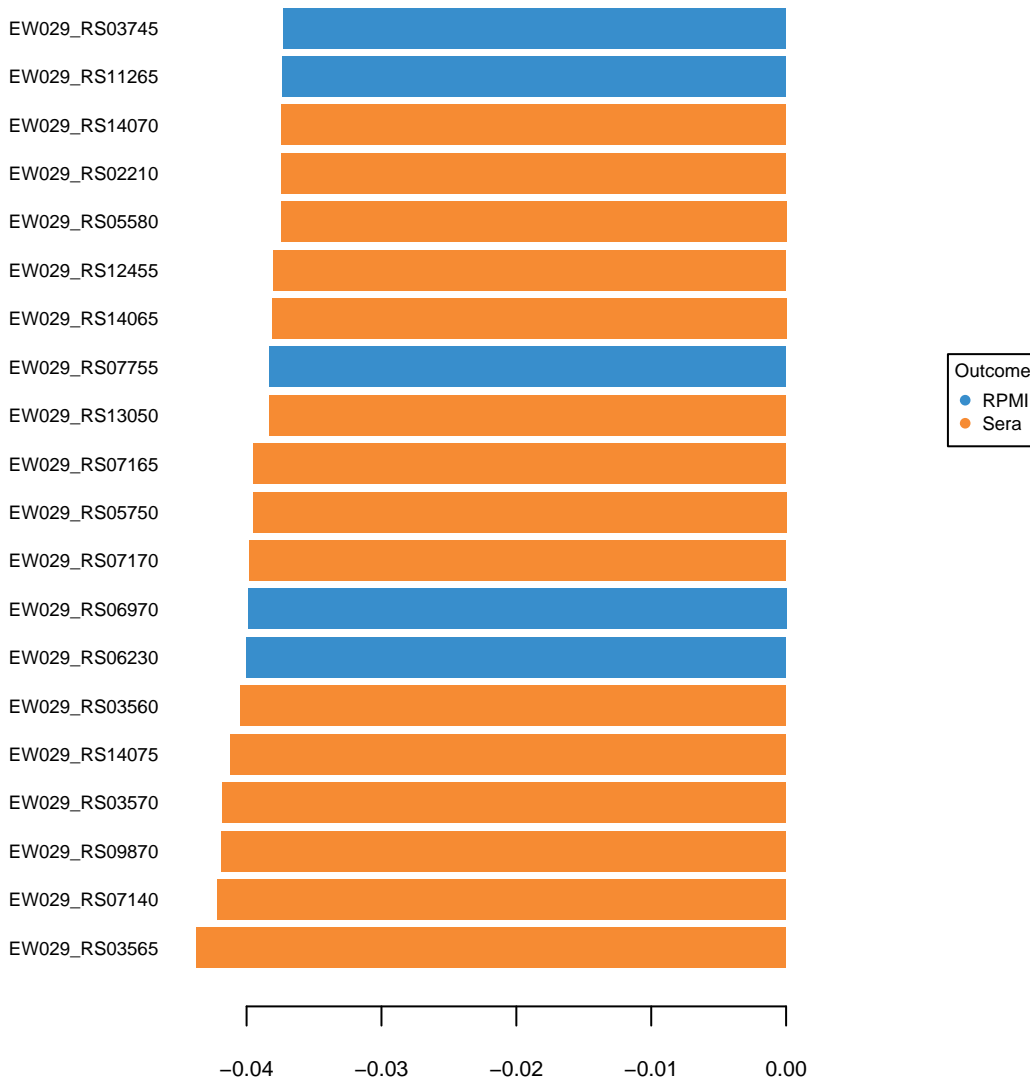
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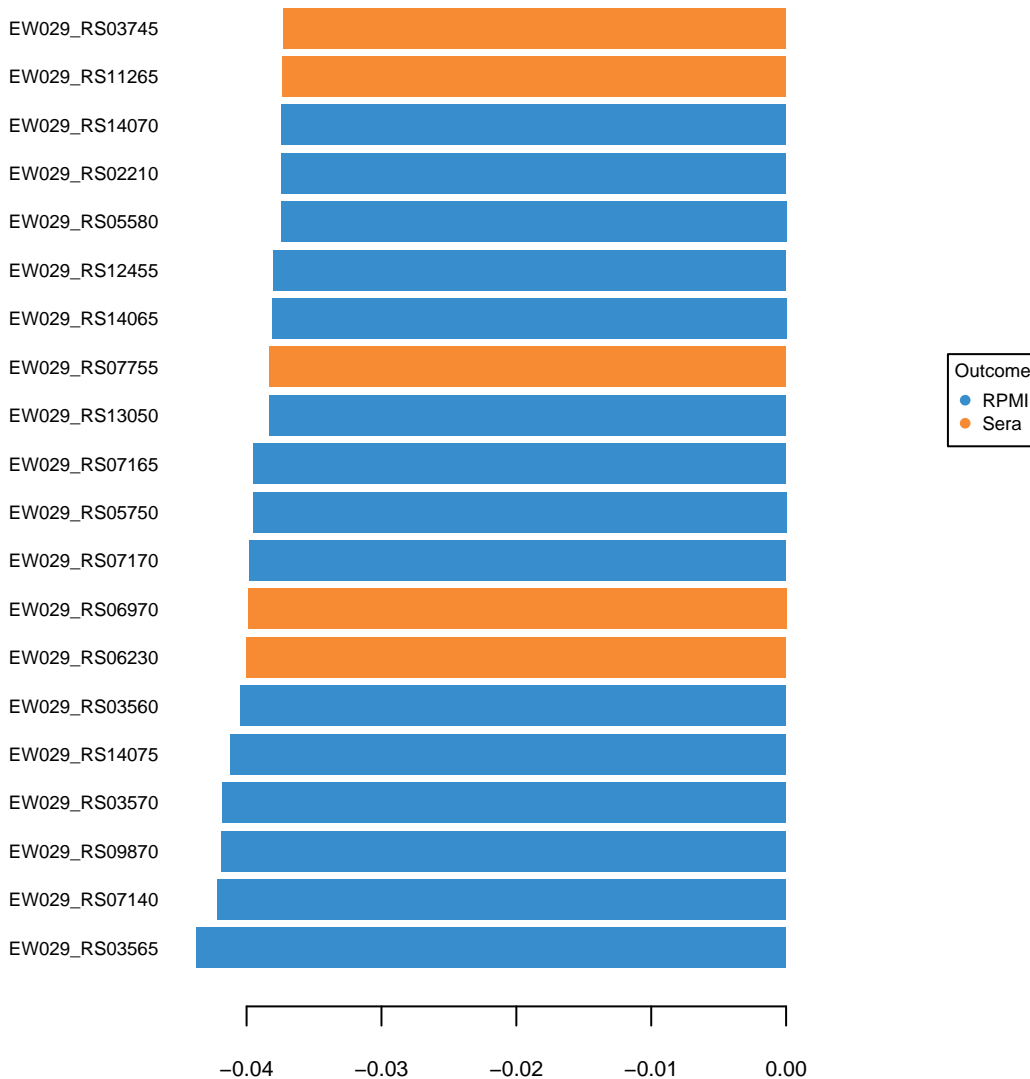
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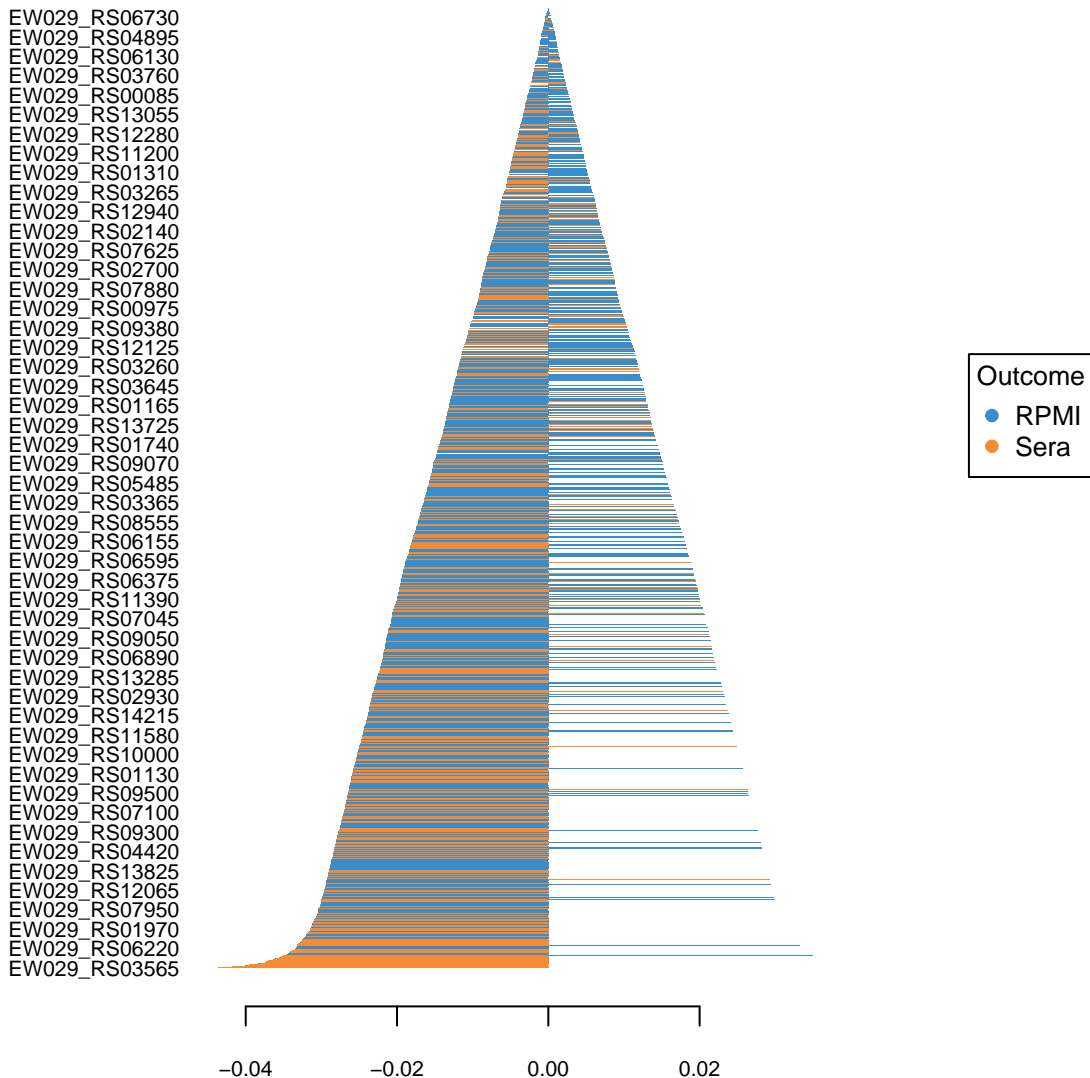
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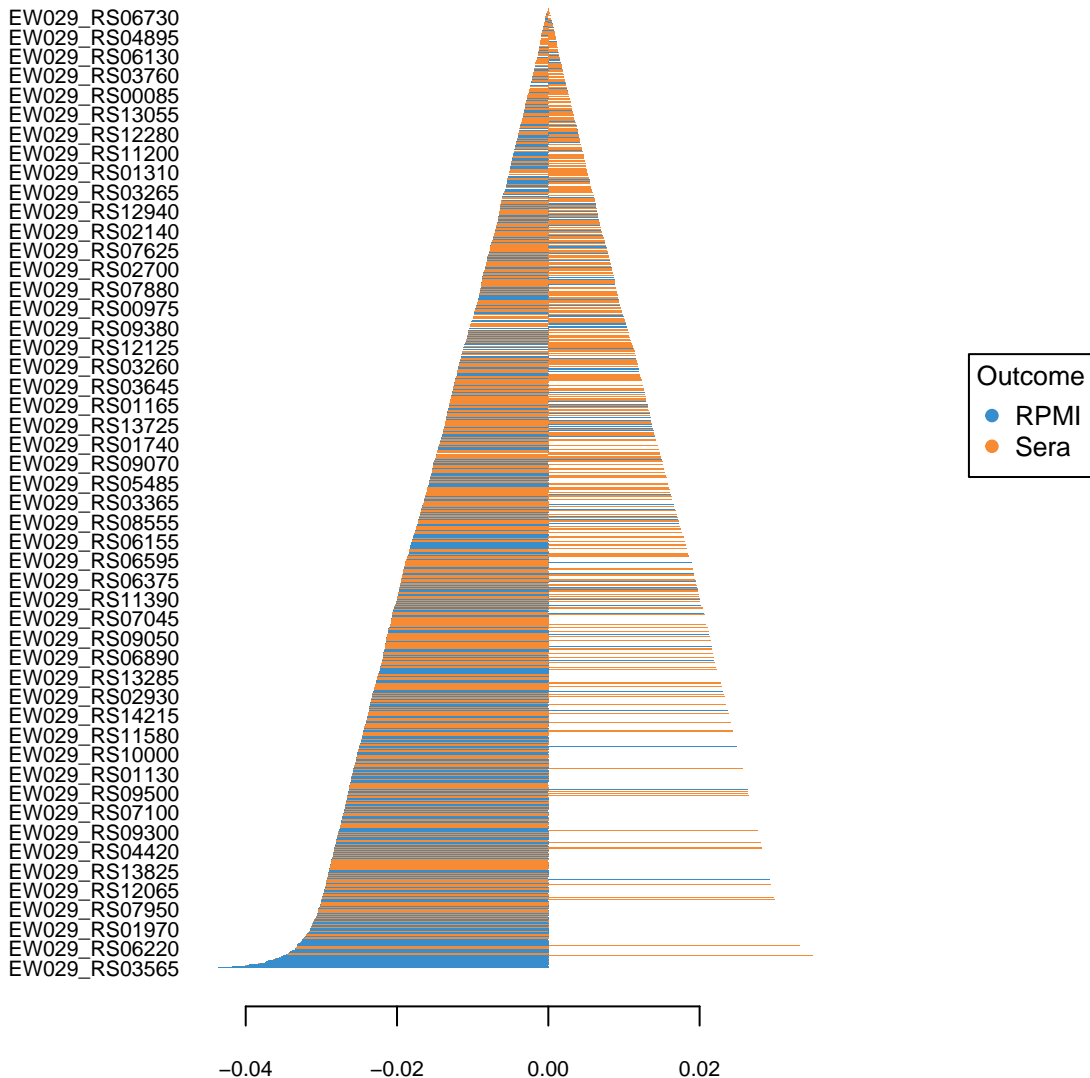
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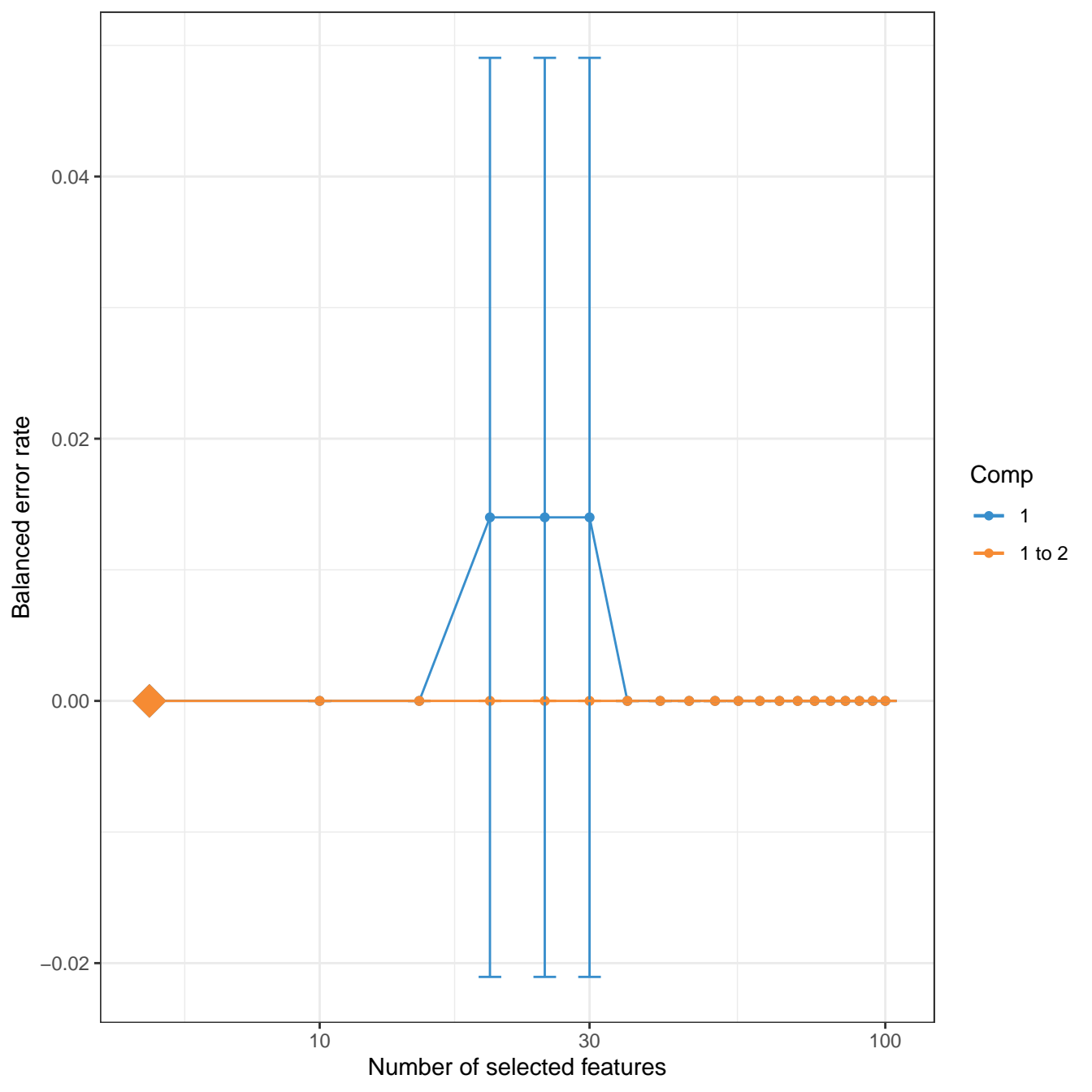


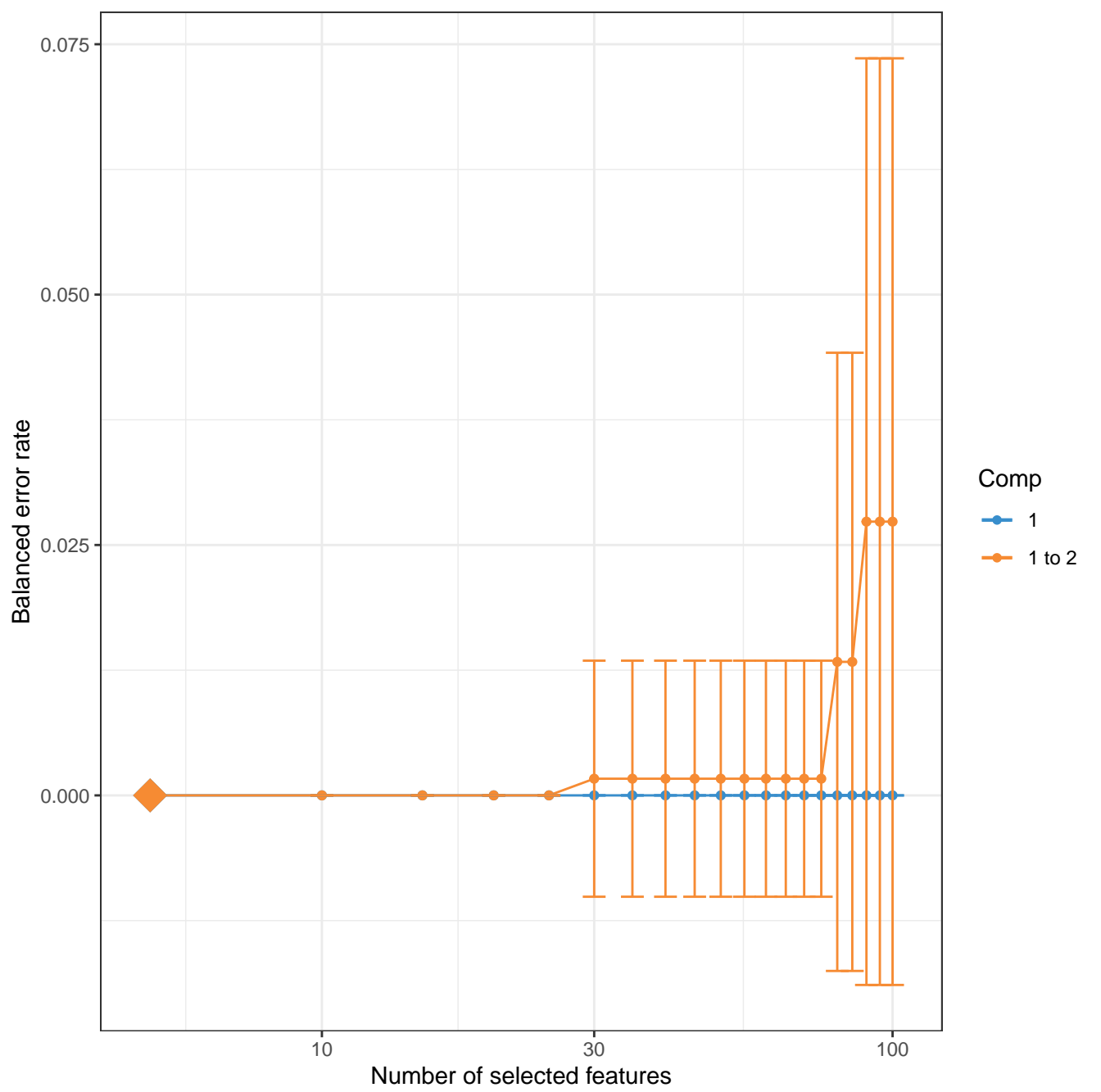
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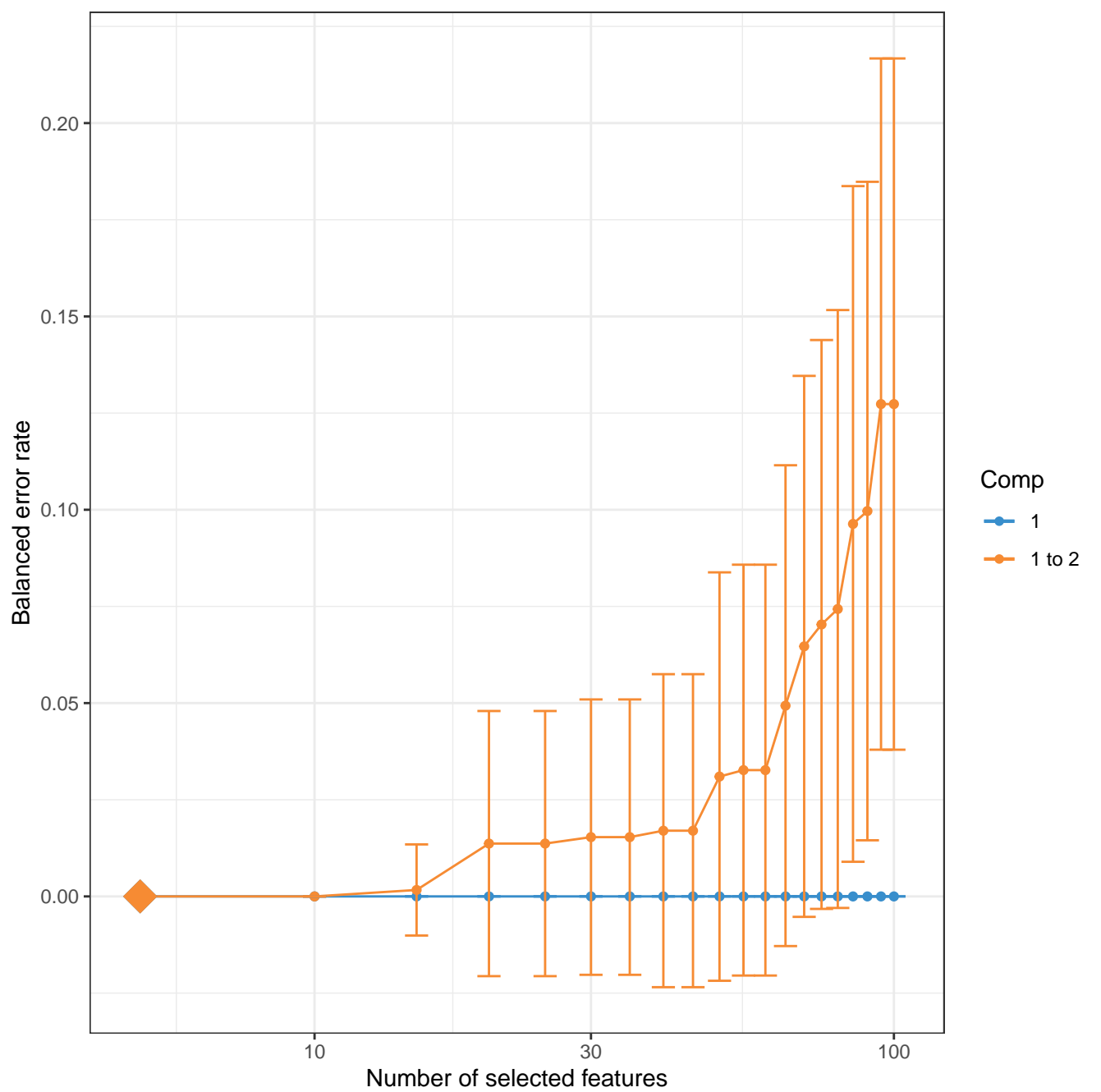


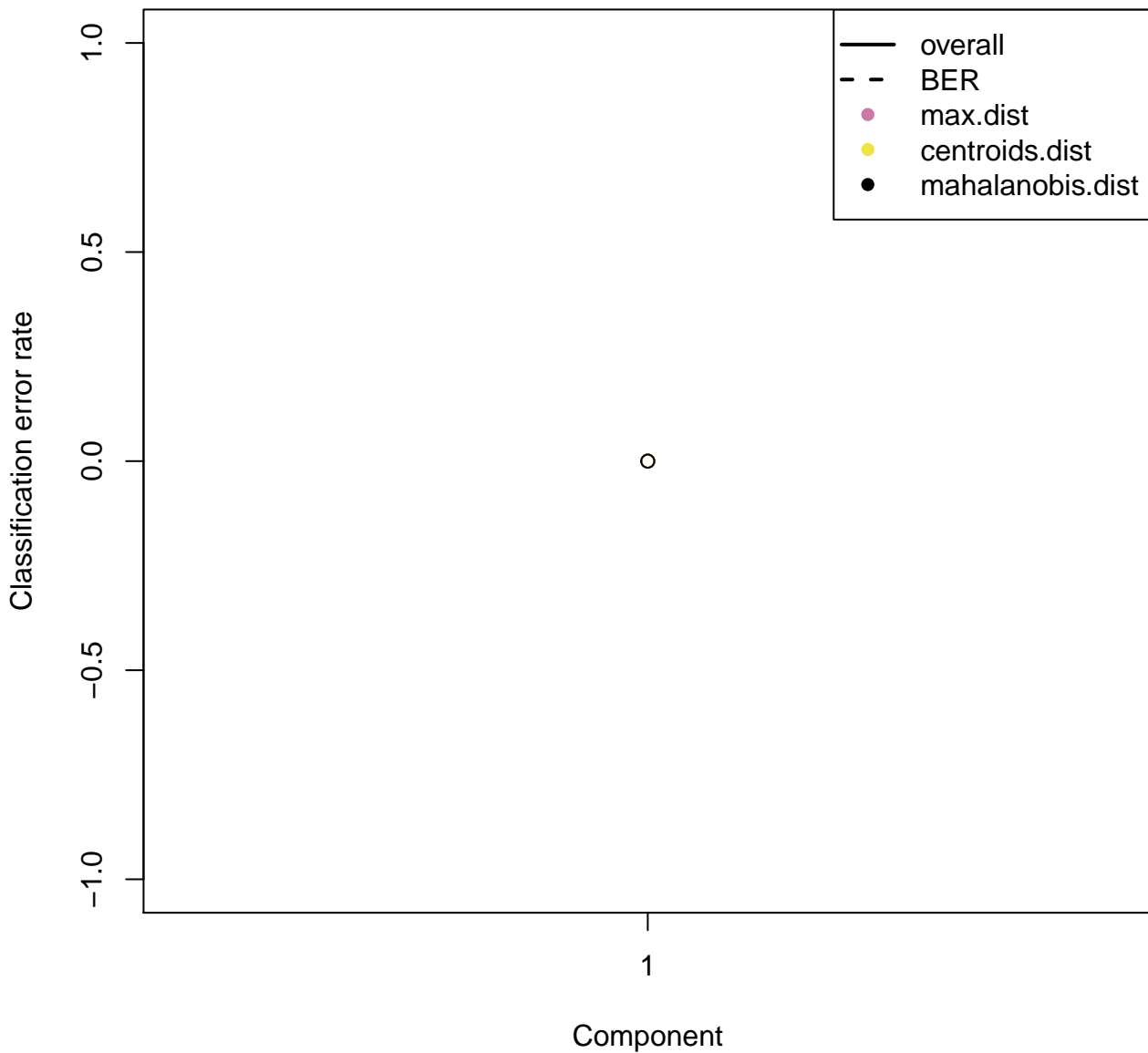
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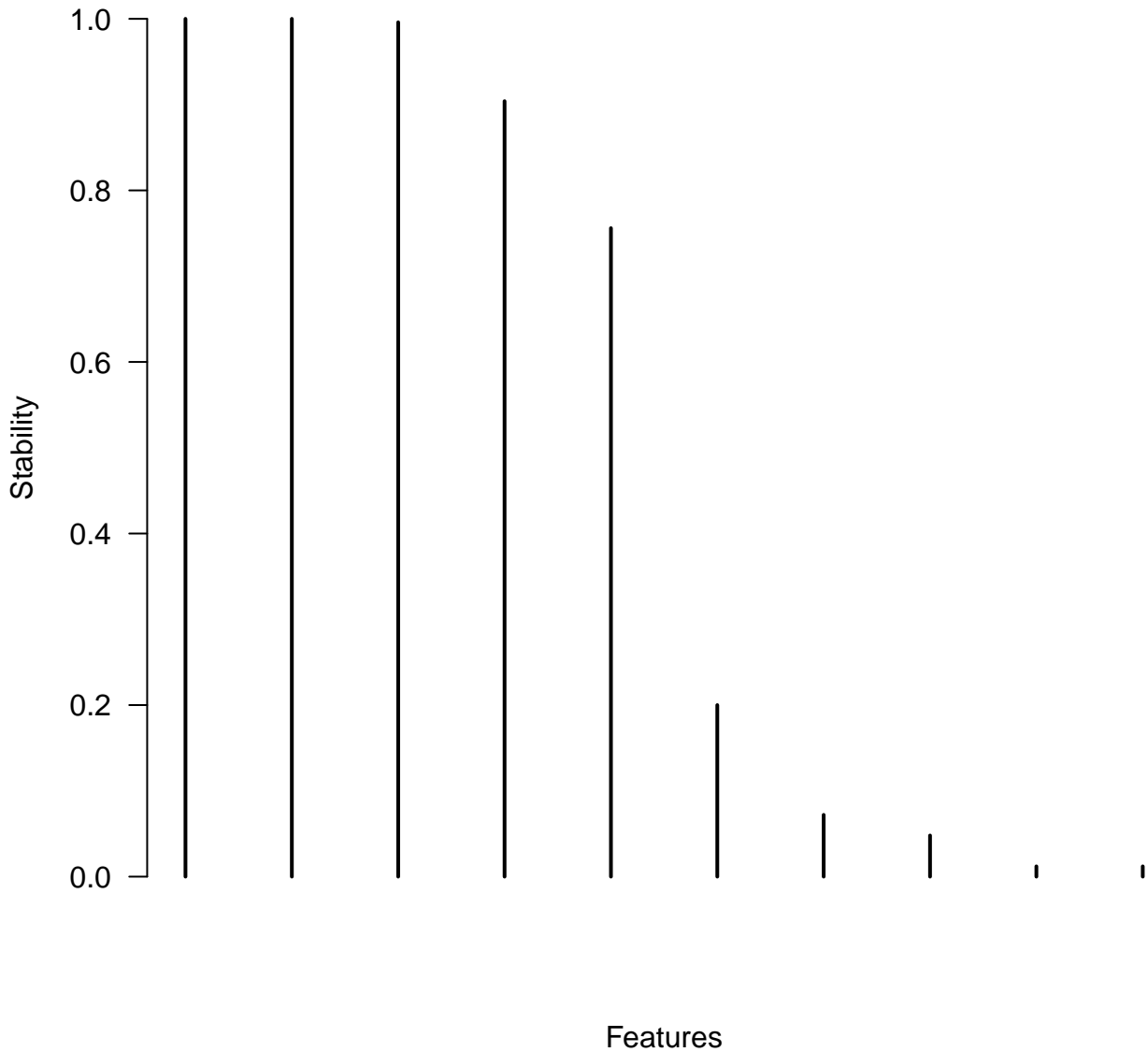




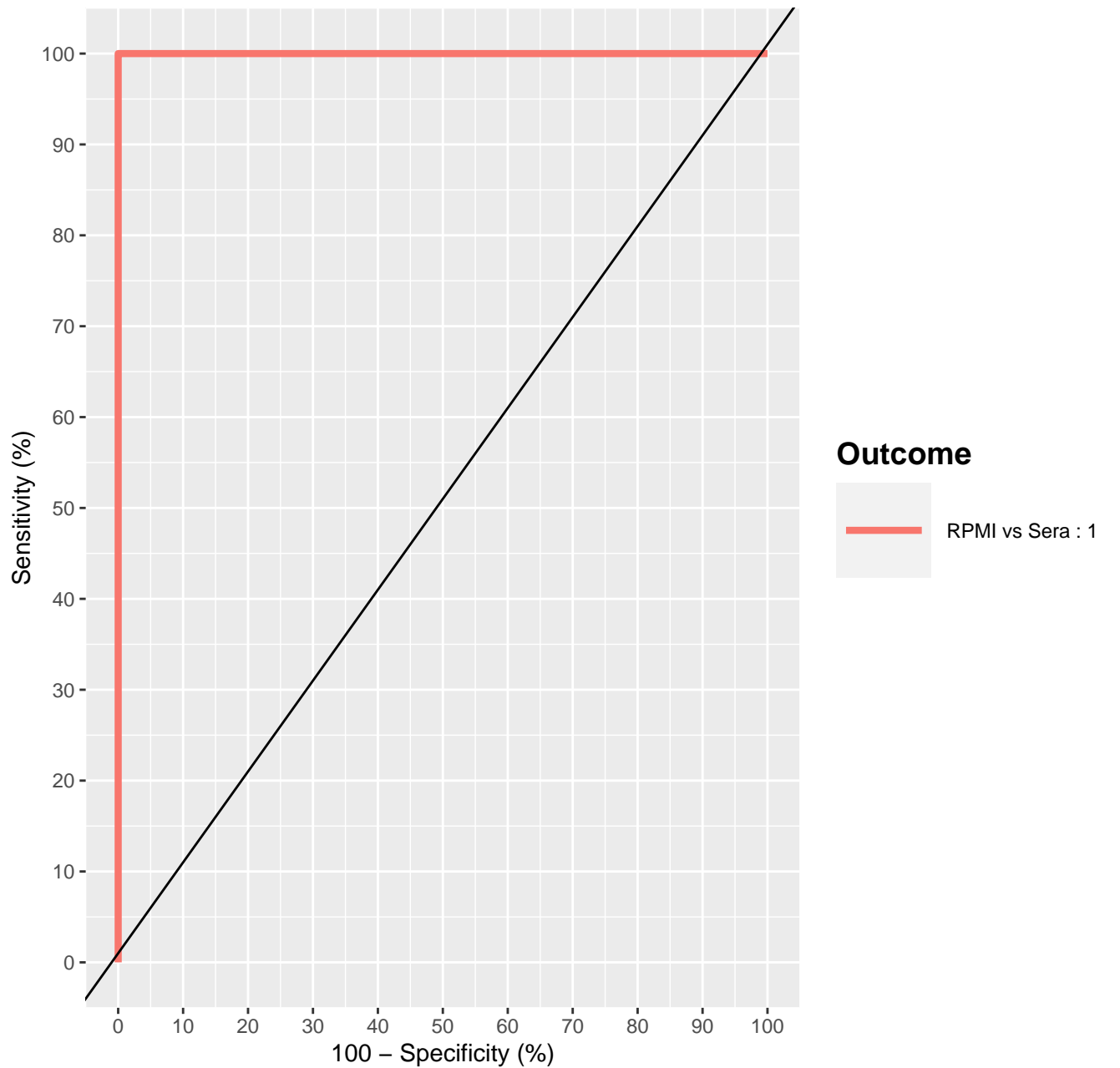




Comp 1

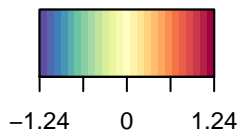


ROC Curve Comp 1



sPLSDA

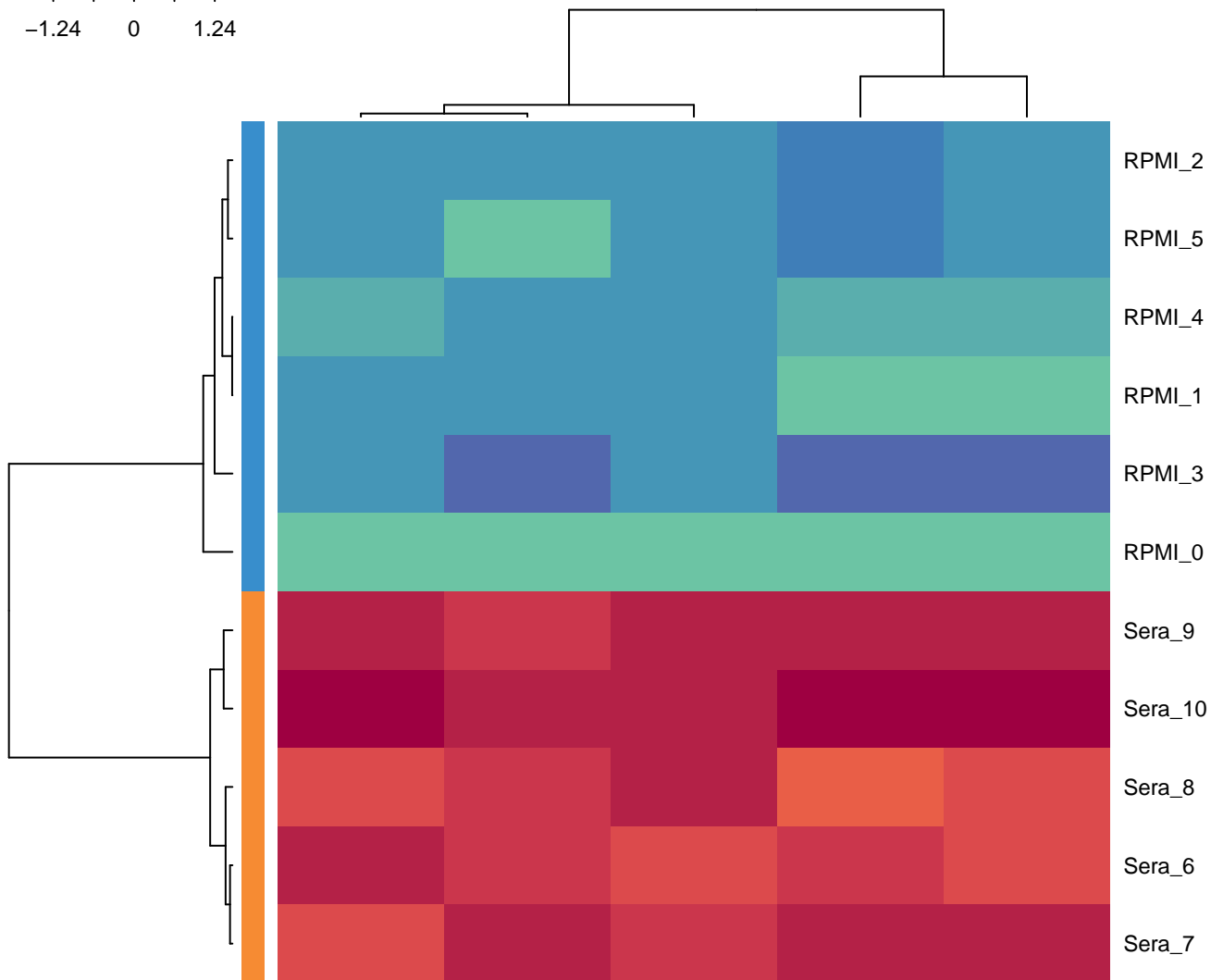
Color key



Status

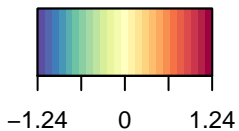
RPMI

Sera



sPLSDA Component 1

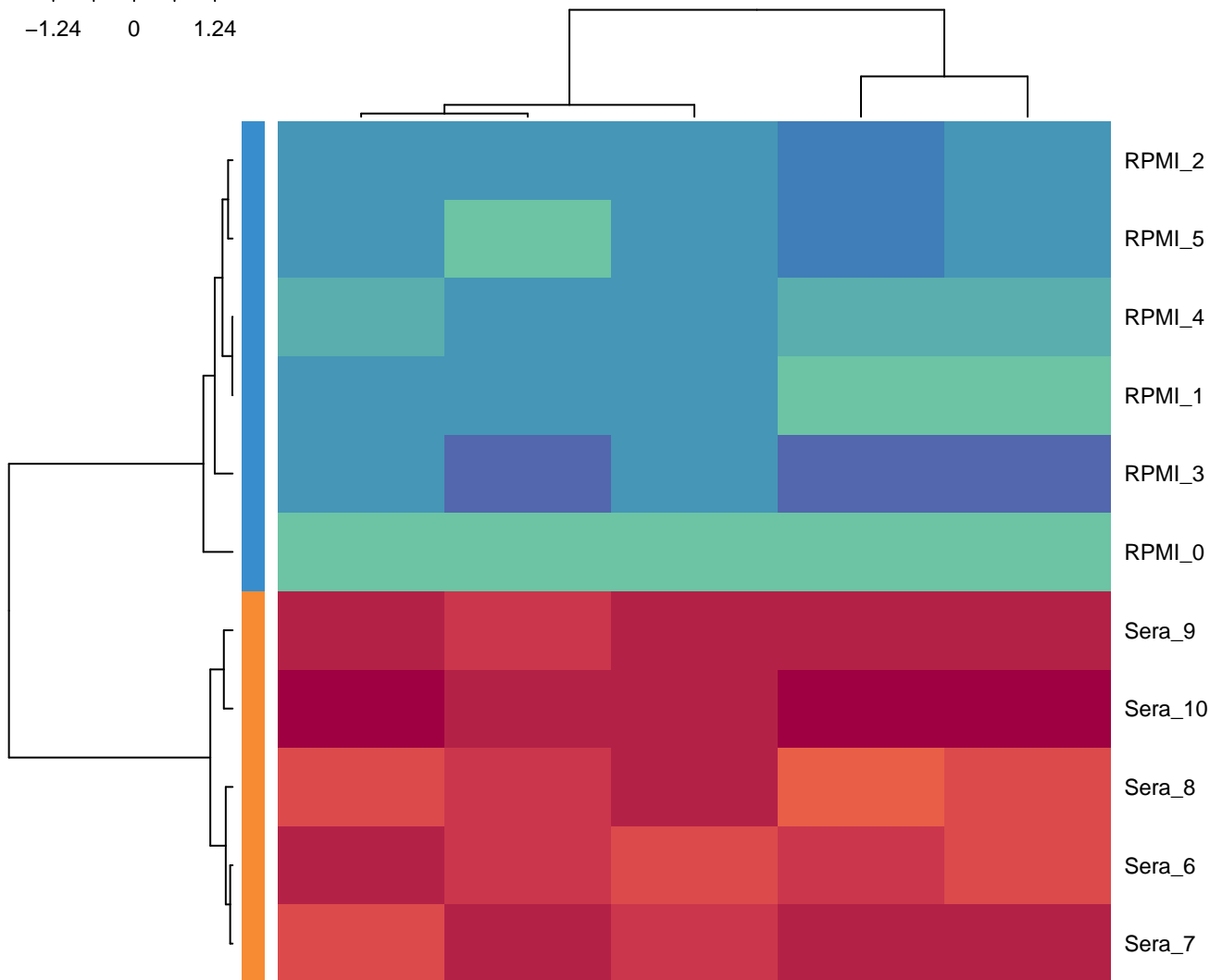
Color key



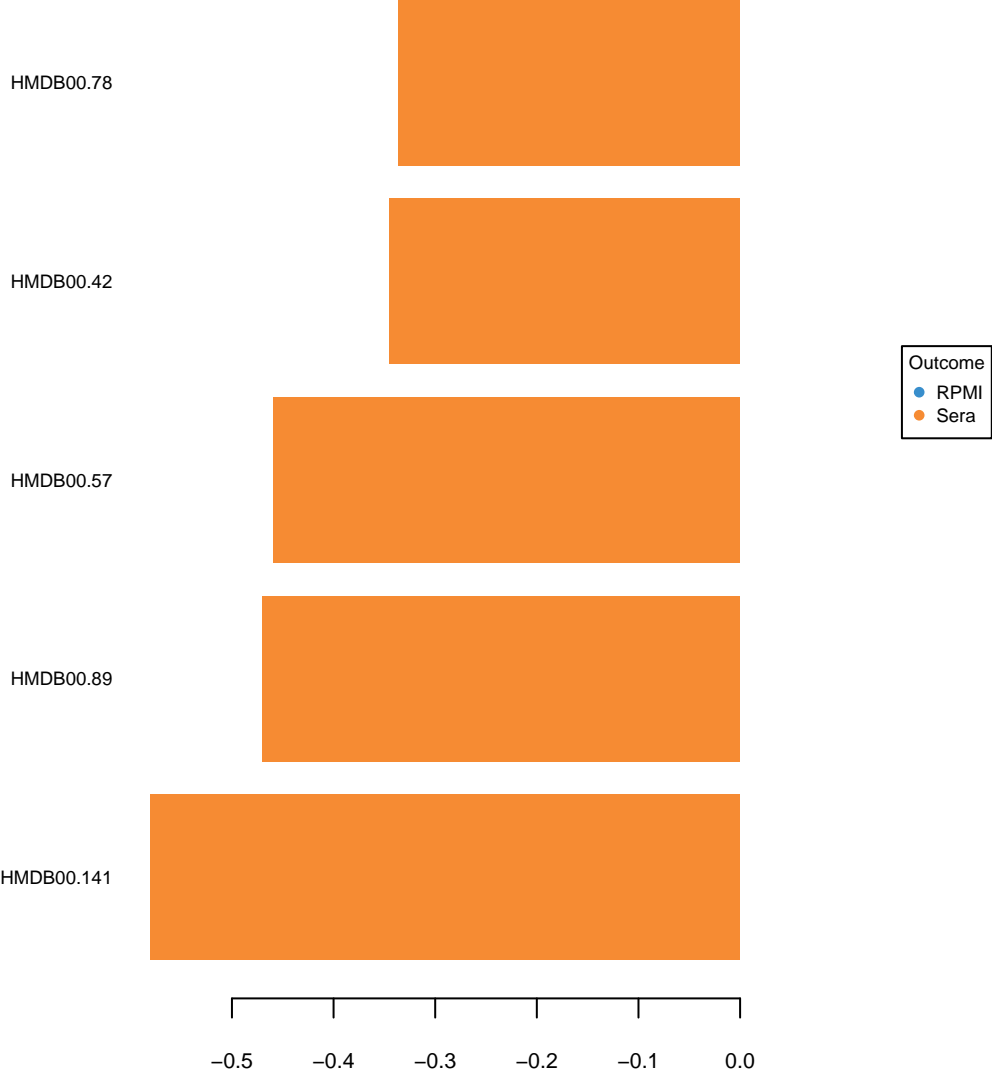
Status

RPMI

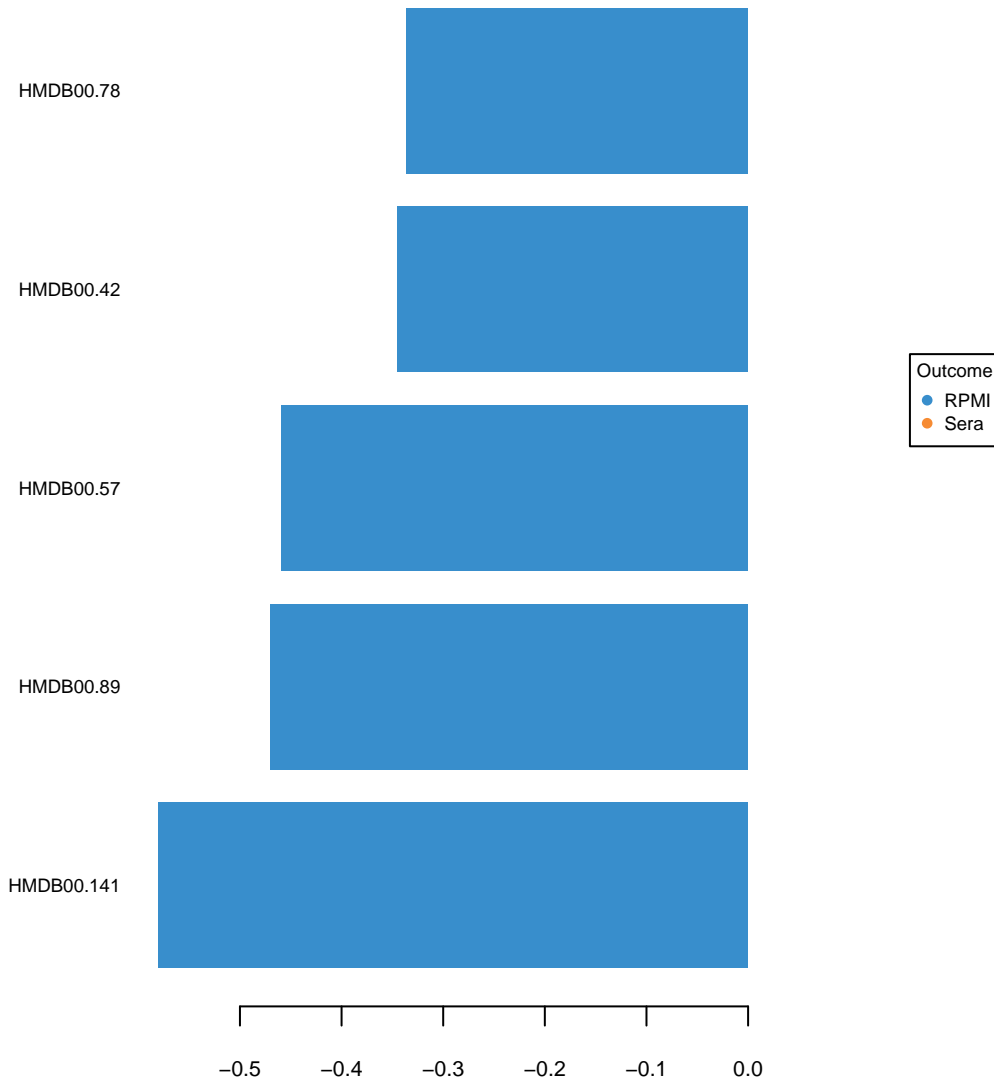
Sera



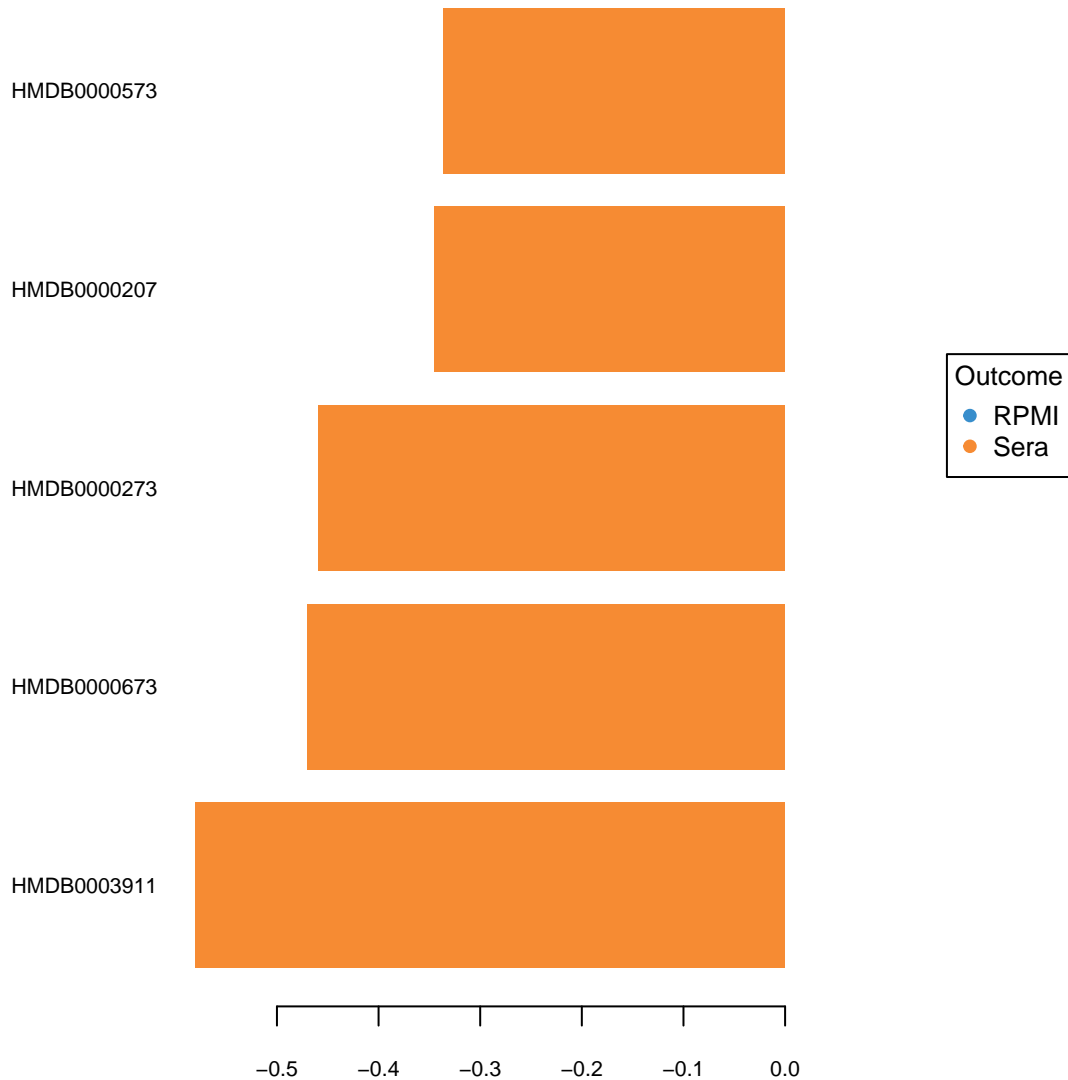
Metabolomics 1 sPLSDA max loa



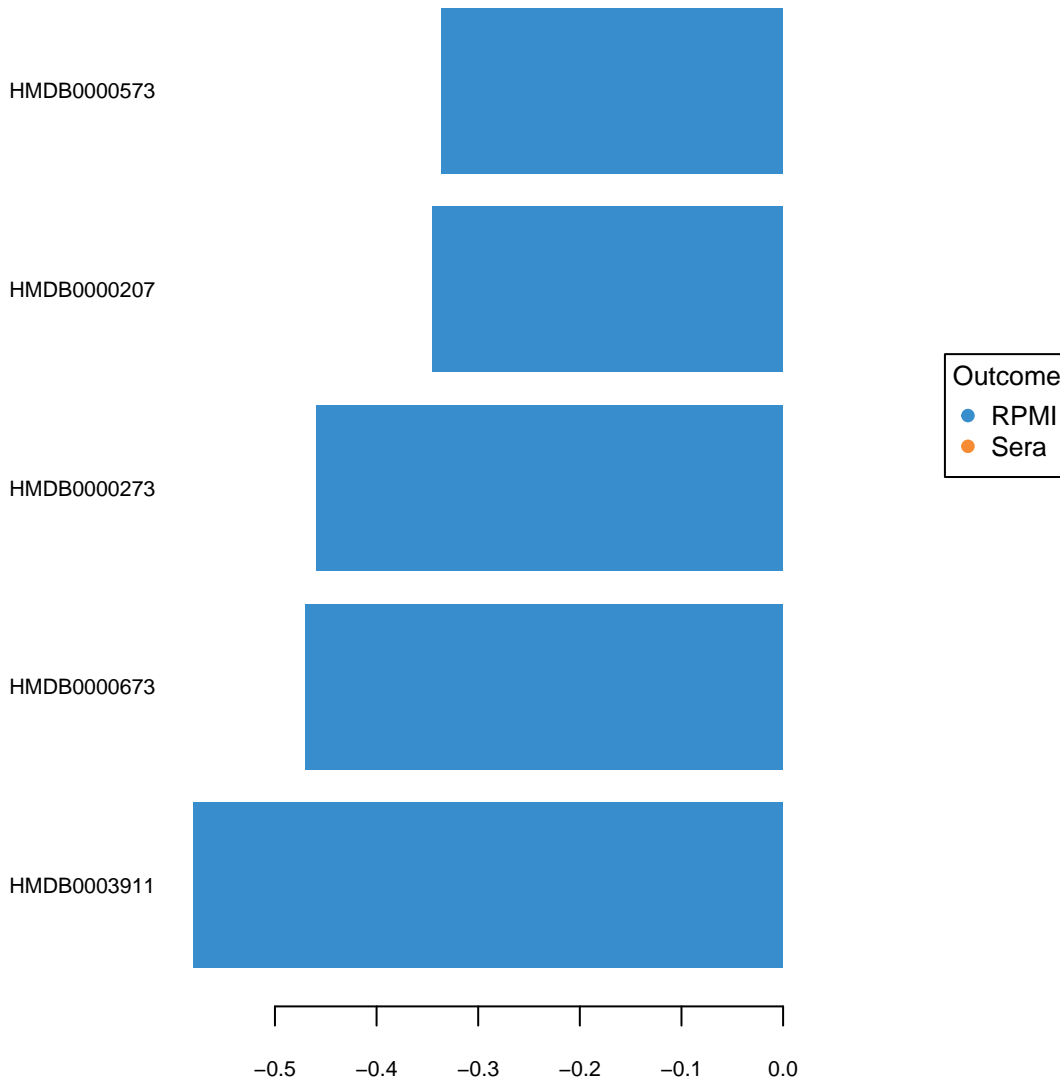
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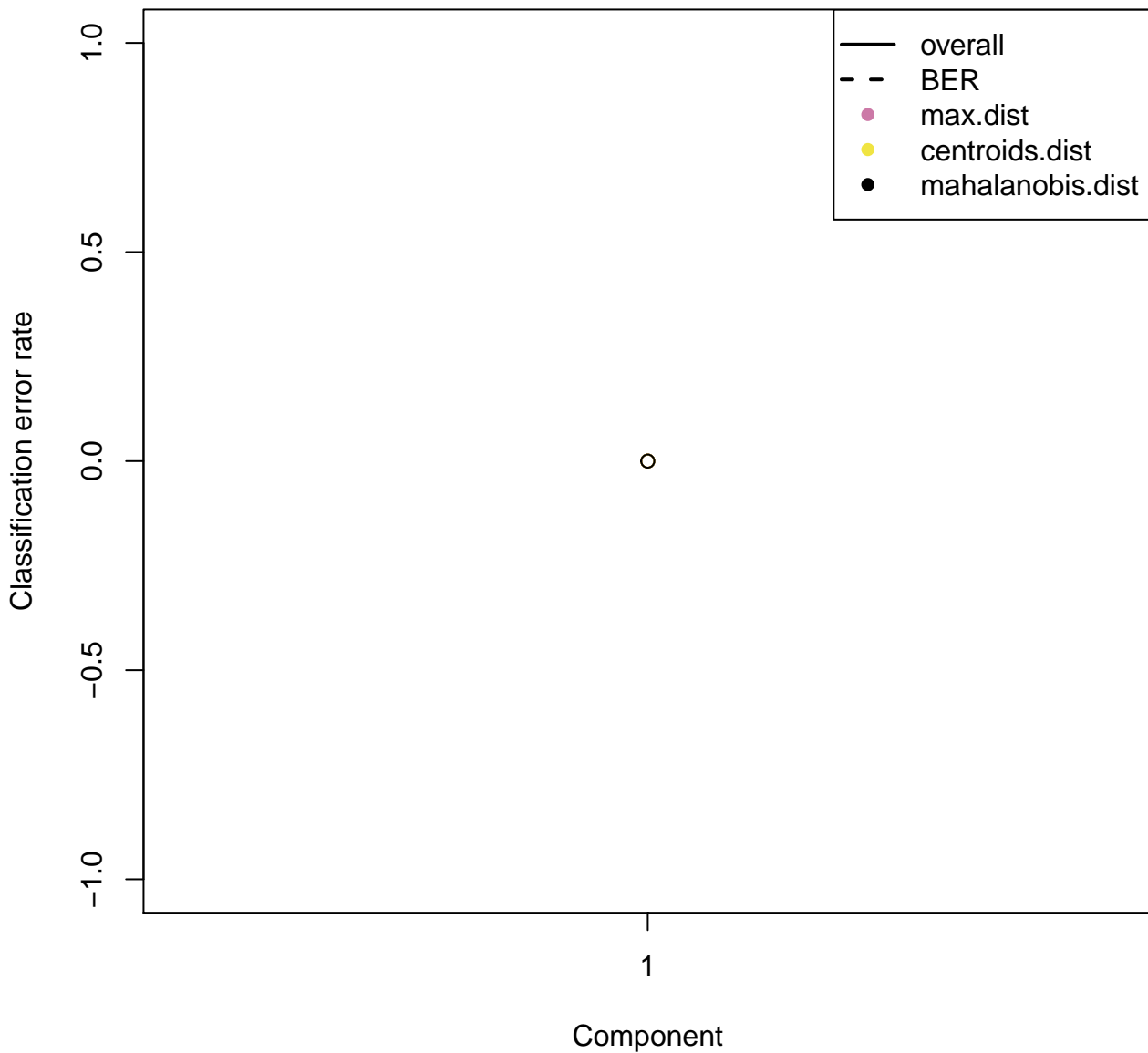


Contribution on comp 1

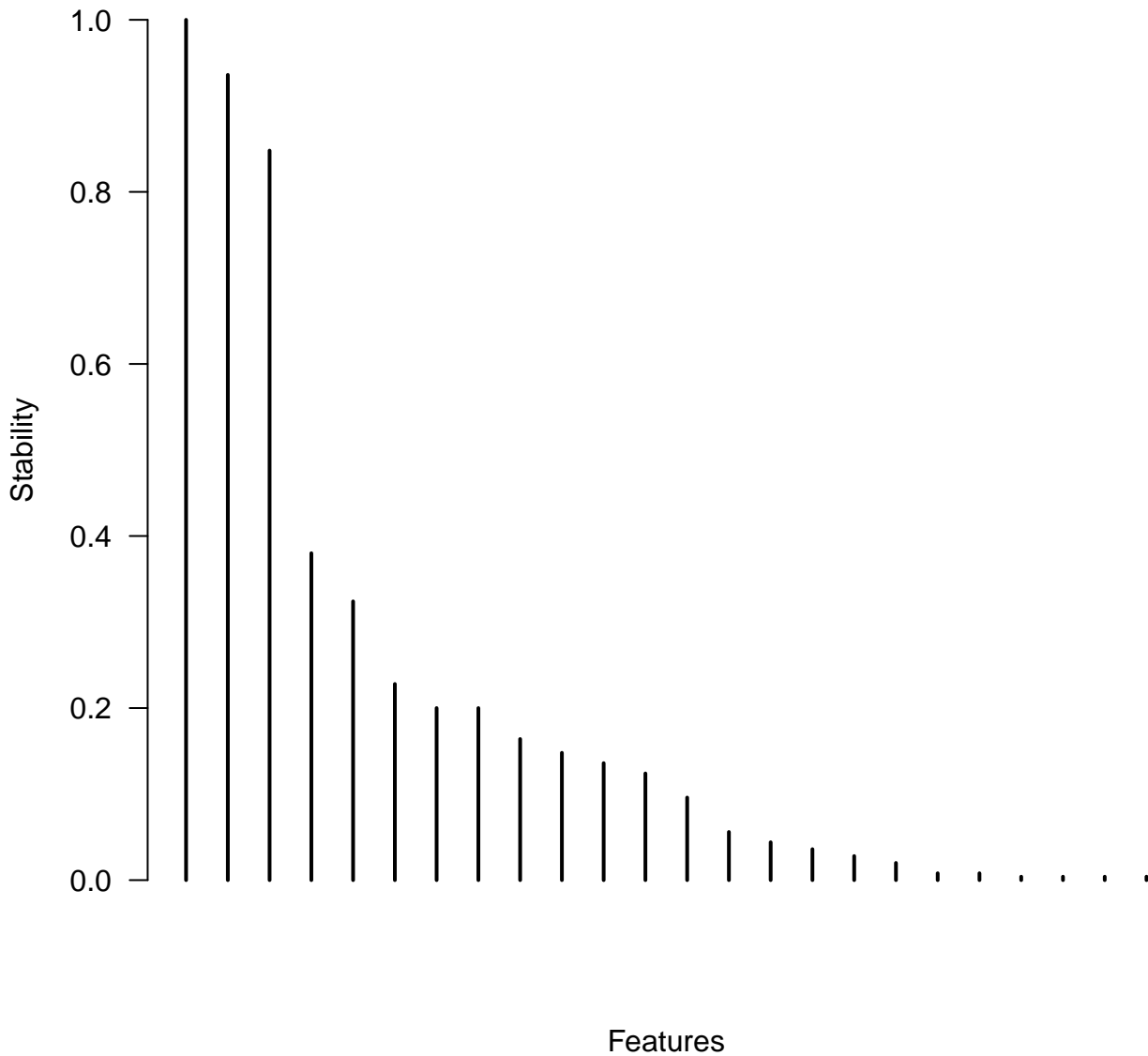


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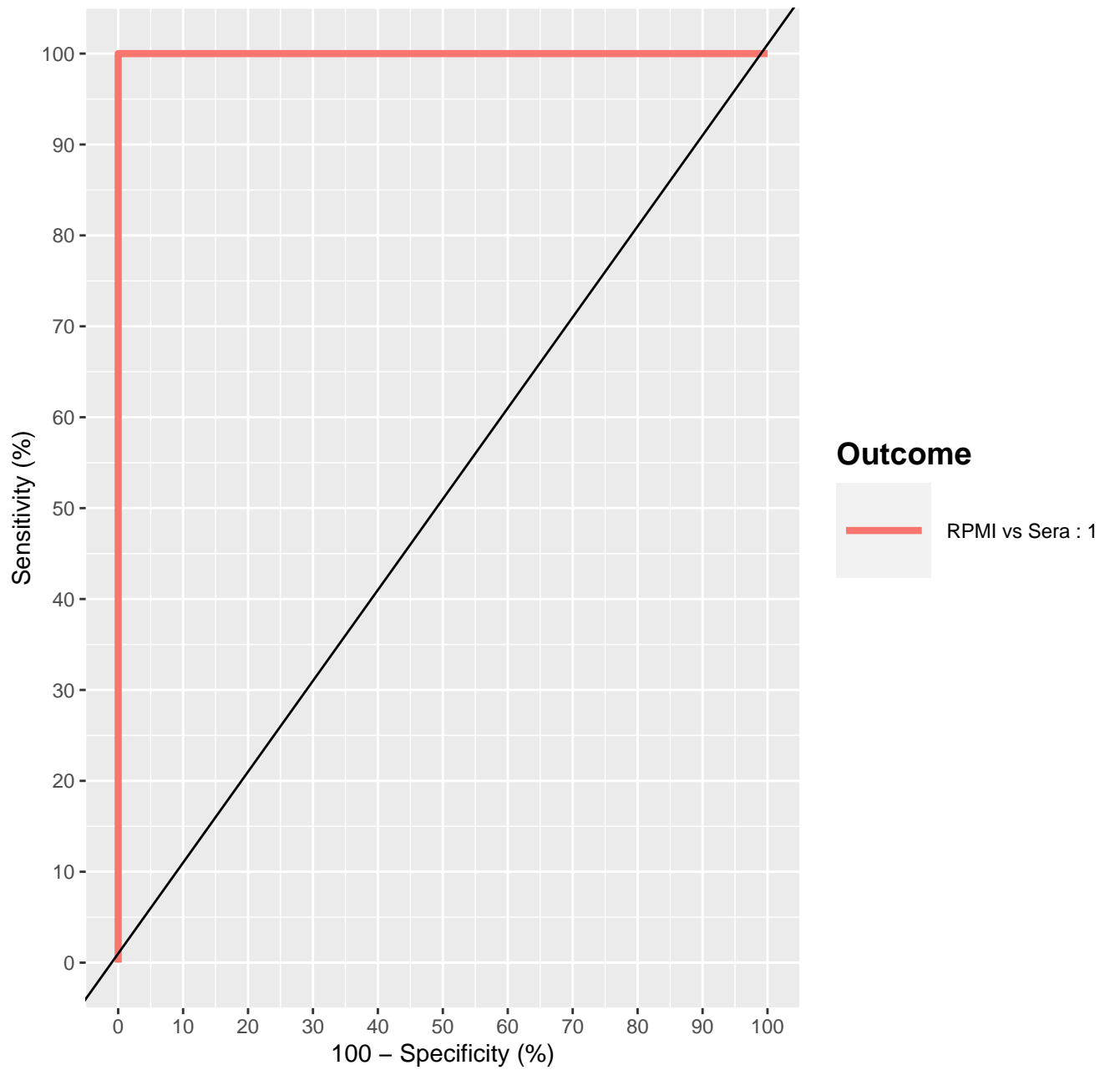




Comp 1

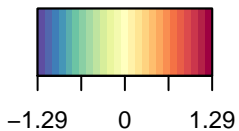


ROC Curve Comp 1



sPLSDA

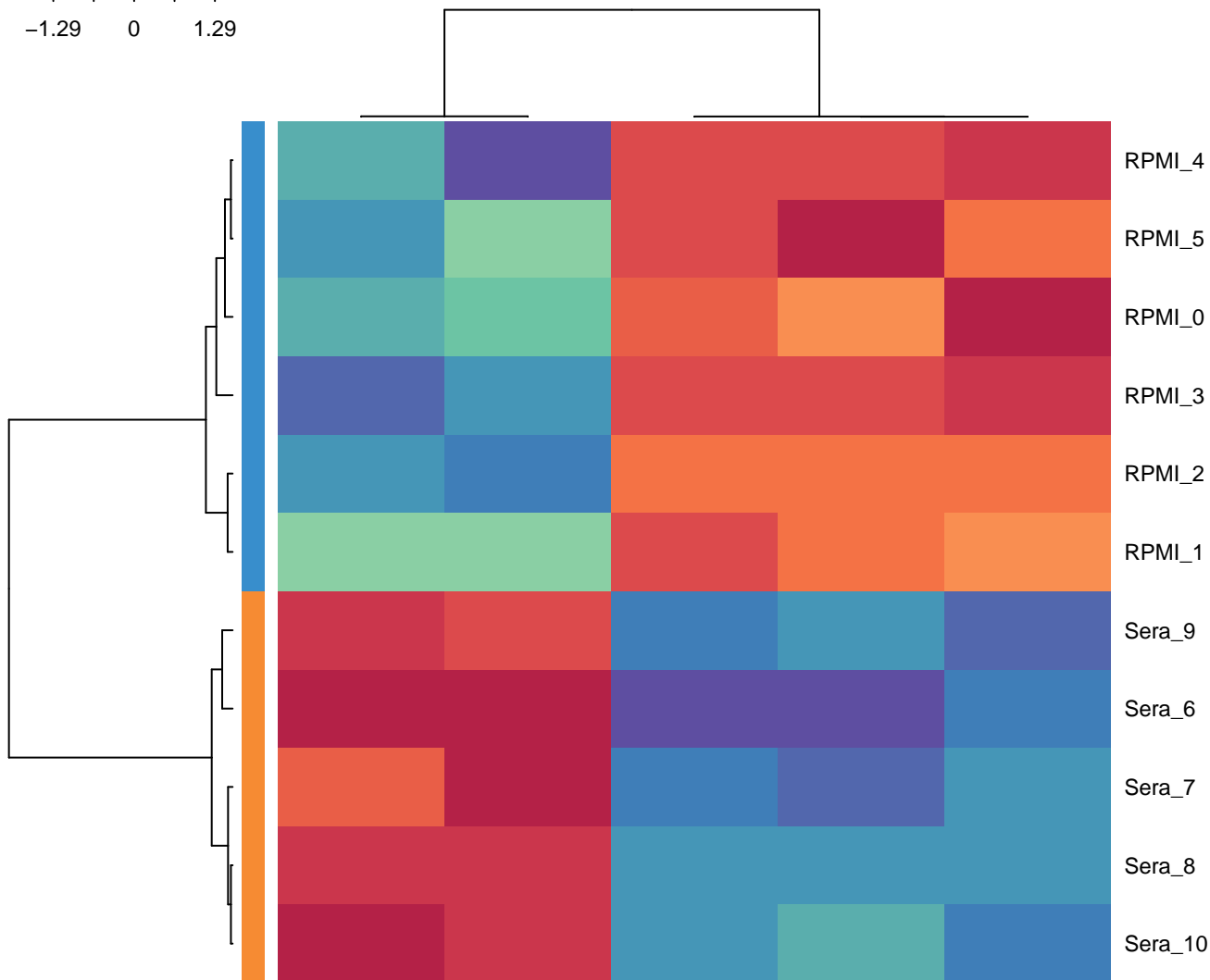
Color key



Status

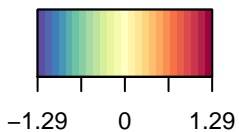
RPMI

Sera



sPLSDA Component 1

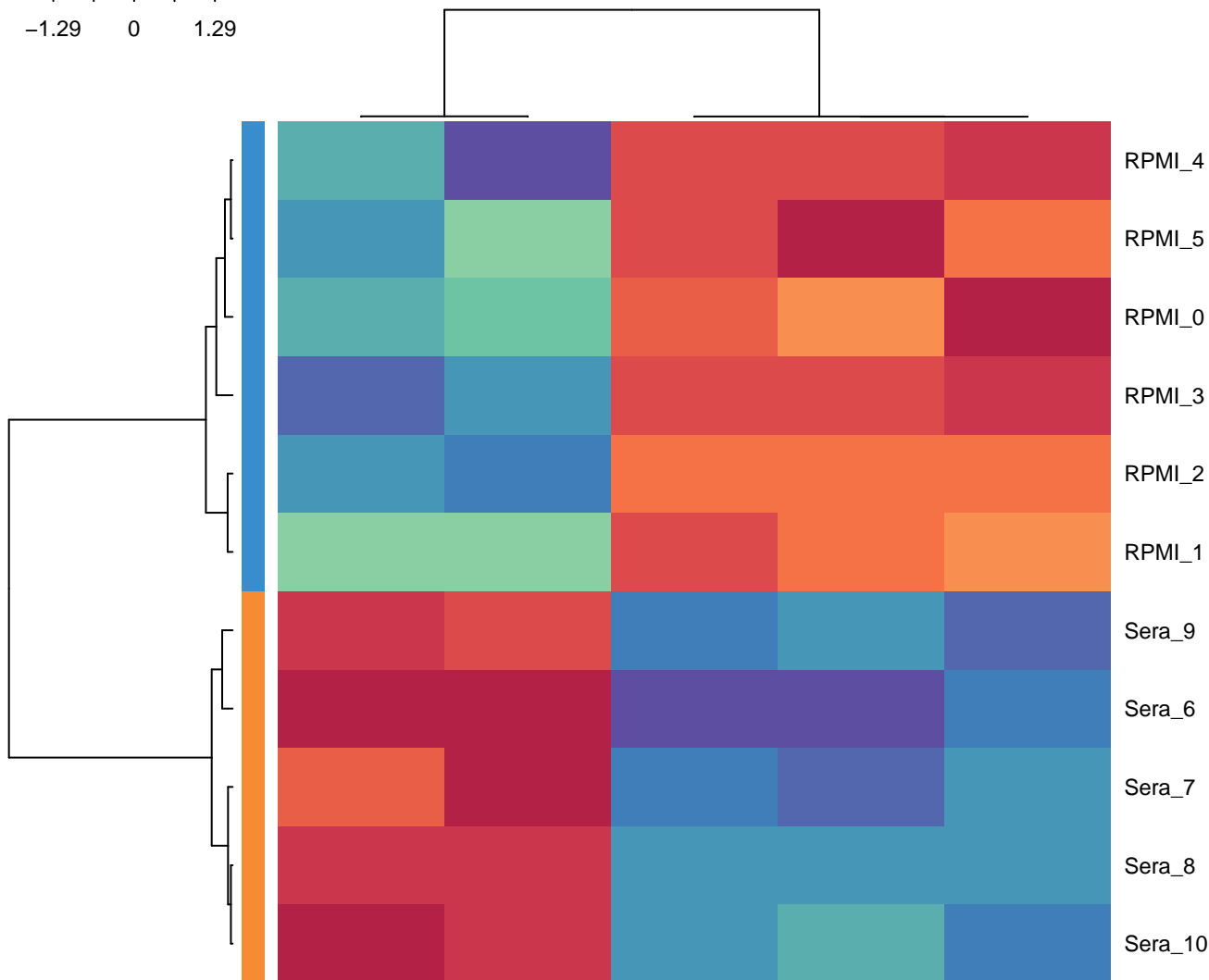
Color key



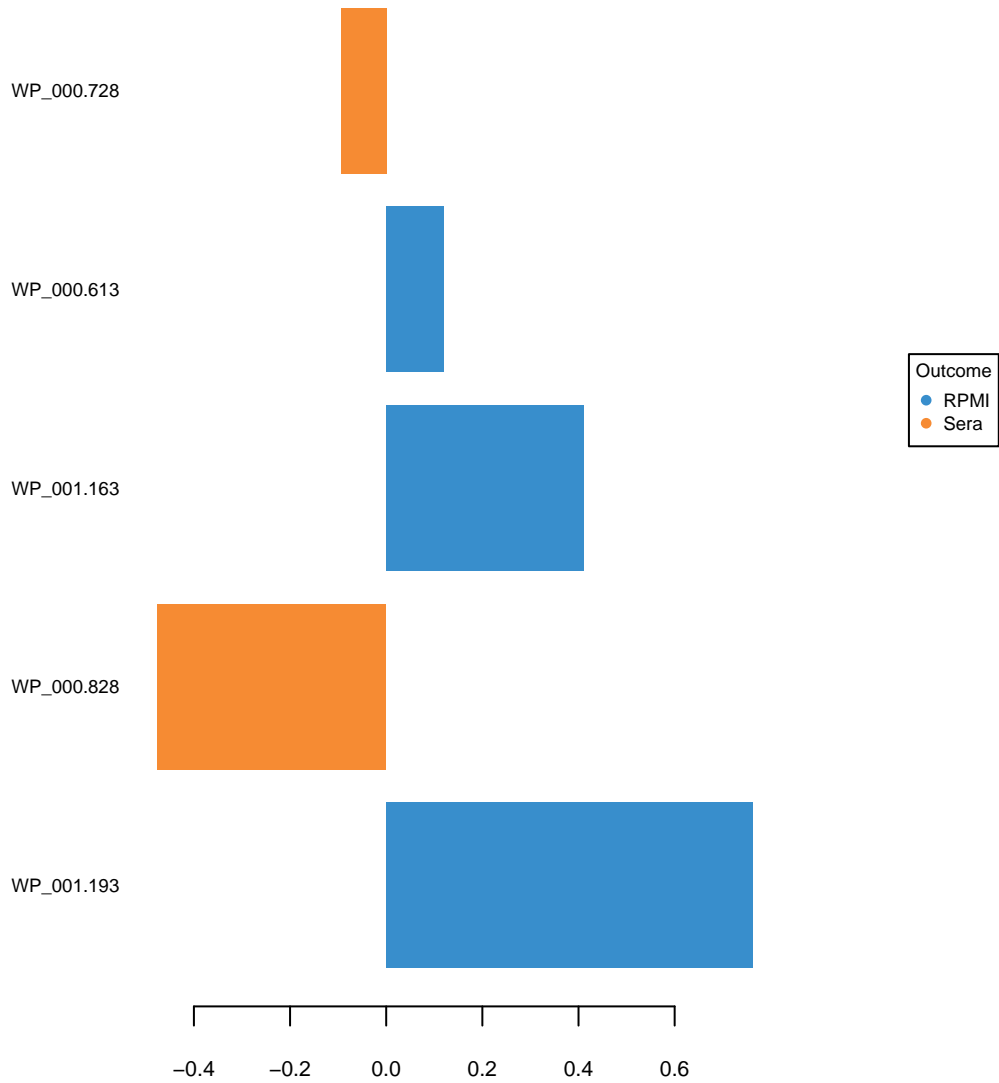
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RPMI

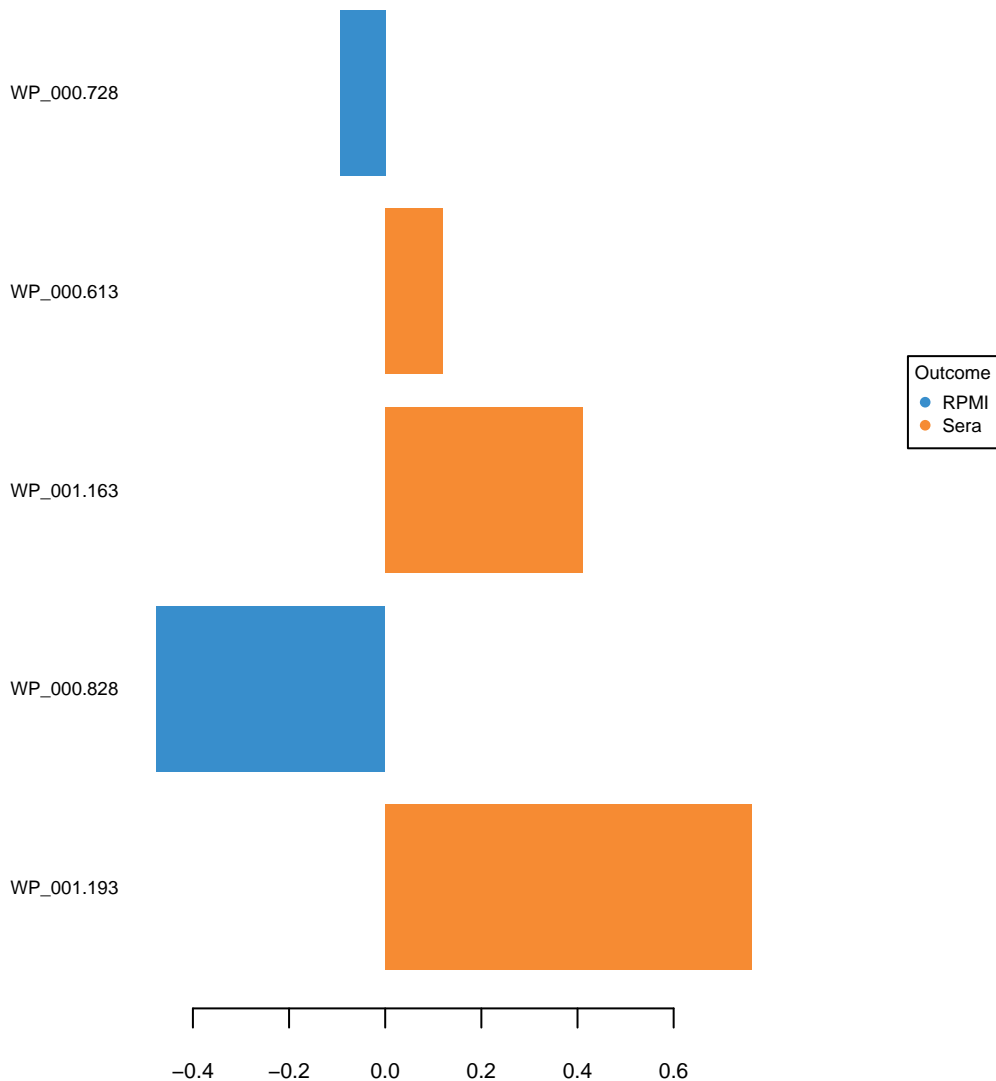
Sera



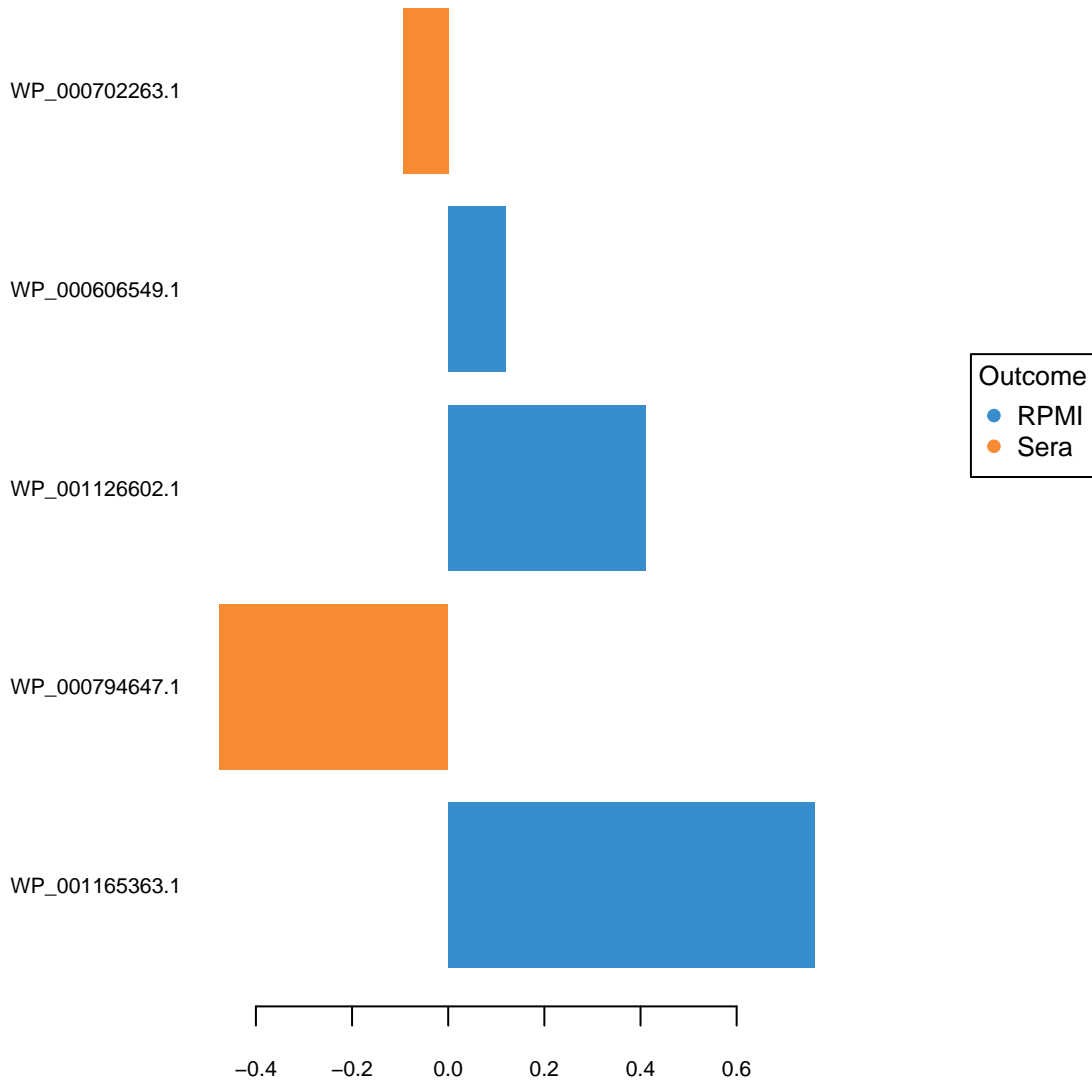
Proteomics 1 sPLSDA max load



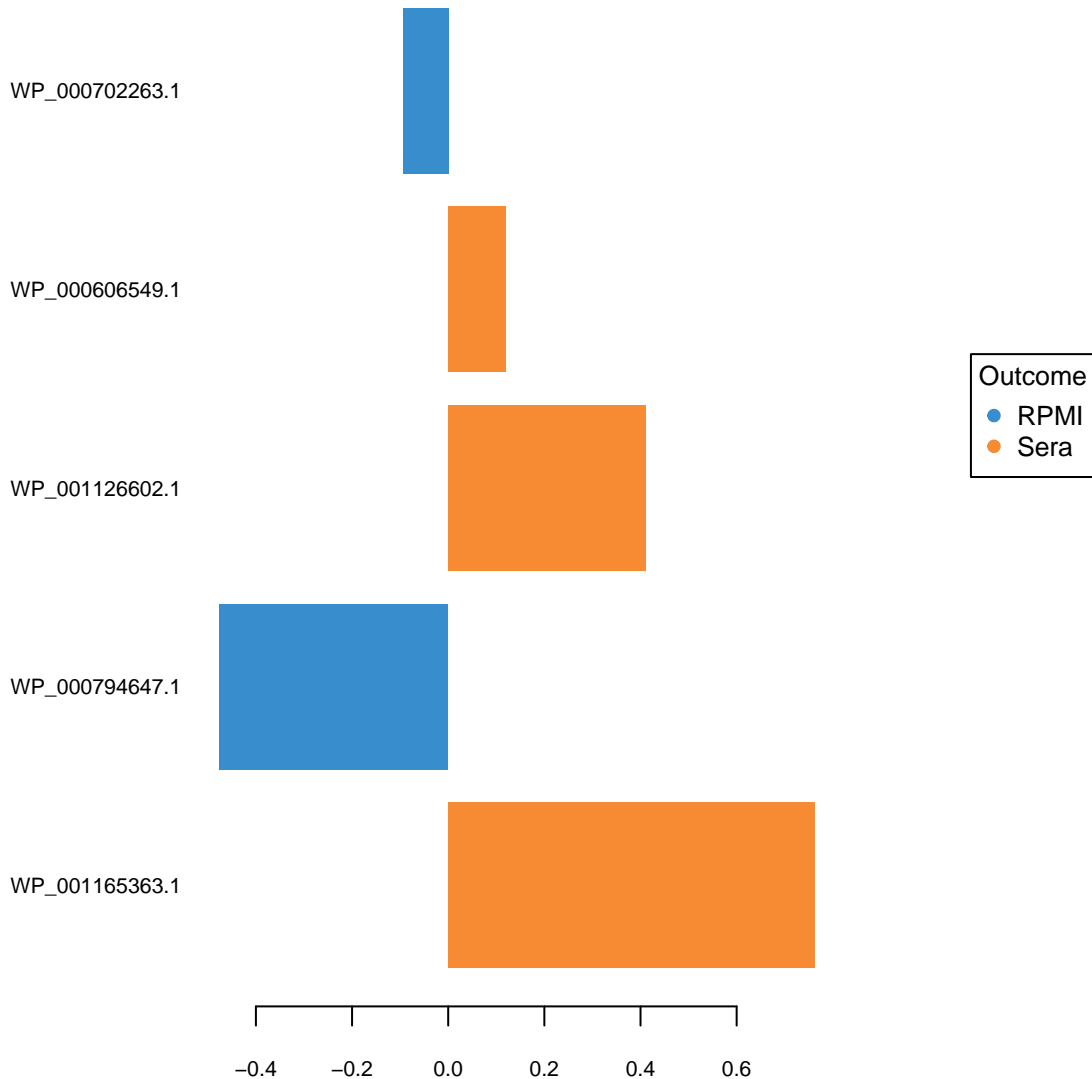
Proteomics 1 sPLSDA min load

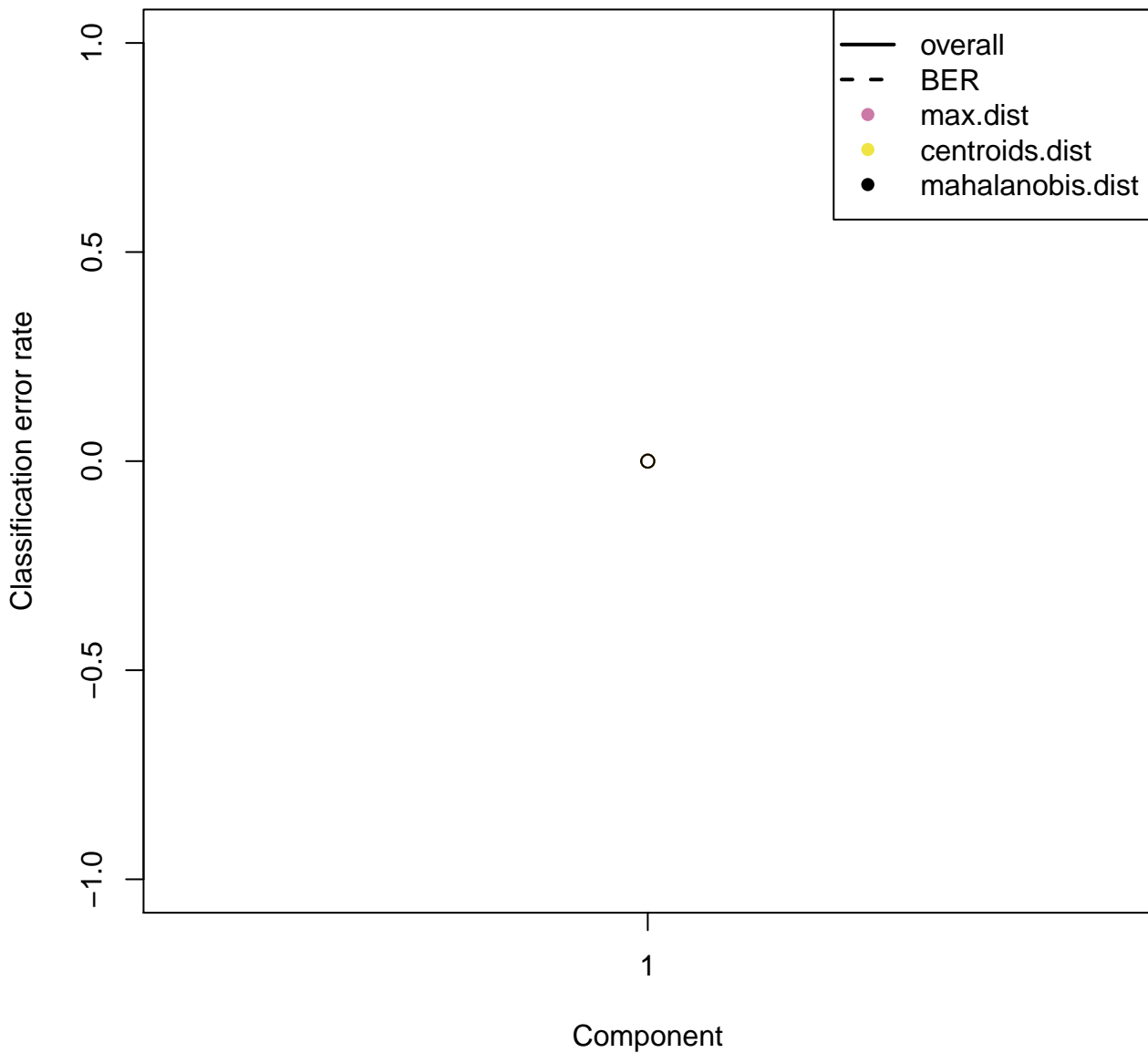


Contribution on comp 1

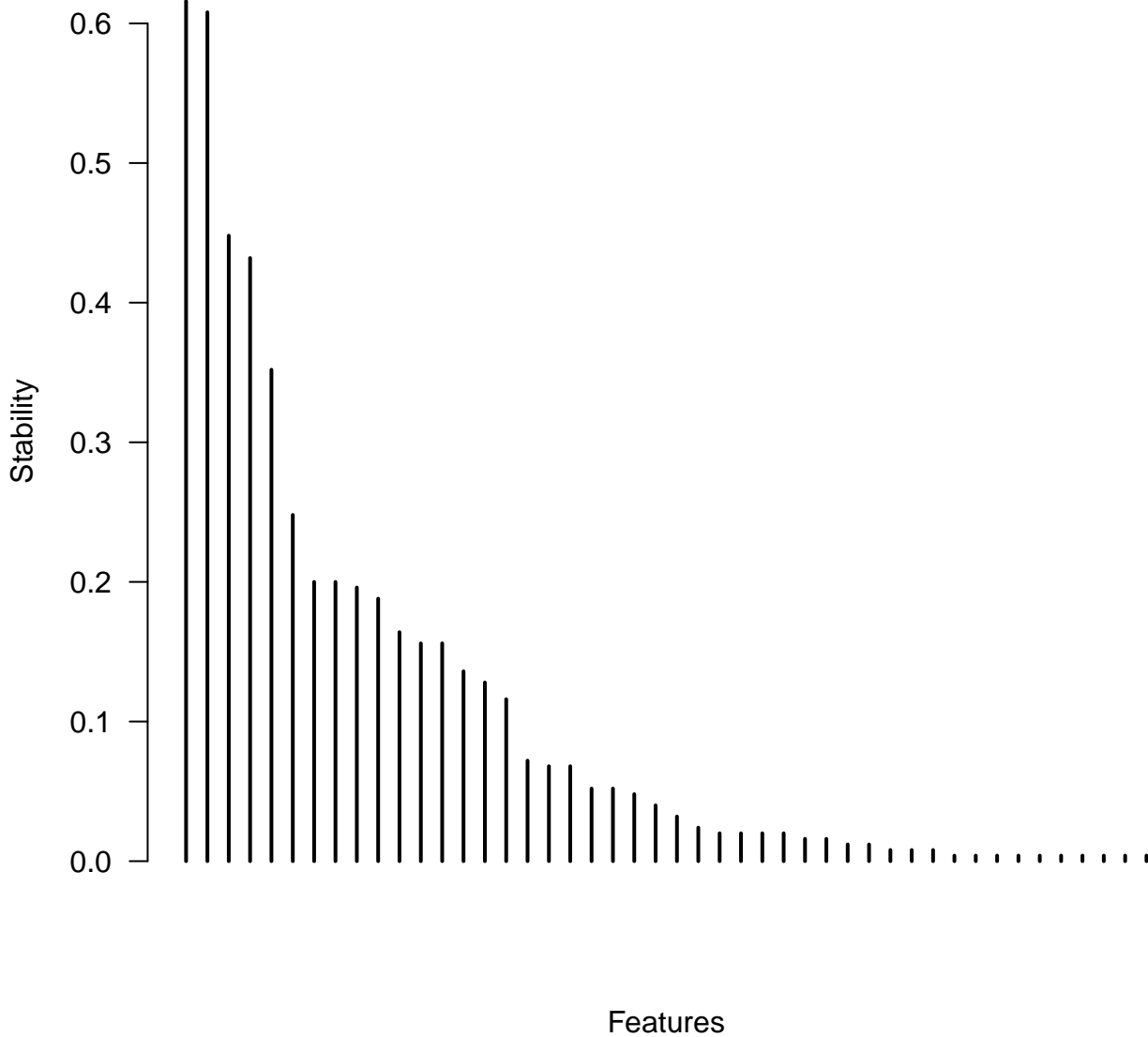


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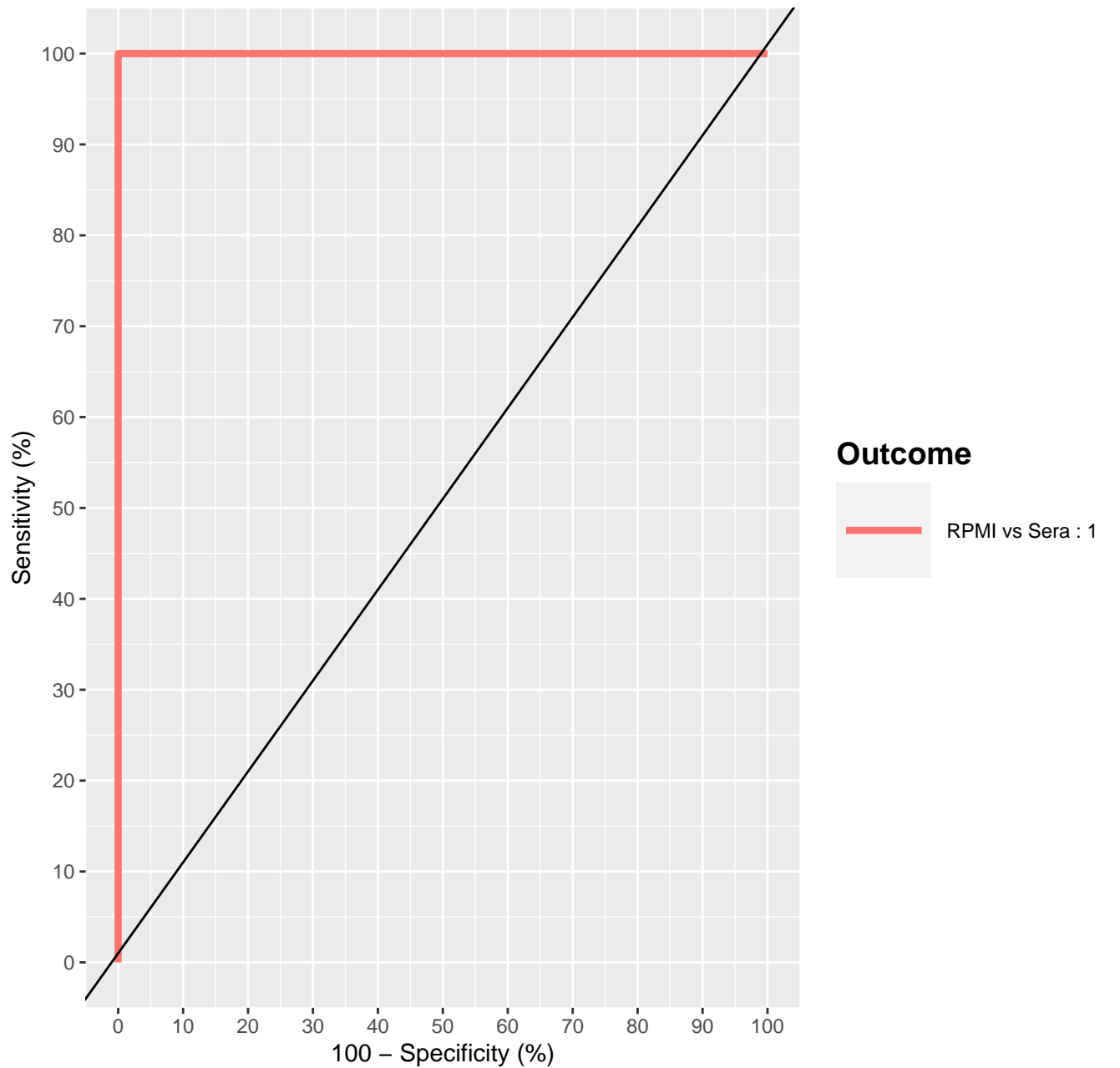




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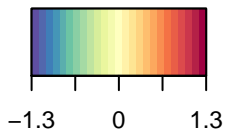


ROC Curve Comp 1



sPLSDA

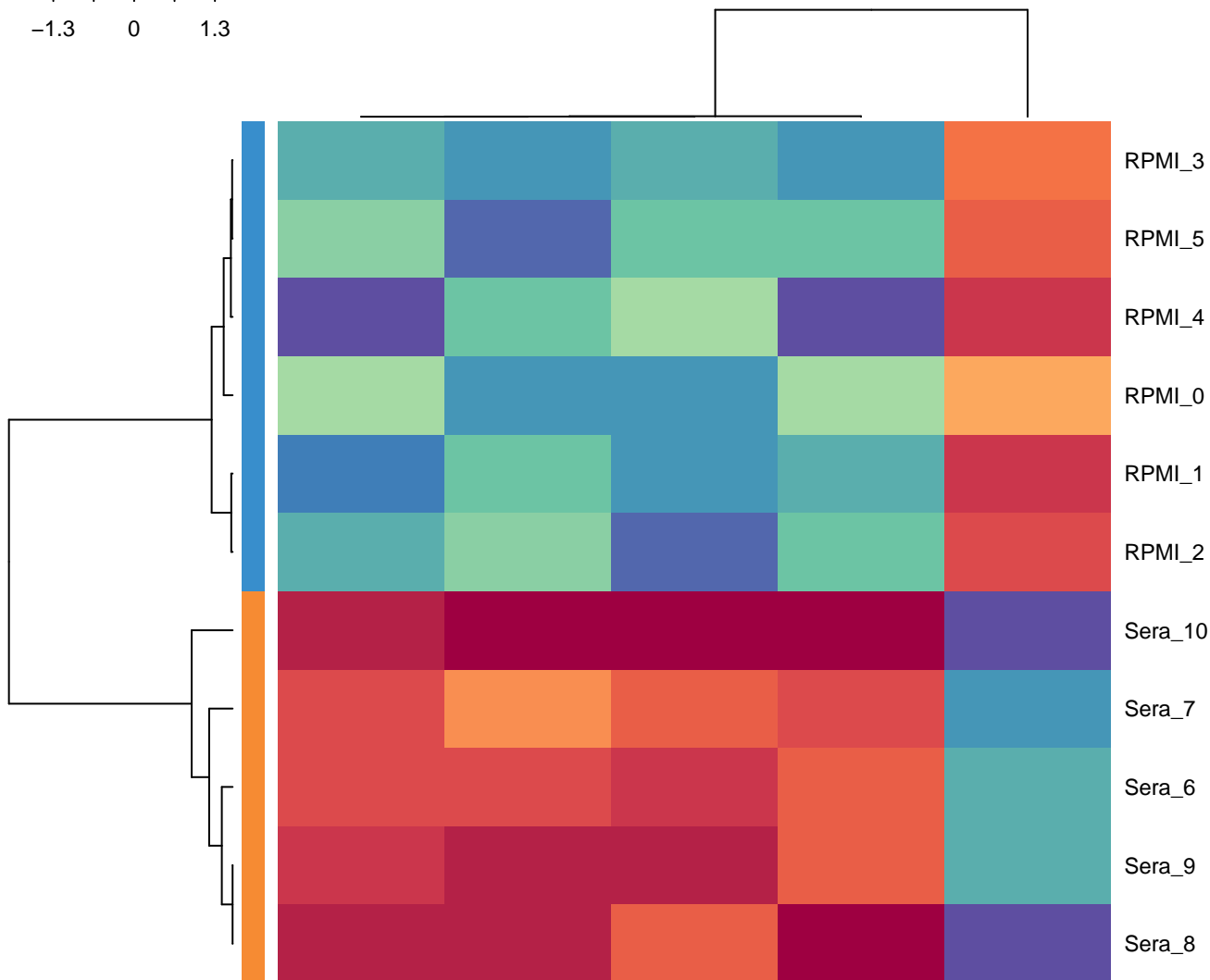
Color key



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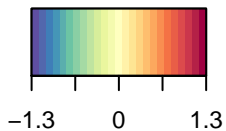
RPMI

Sera



sPLSDA Component 1

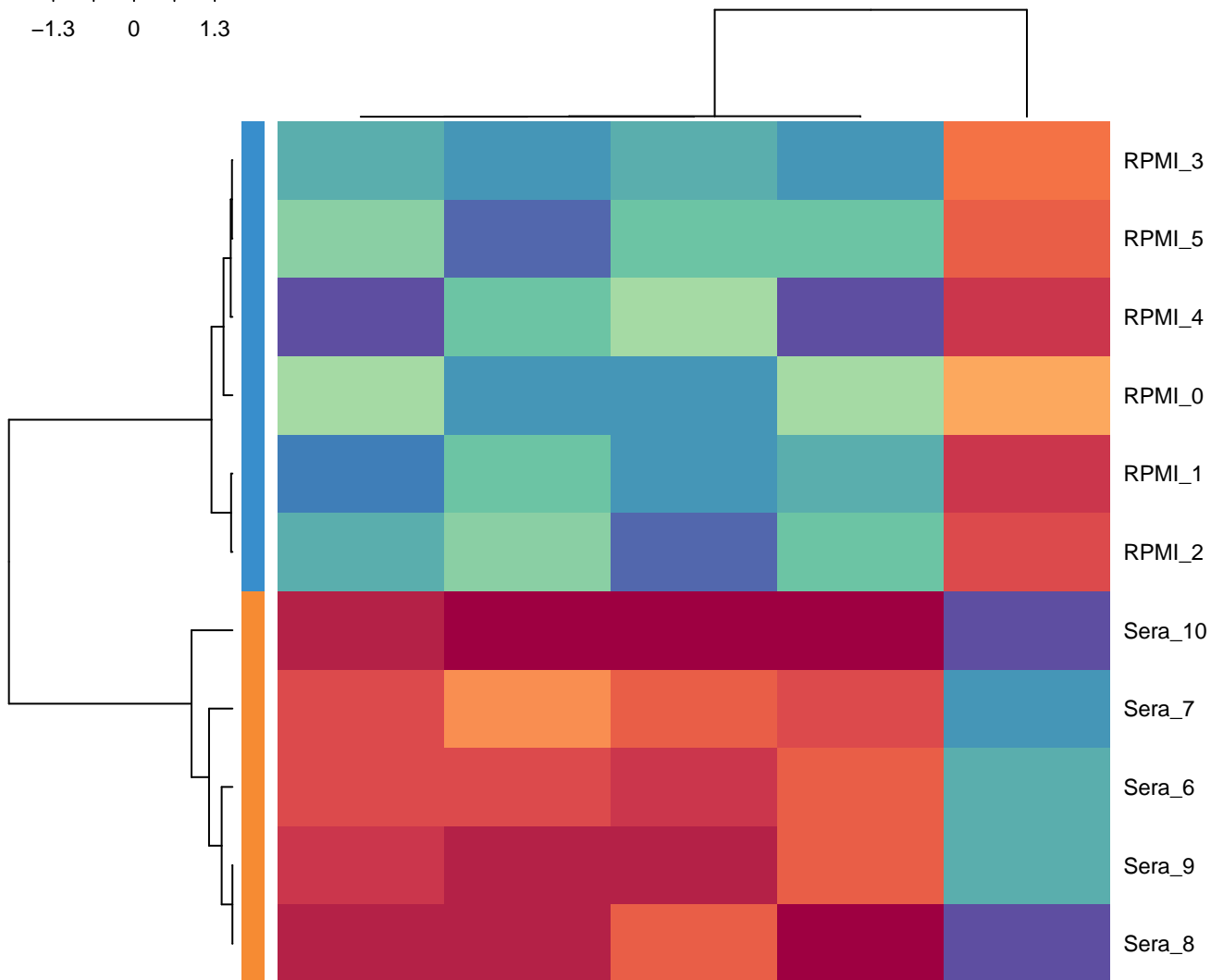
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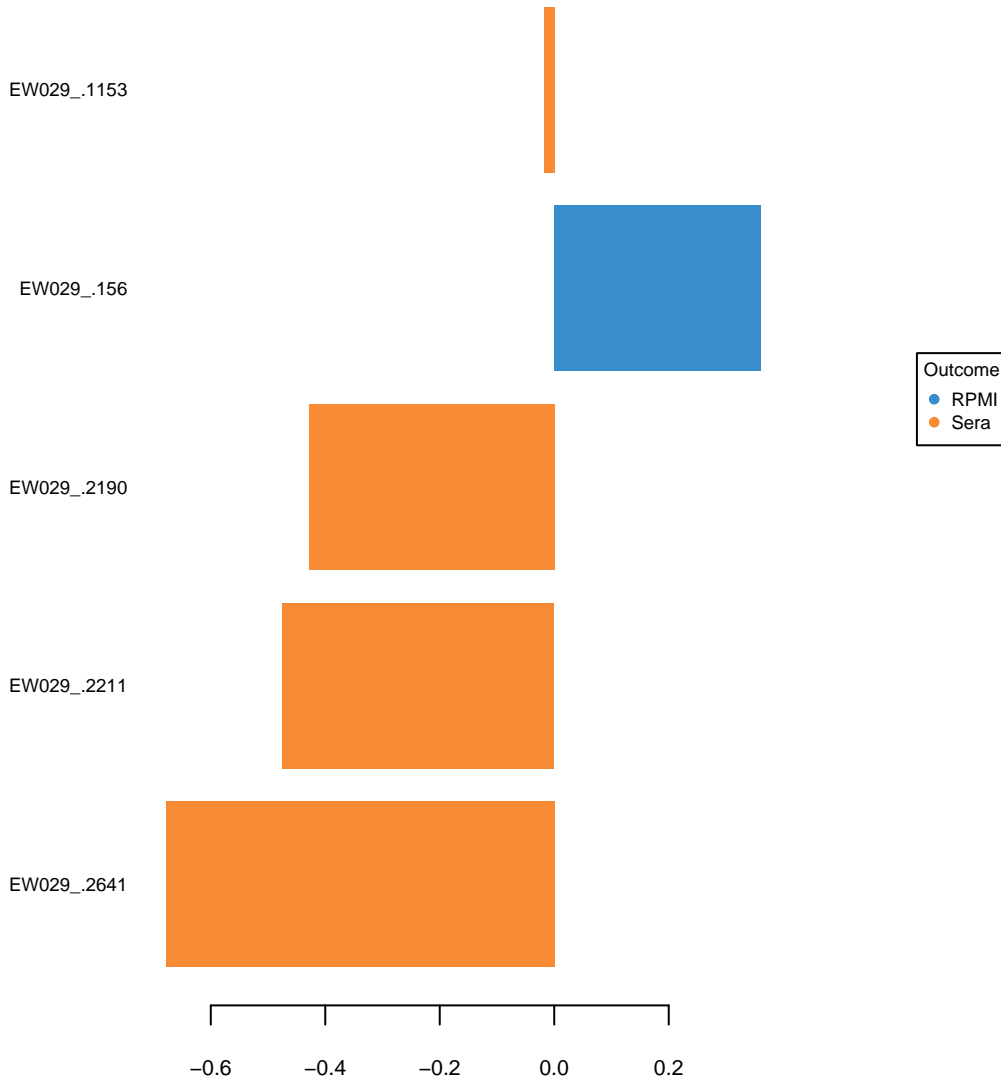
Status

RPMI

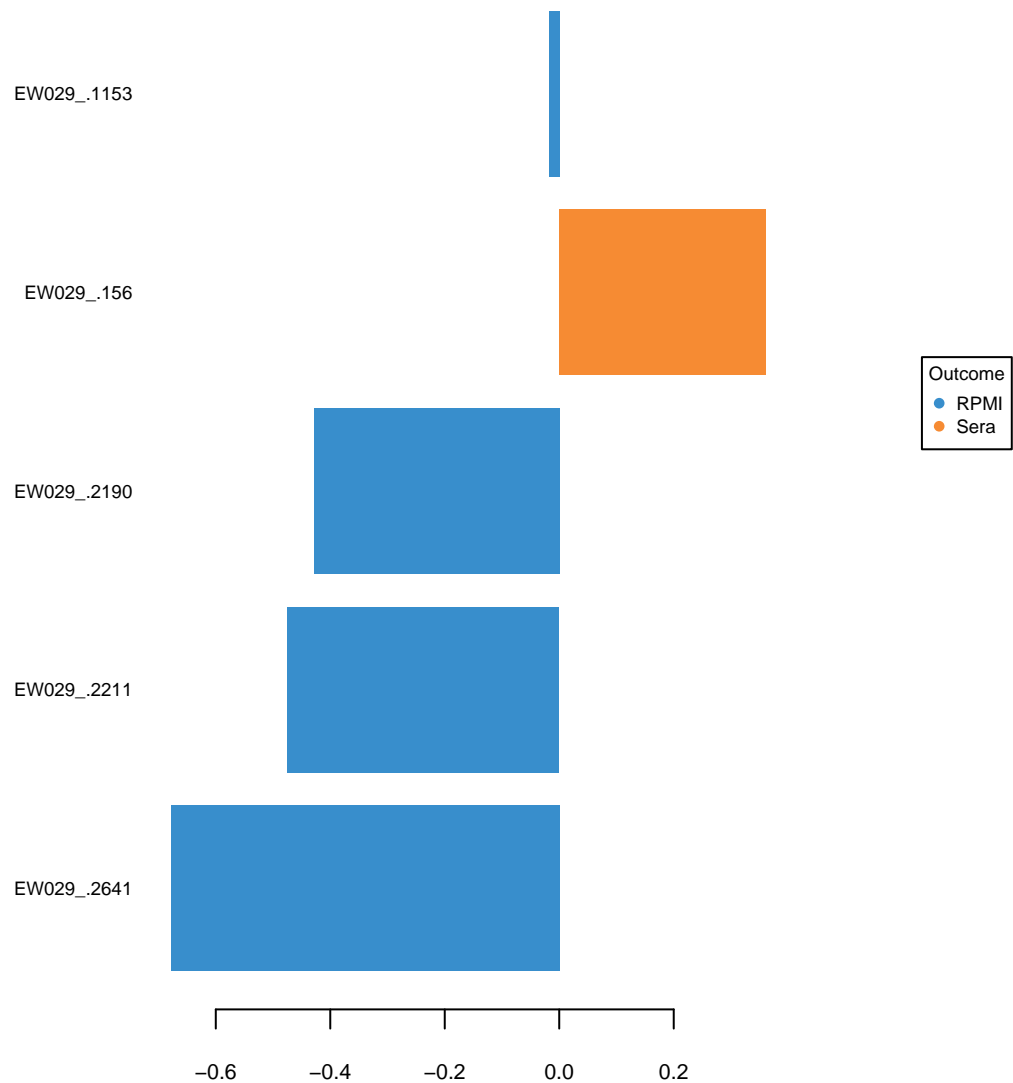
Sera



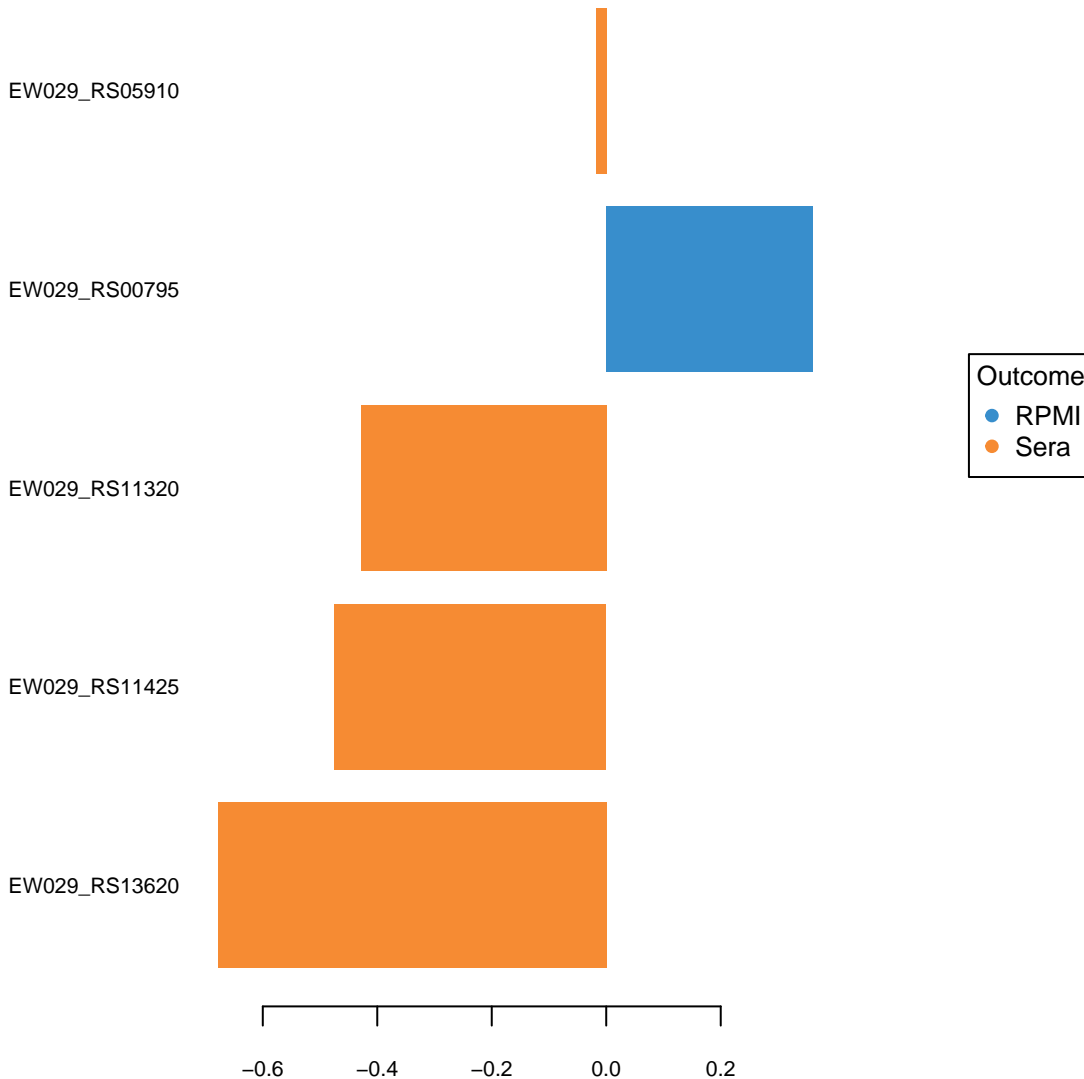
RNA_Seq 1 sPLSDA max loadings



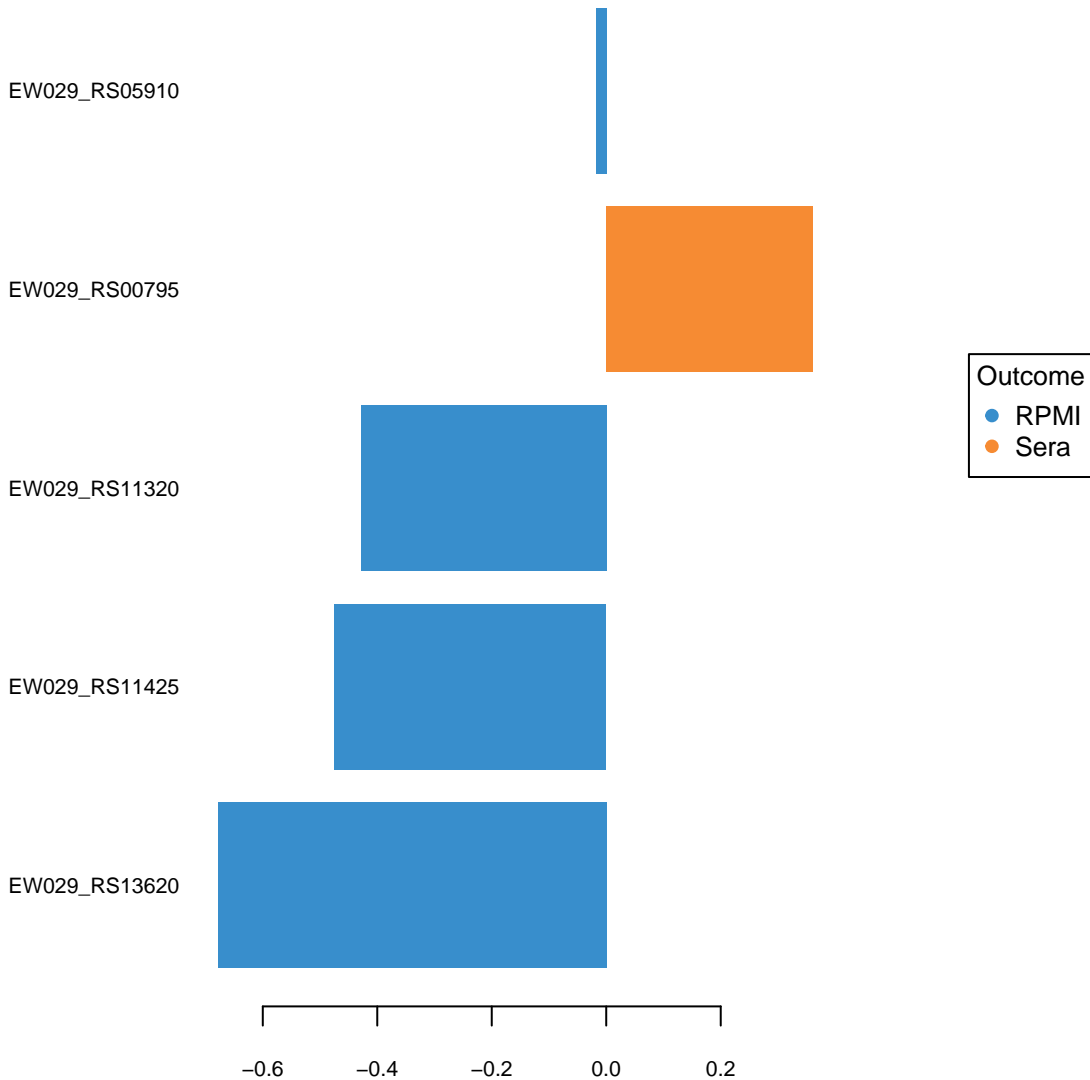
RNA_Seq 1 sPLSDA min loadings

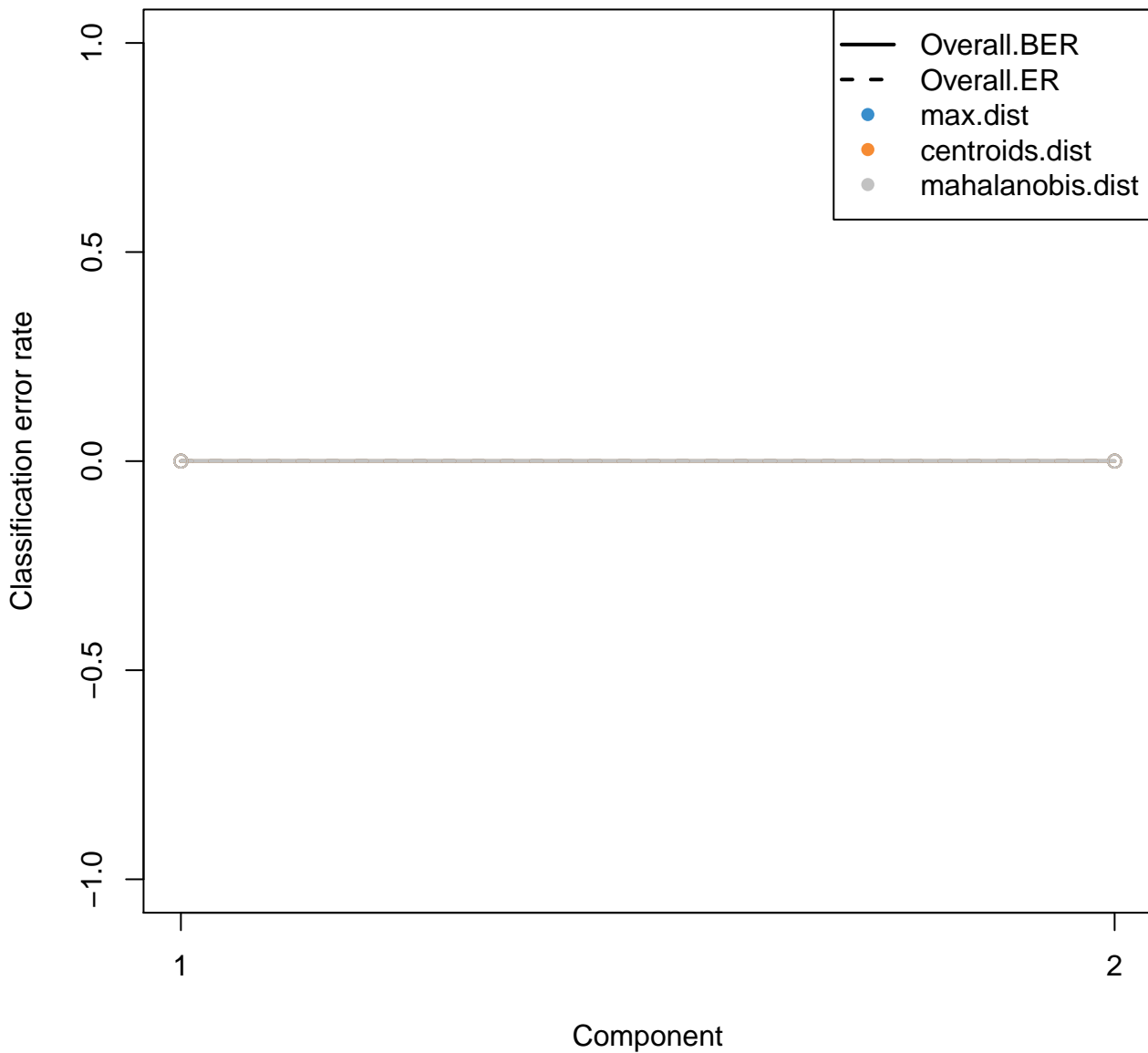


Contribution on comp 1

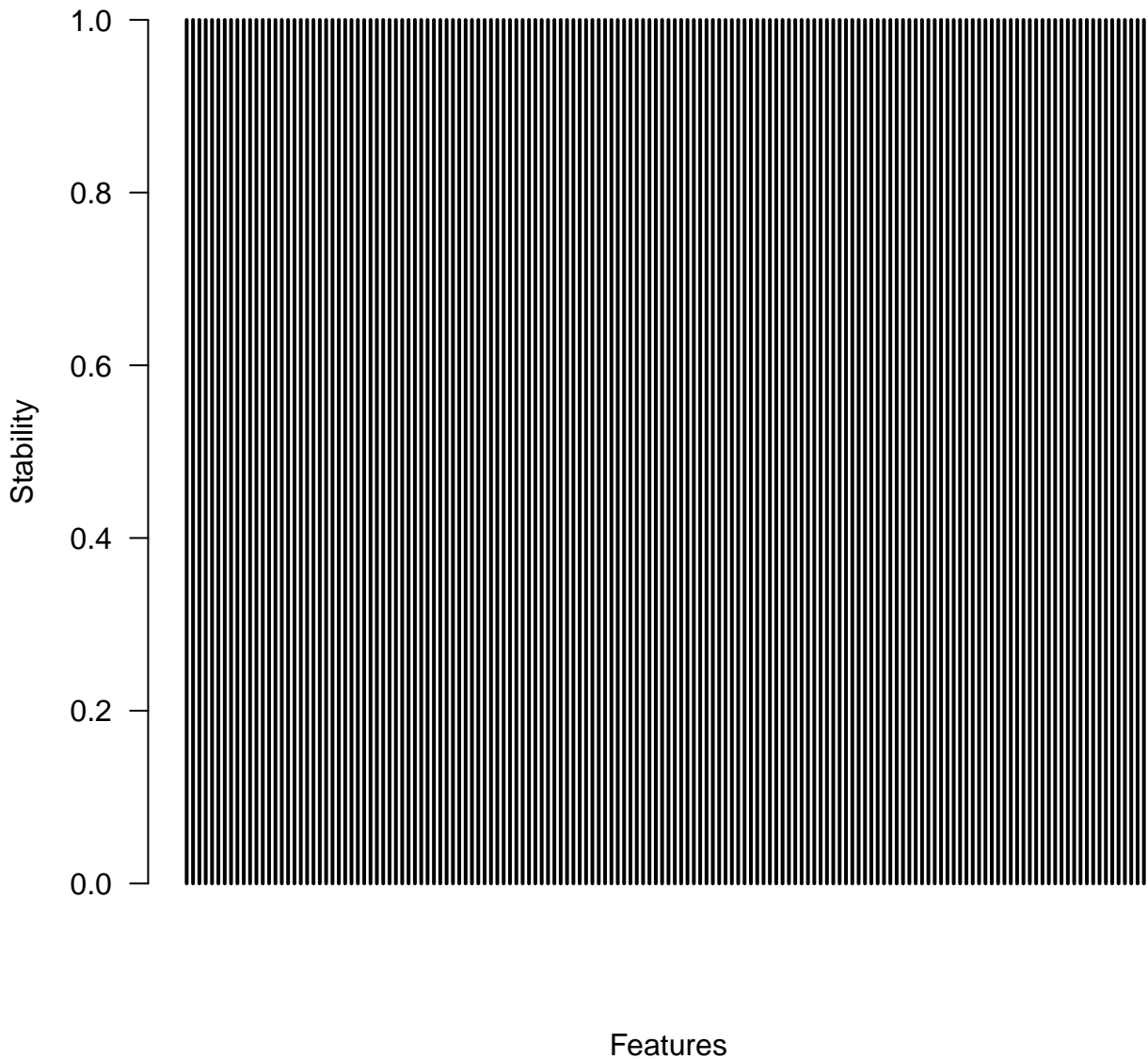


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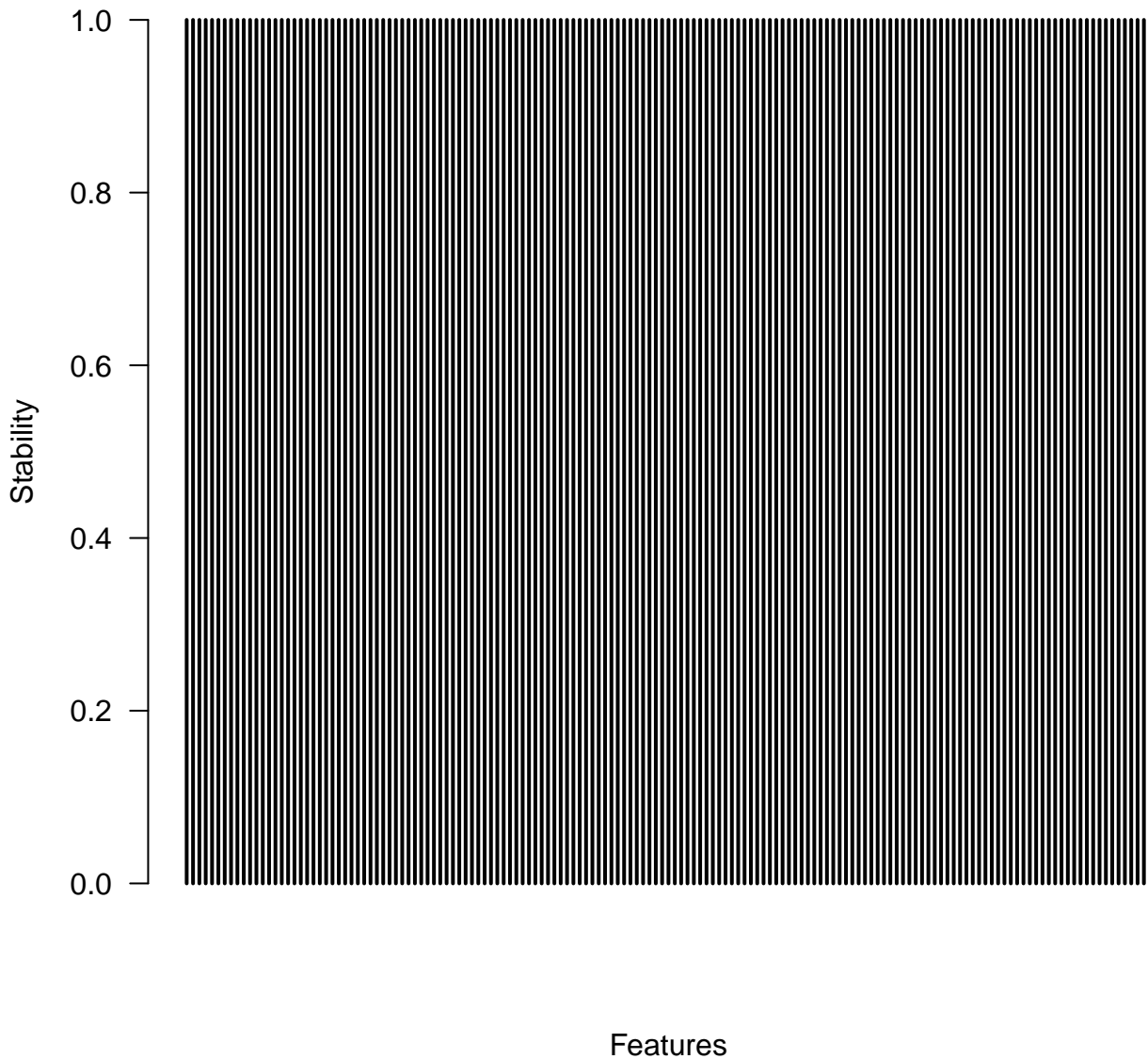




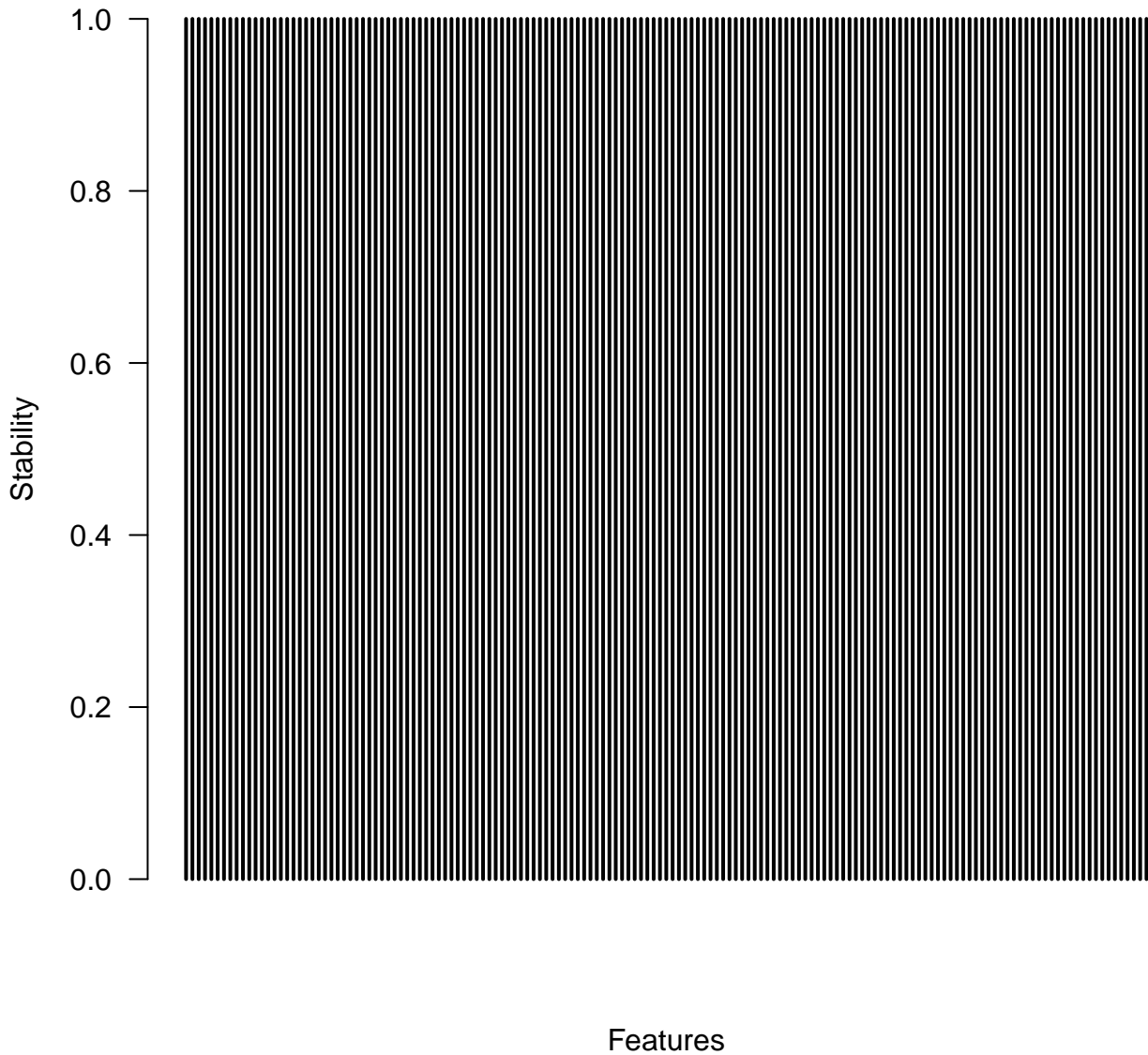
Metabolomics Comp 1



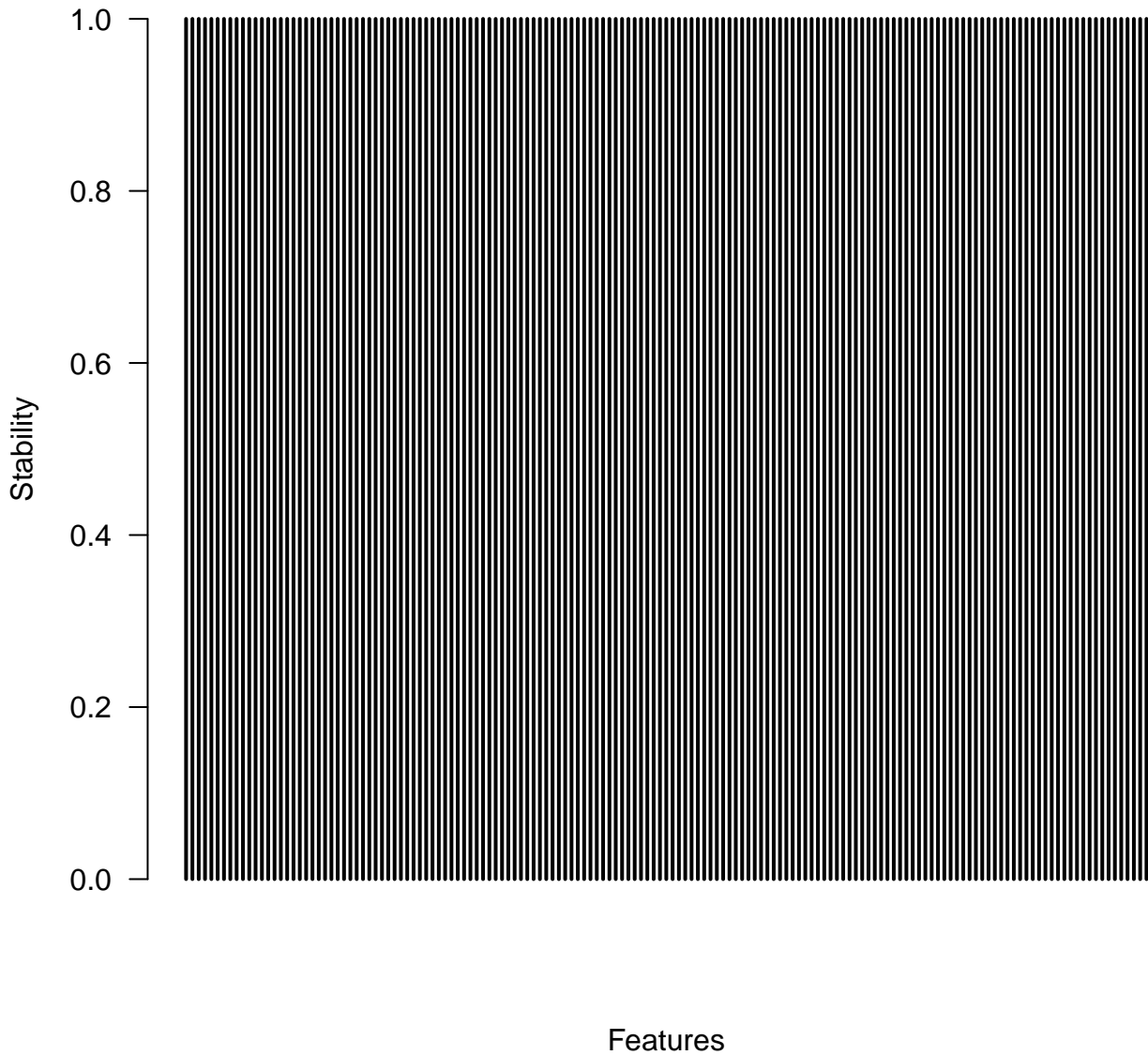
Metabolomics Comp 2



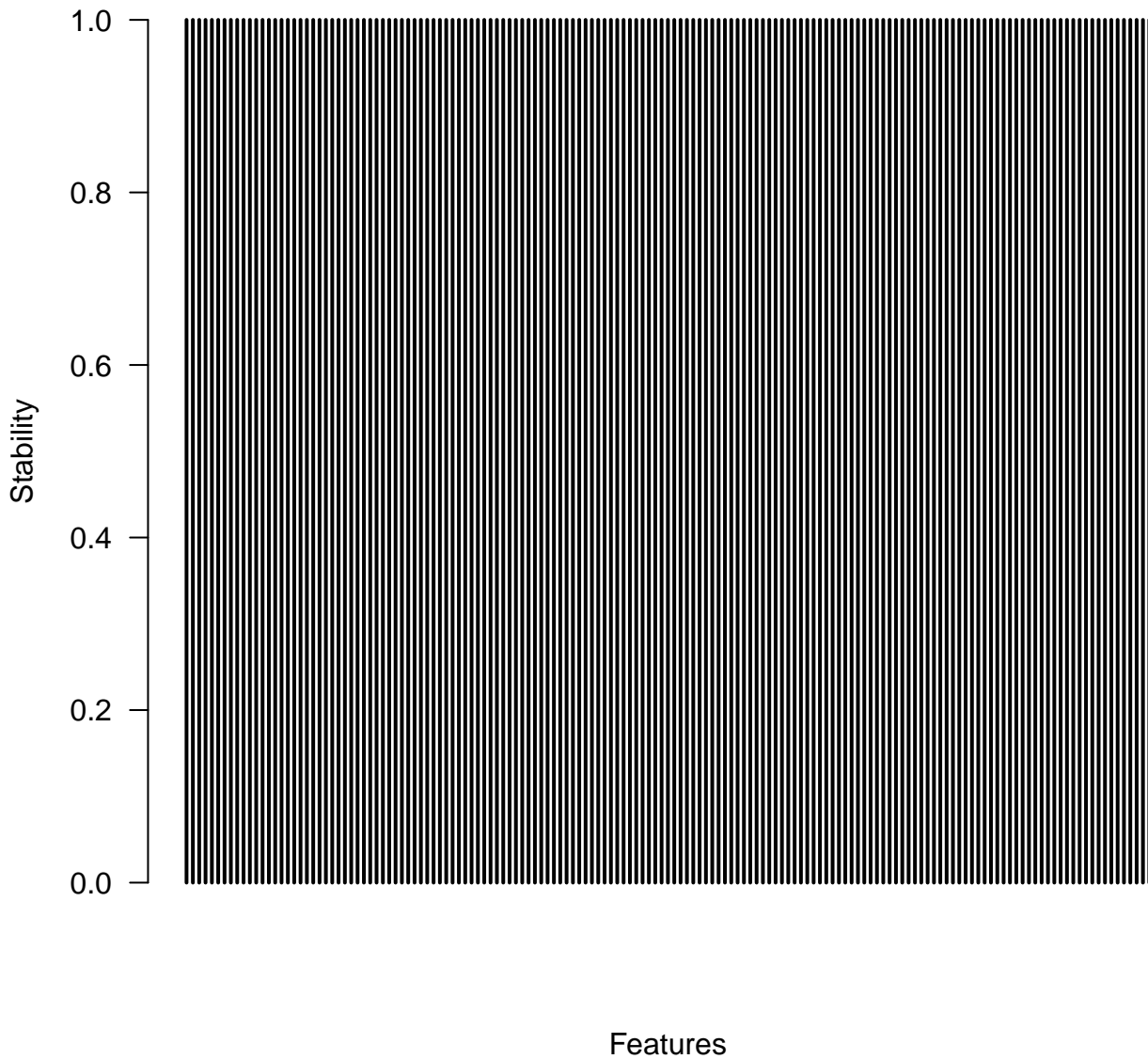
Proteomics Comp 1



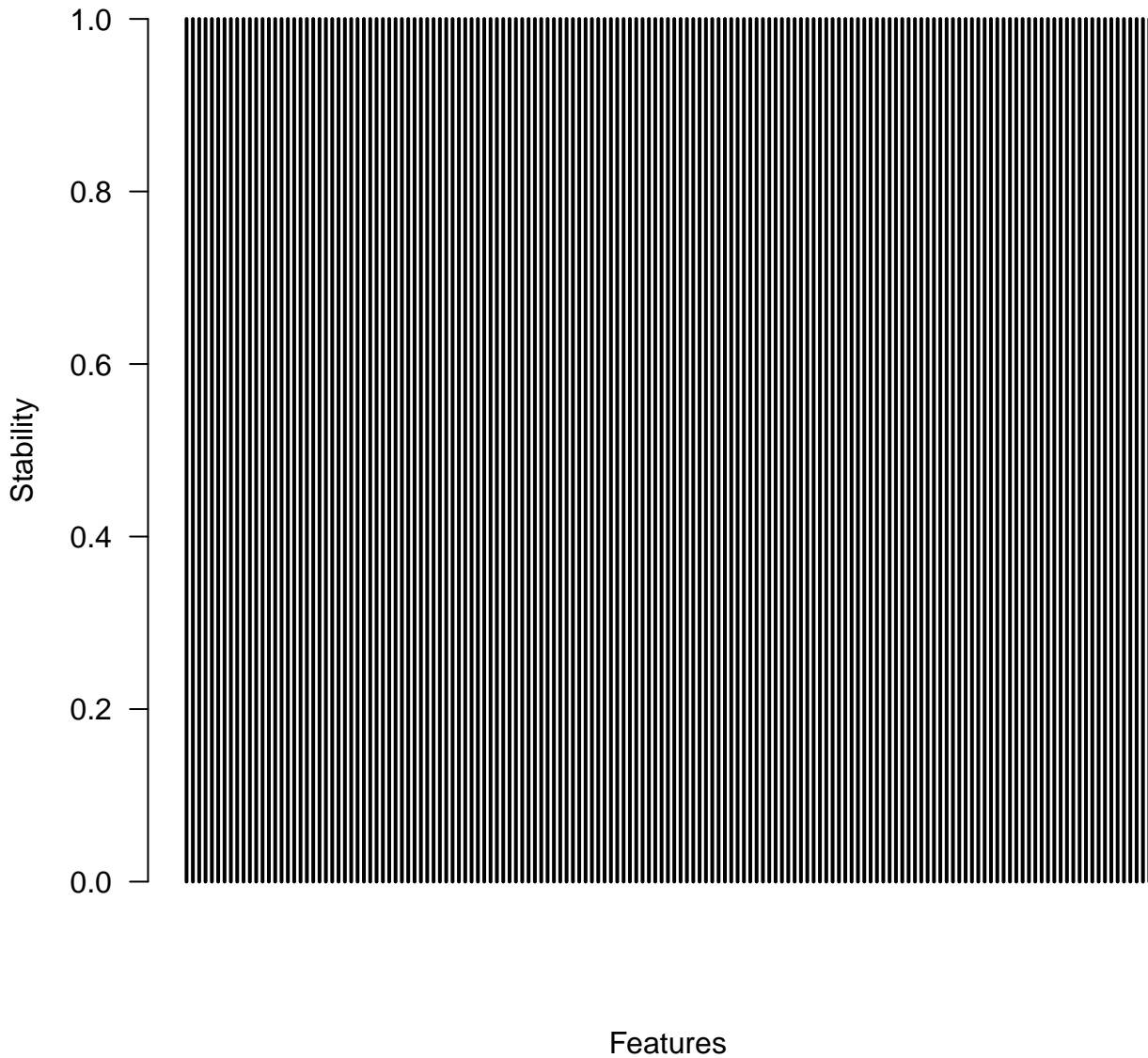
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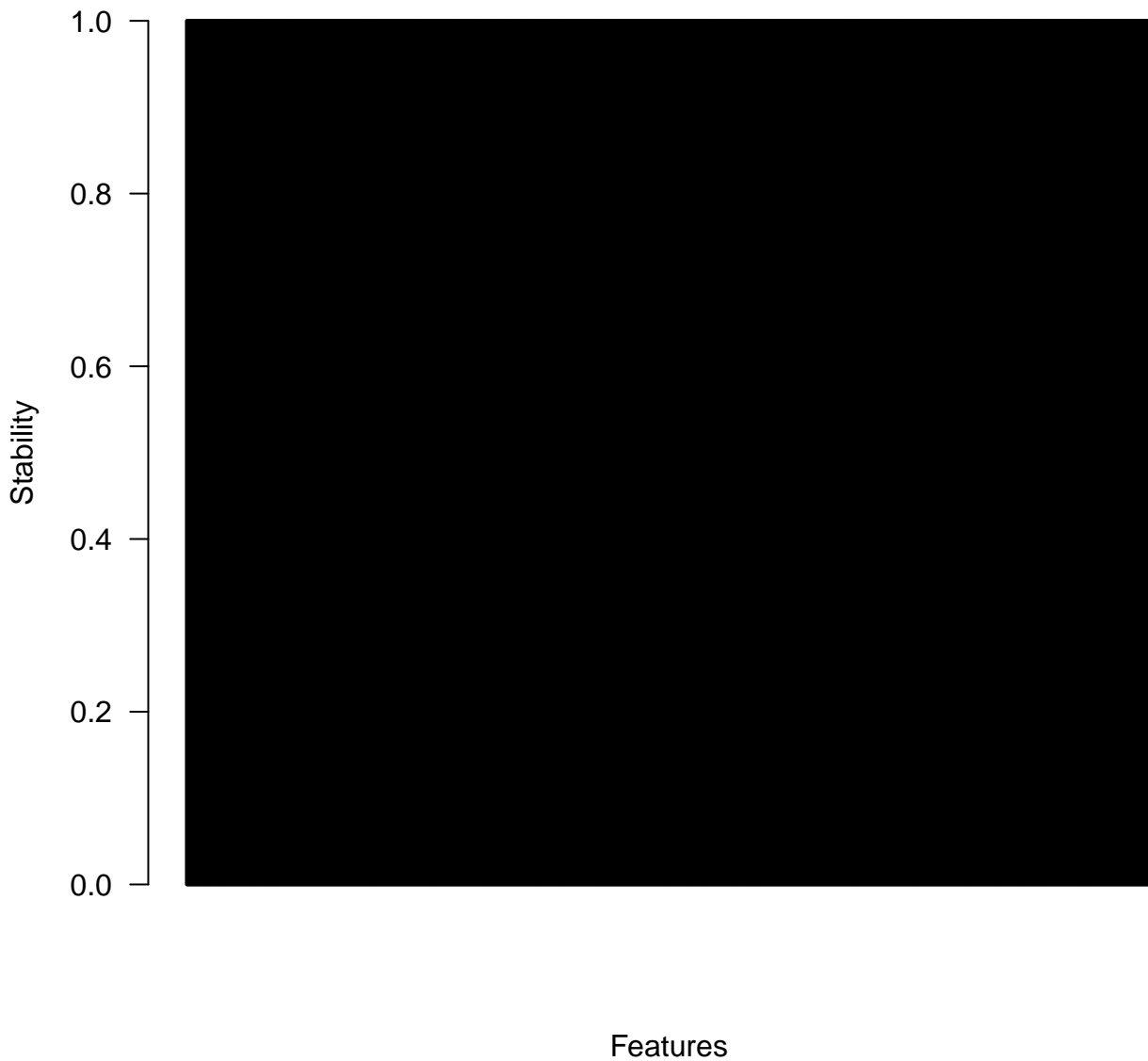
RNA_Seq Comp 1



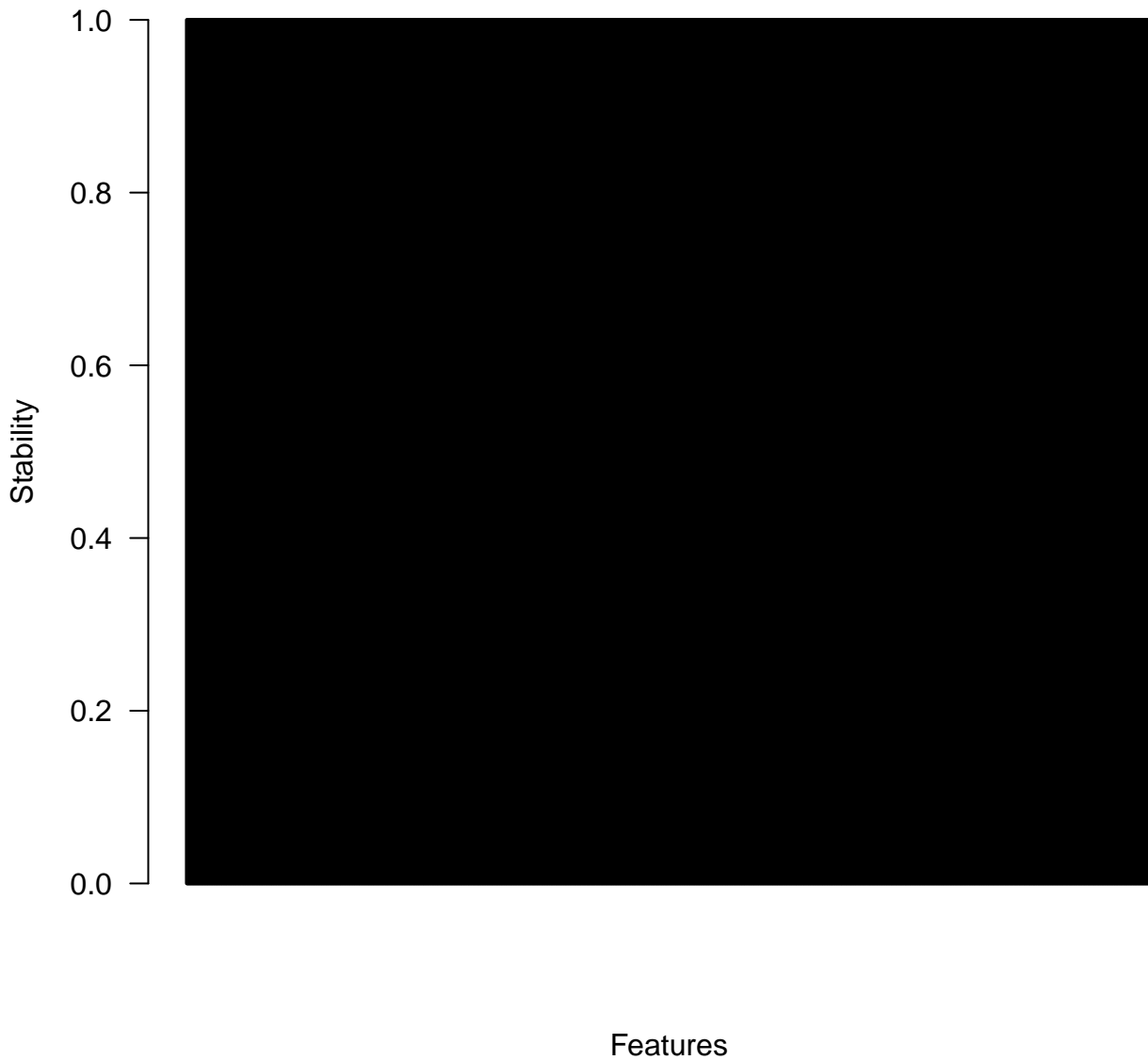
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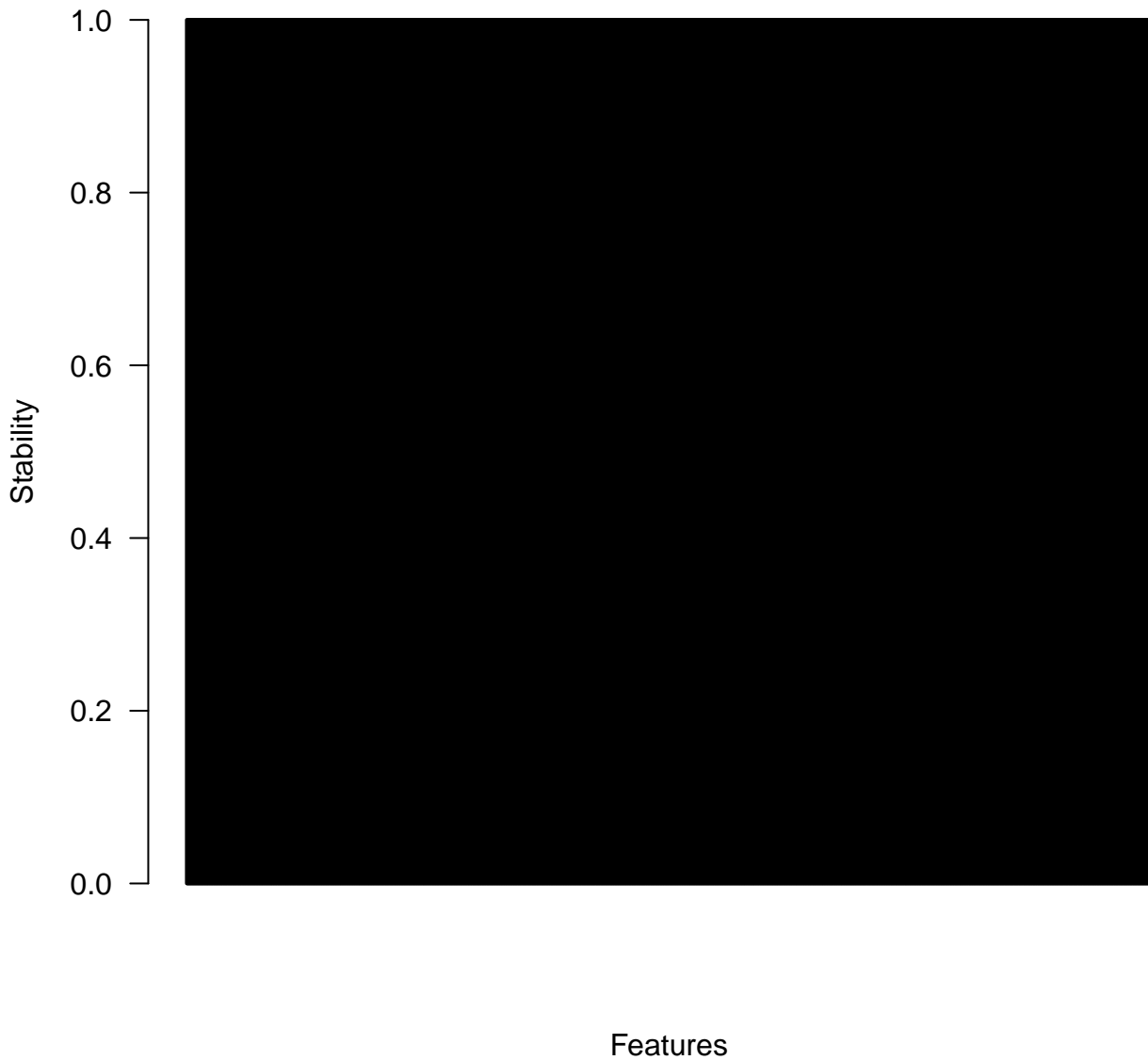
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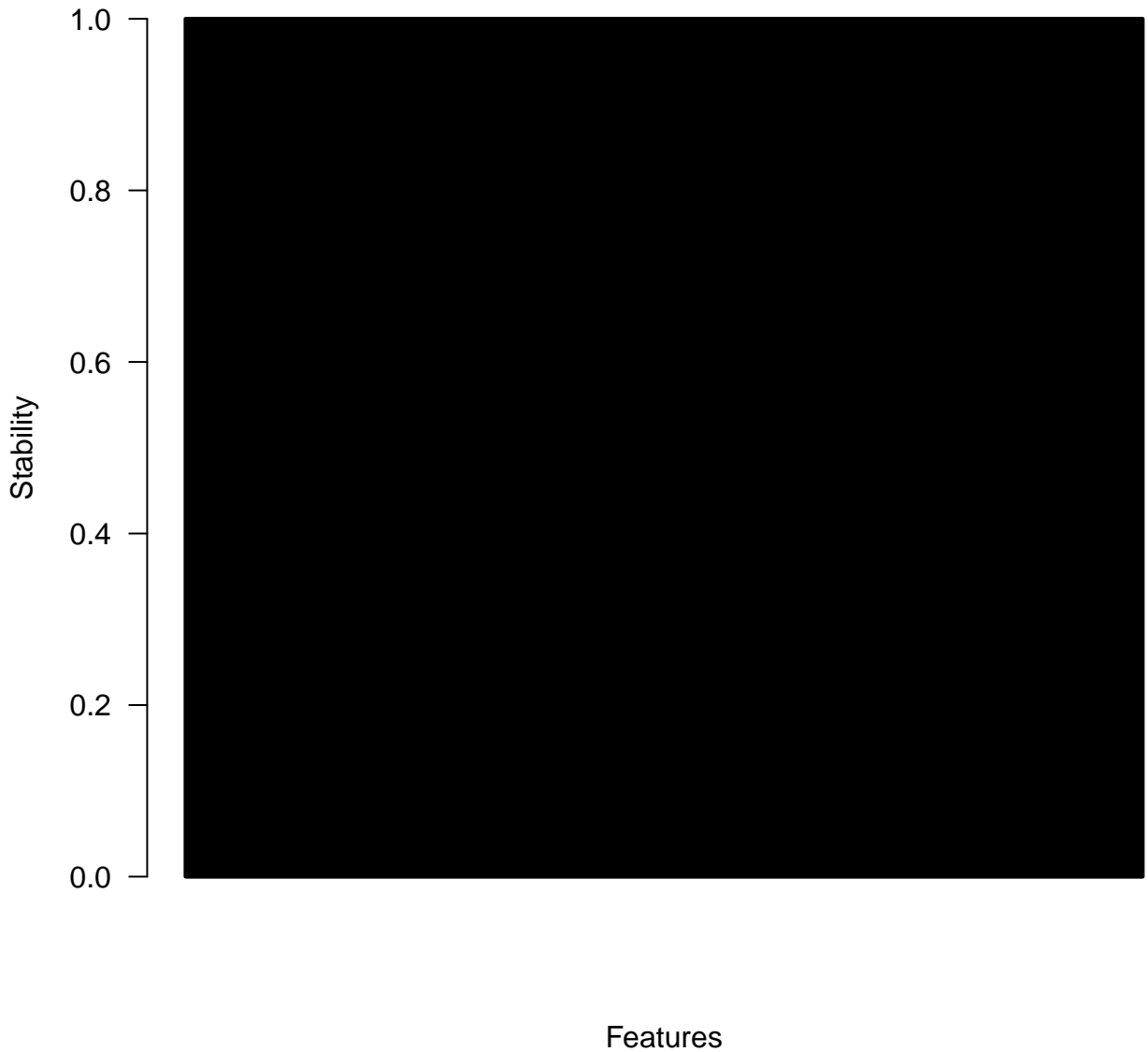
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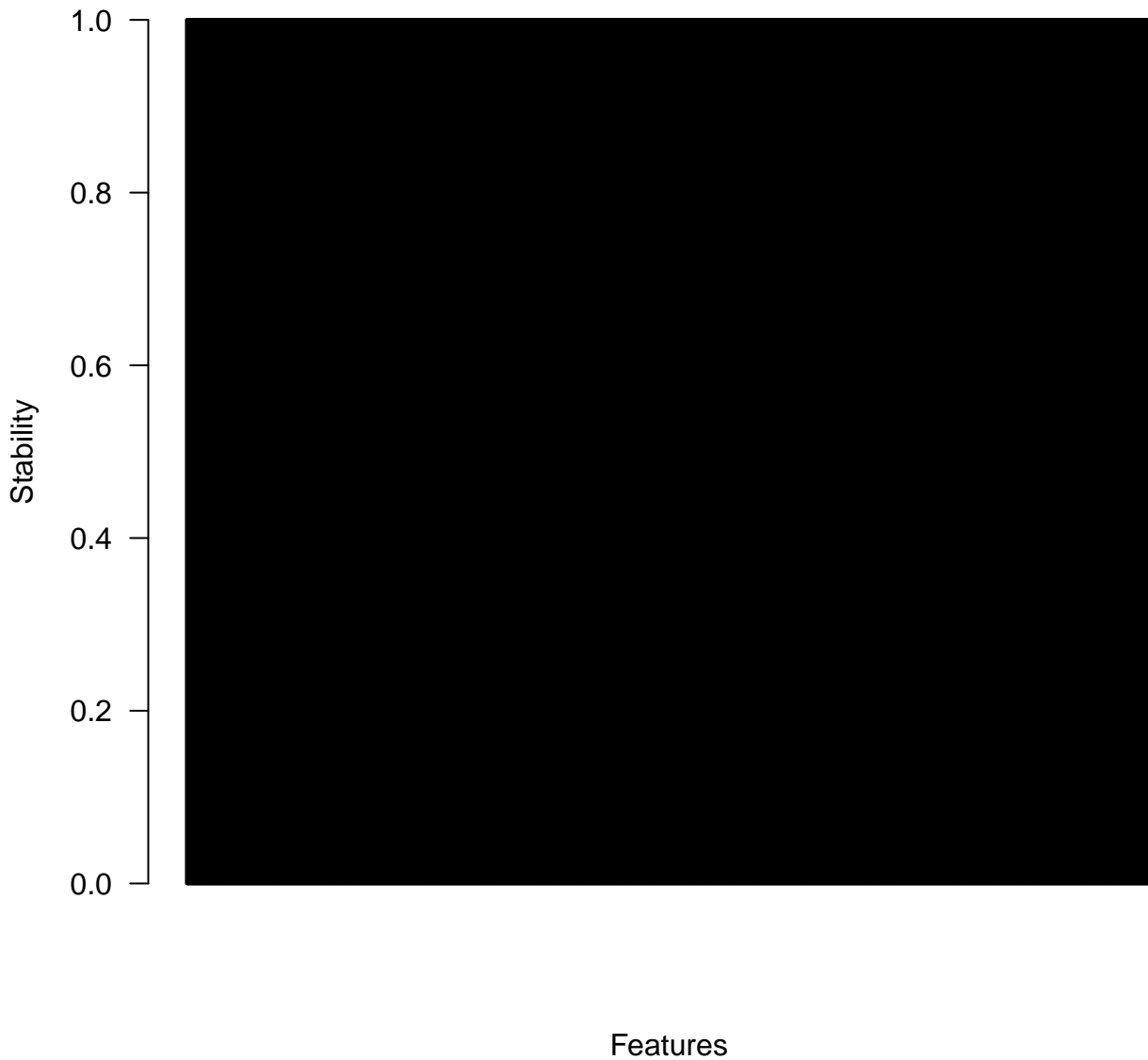
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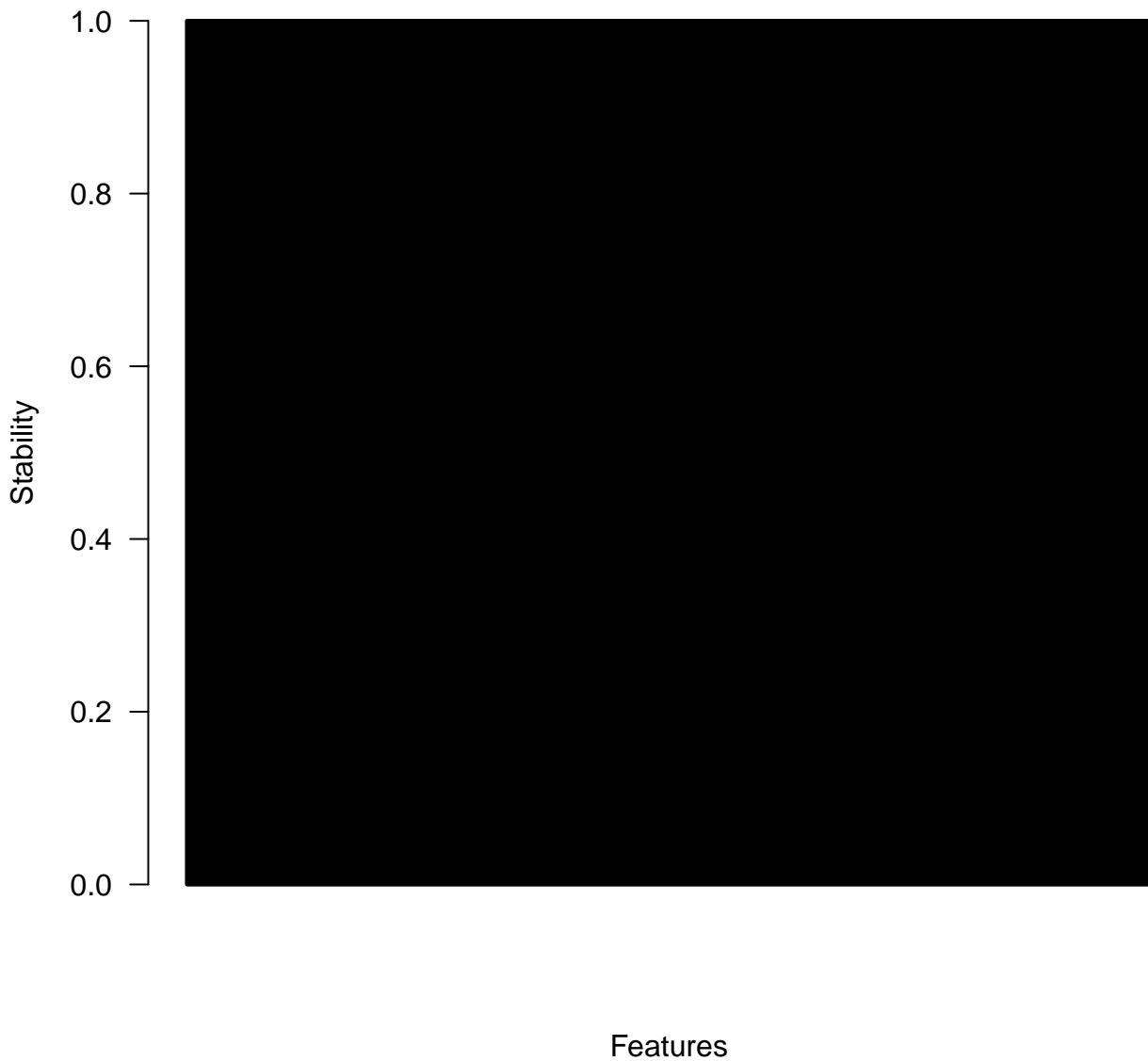
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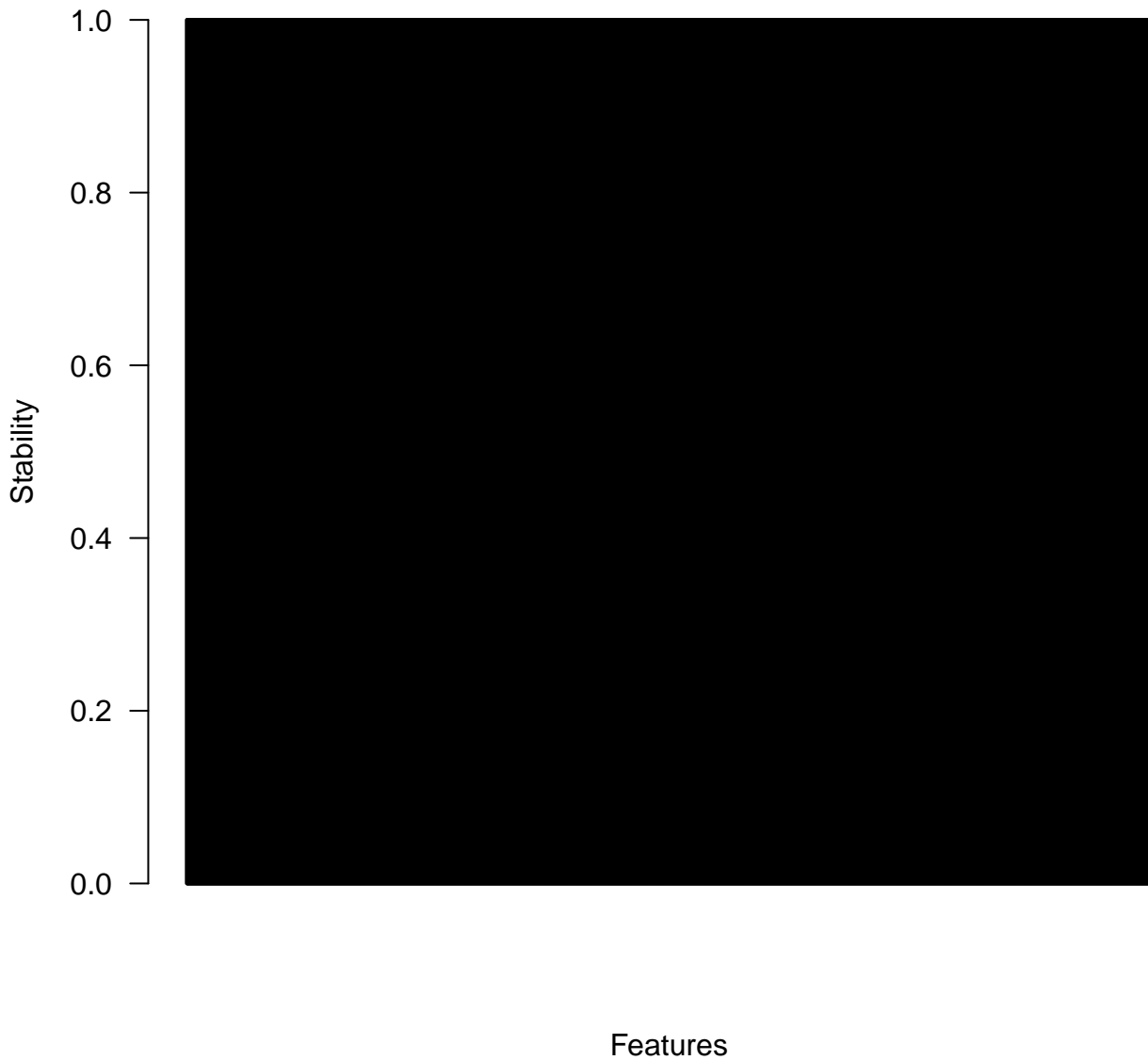
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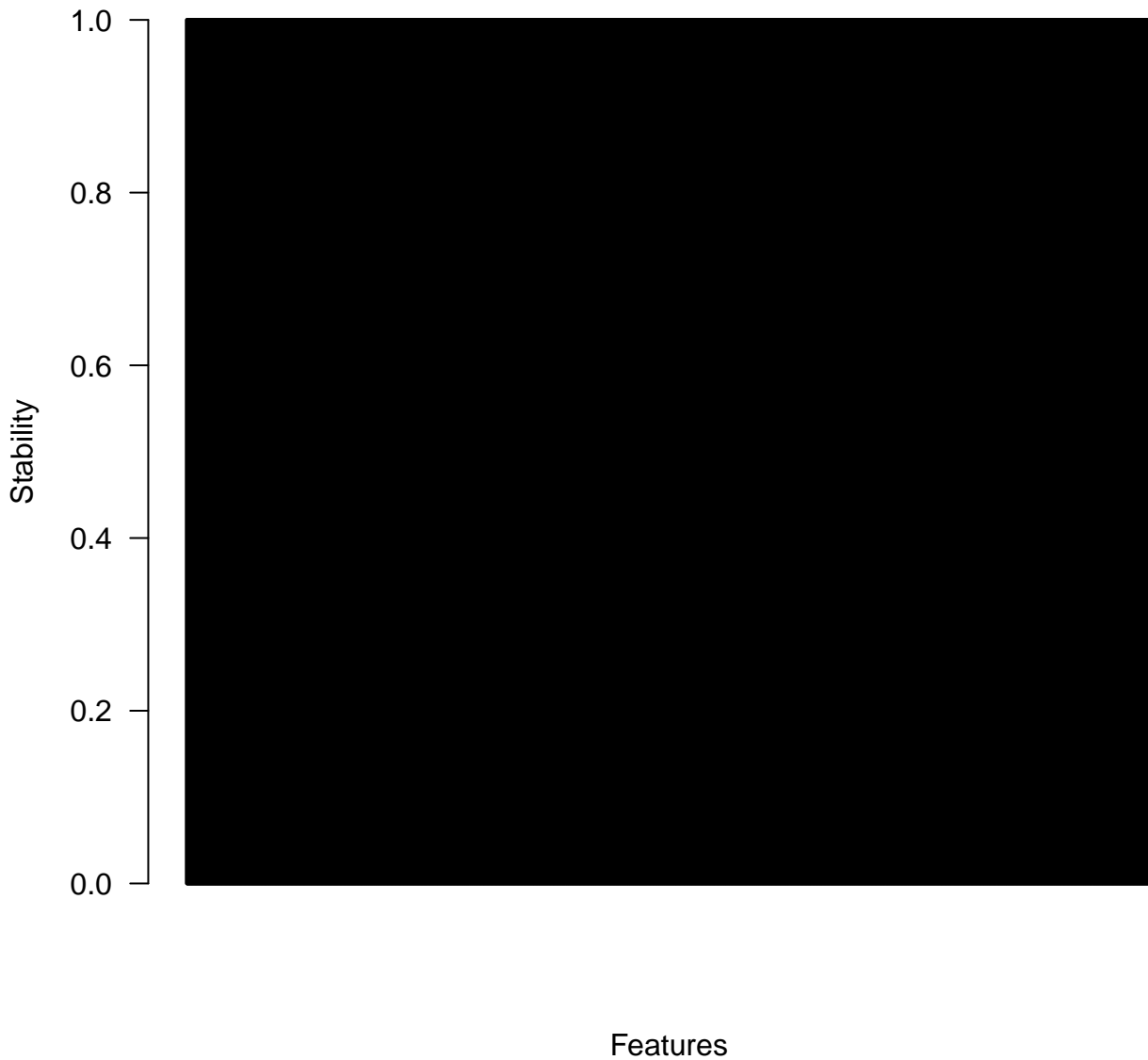
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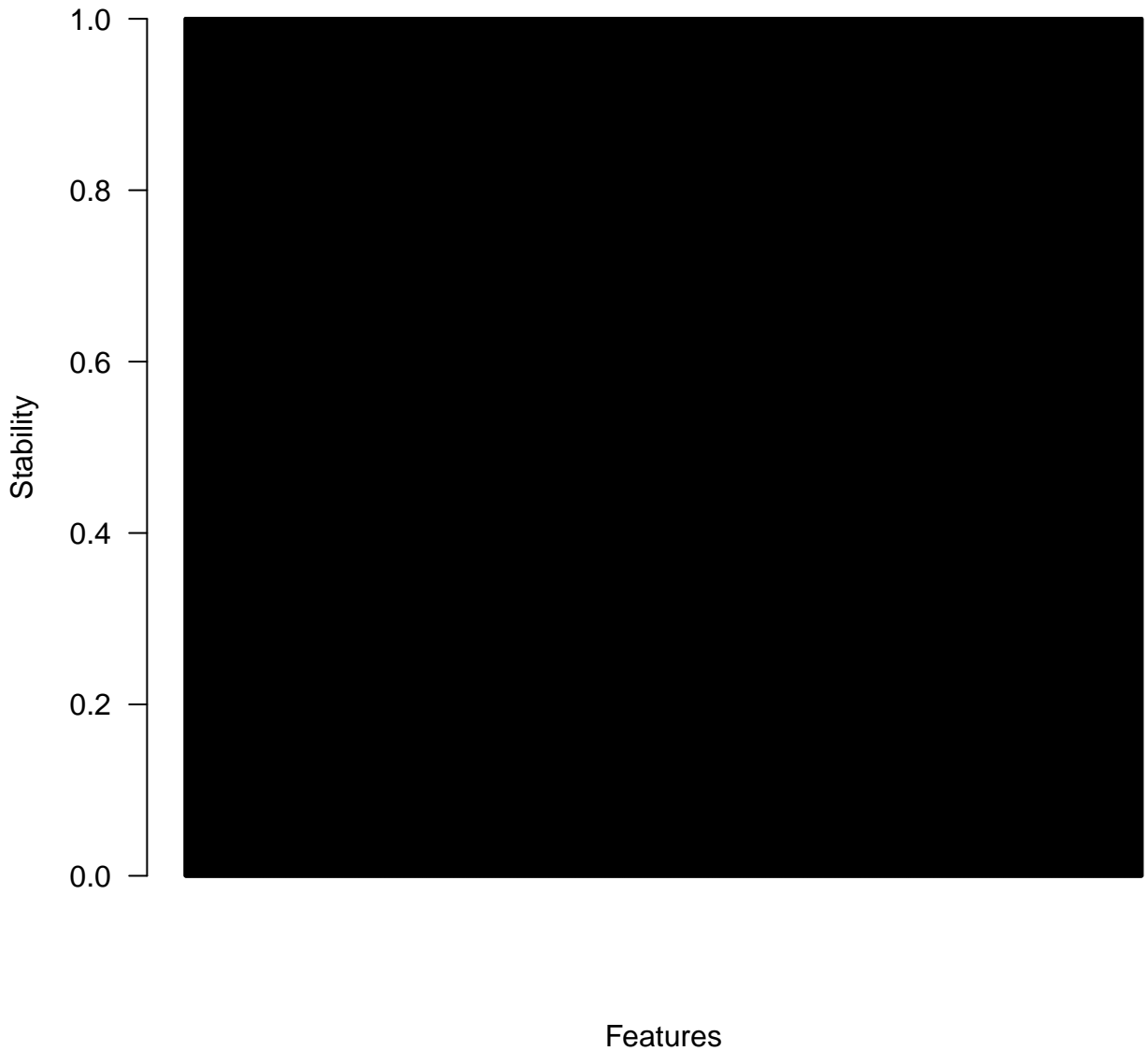
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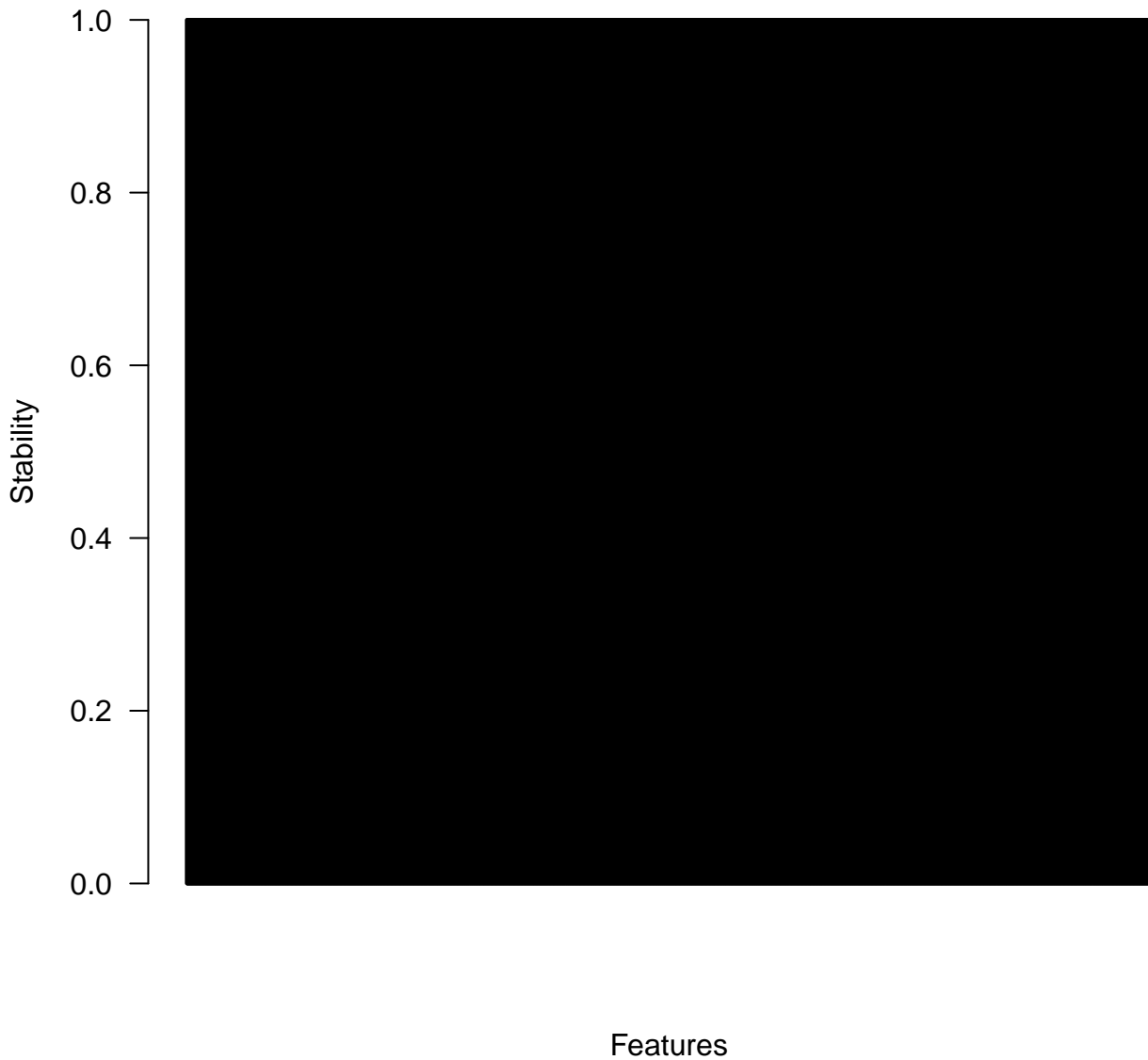
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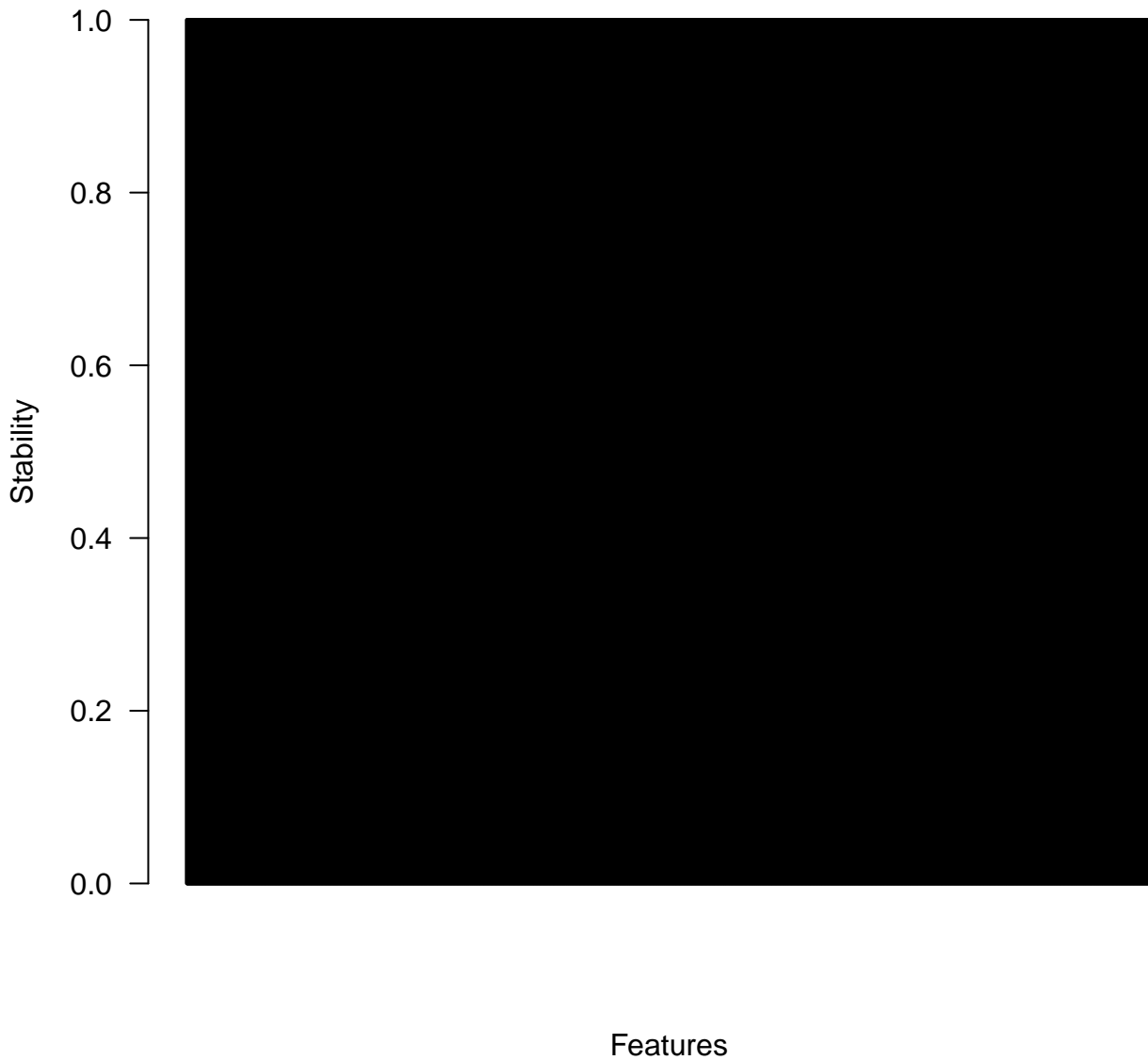
Proteomics Comp 1



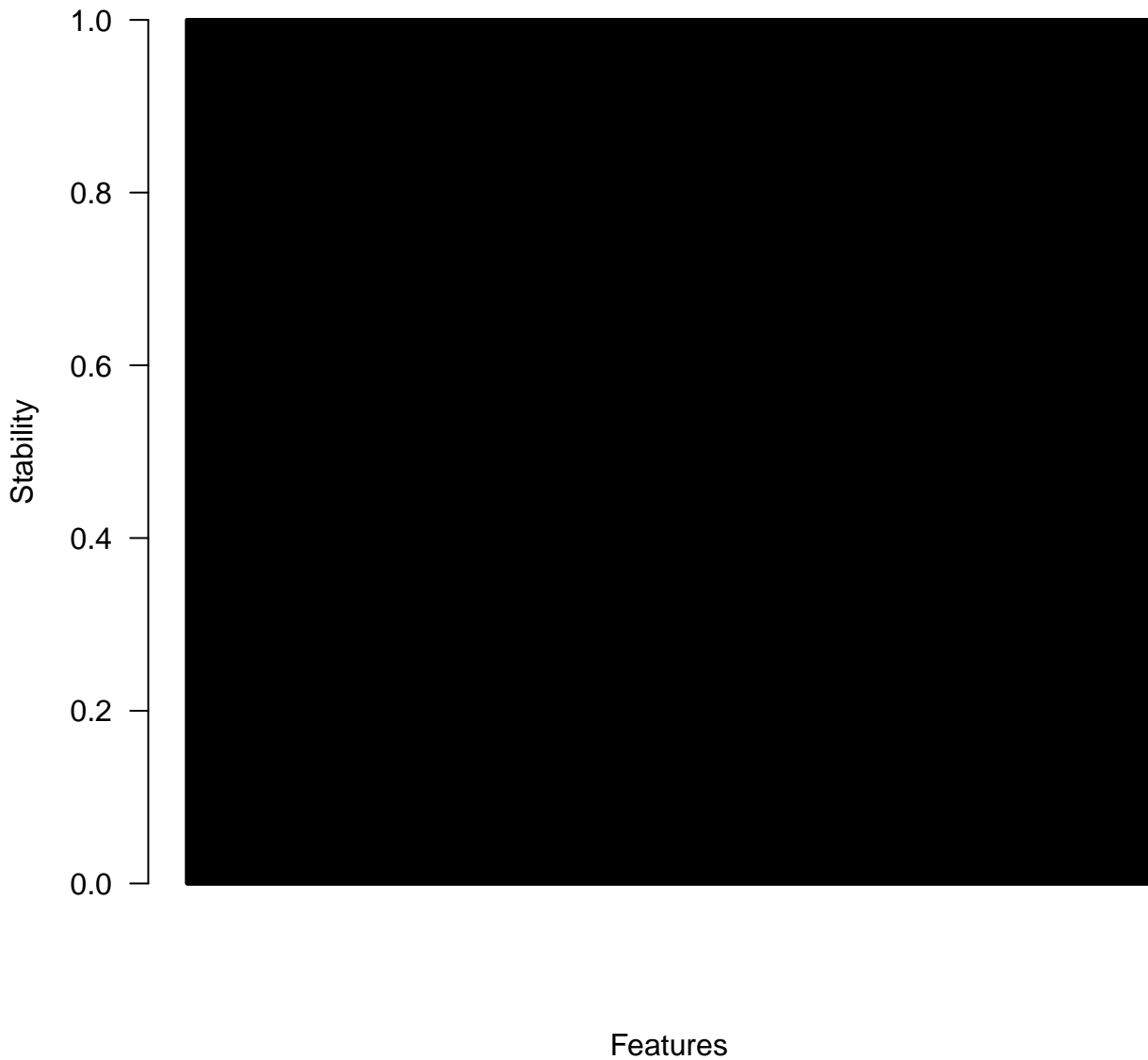
Proteomics Comp 2



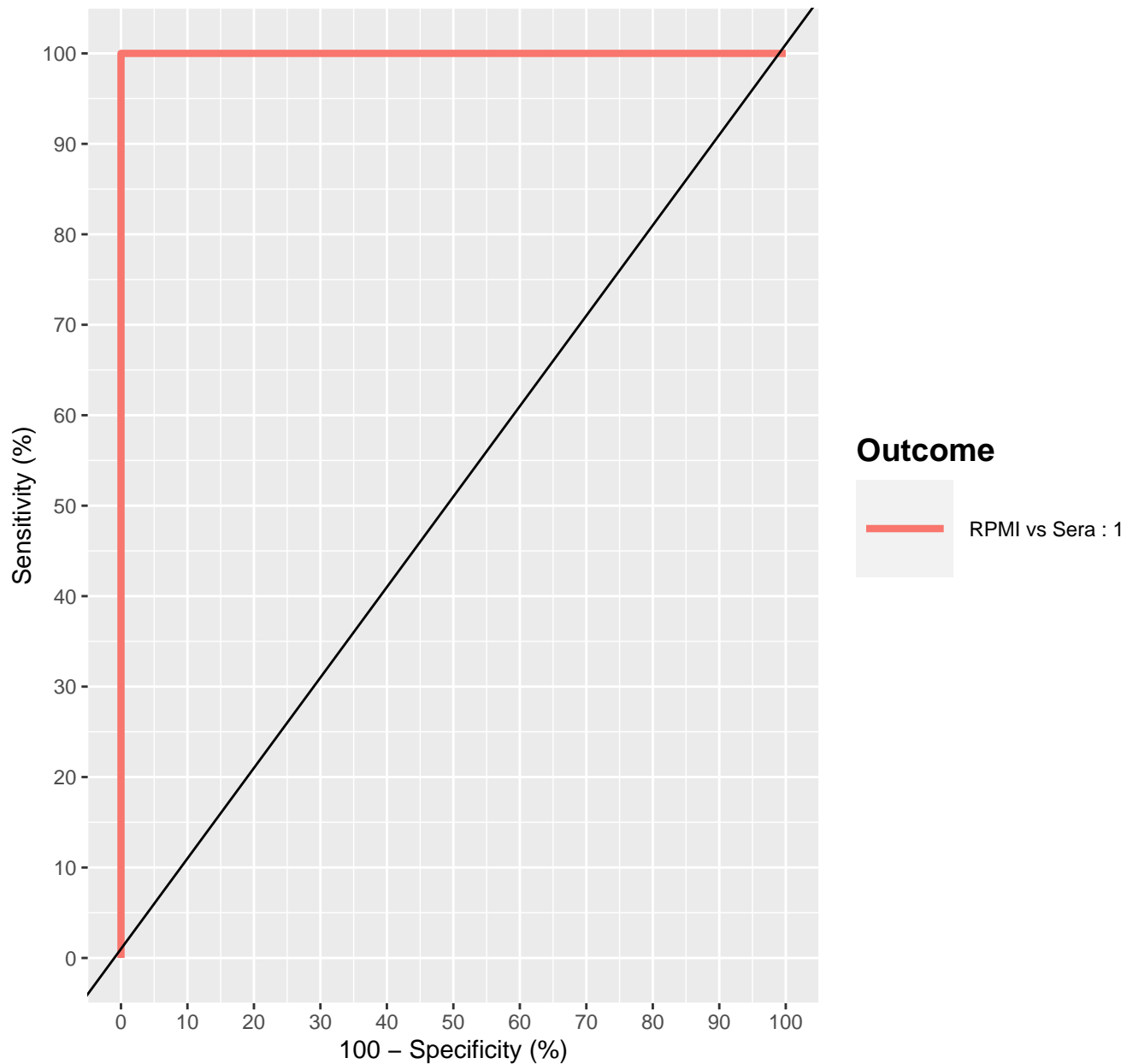
RNA_Seq Comp 1



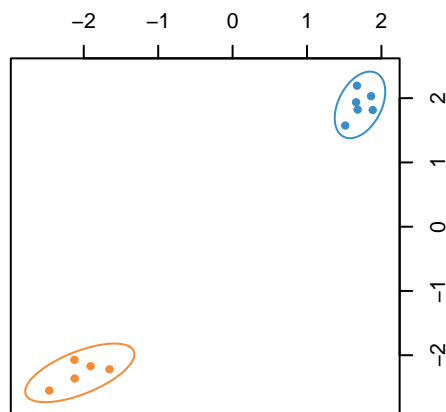
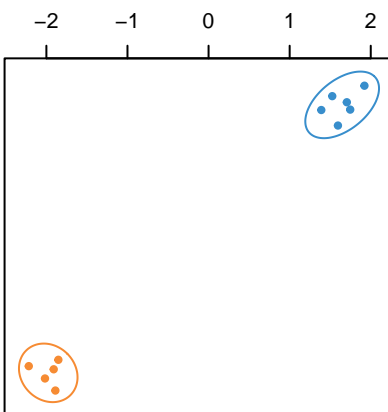
RNA_Seq Comp 2



ROC Curve
Block: Metabolomics, comp: 1

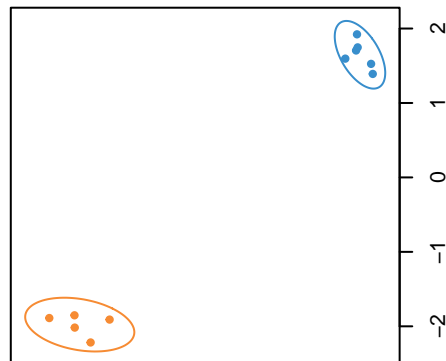


Metabolomics



0.99

Proteomics



1

0.99

RNA_Seq



Comp 1

Correlation cut-off
 $r=0.1$

RNA_Seq

Metabolomics

Proteomics

Expression

- RPMI
- Sera

Correlations

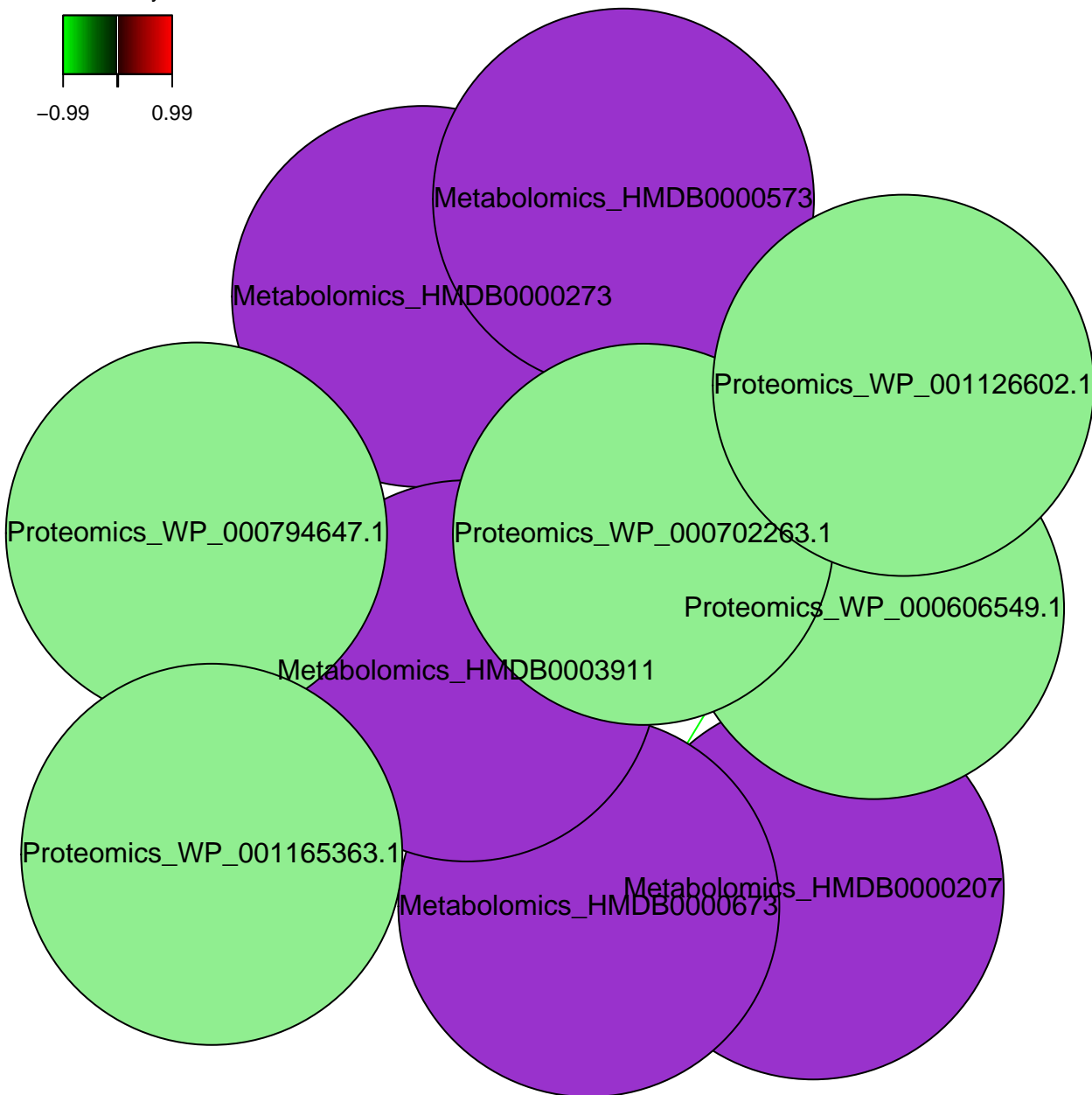
- Positive Correlation
- Negative Correlation

Color key



-0.99

0.99



Color key

-1.3 0 1.3

Rows

● RPMI

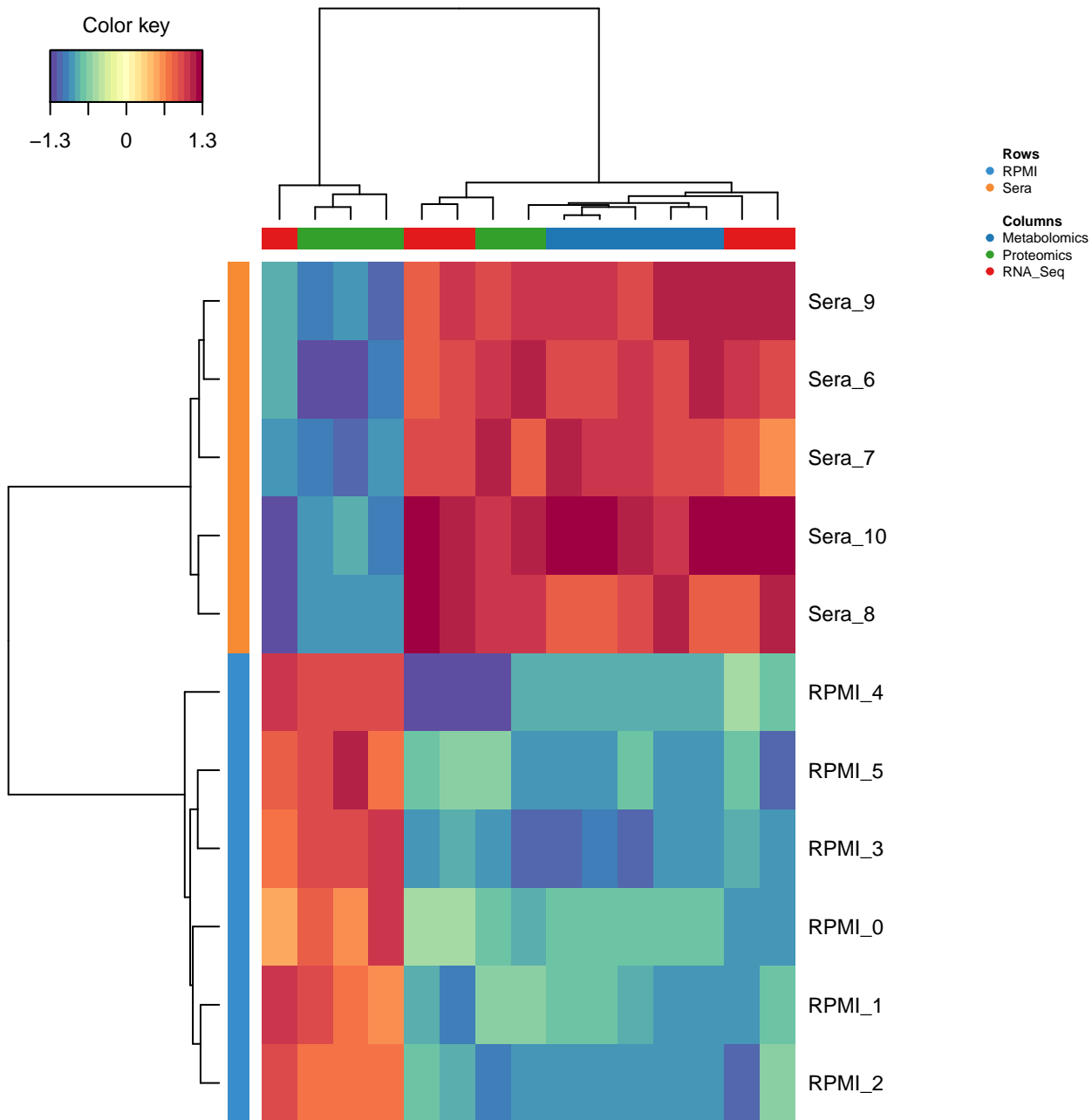
● Sera

Columns

● Metabolomics

● Proteomics

● RNA_Seq



Color key

-1.3 0 1.3

Rows

● RPMI

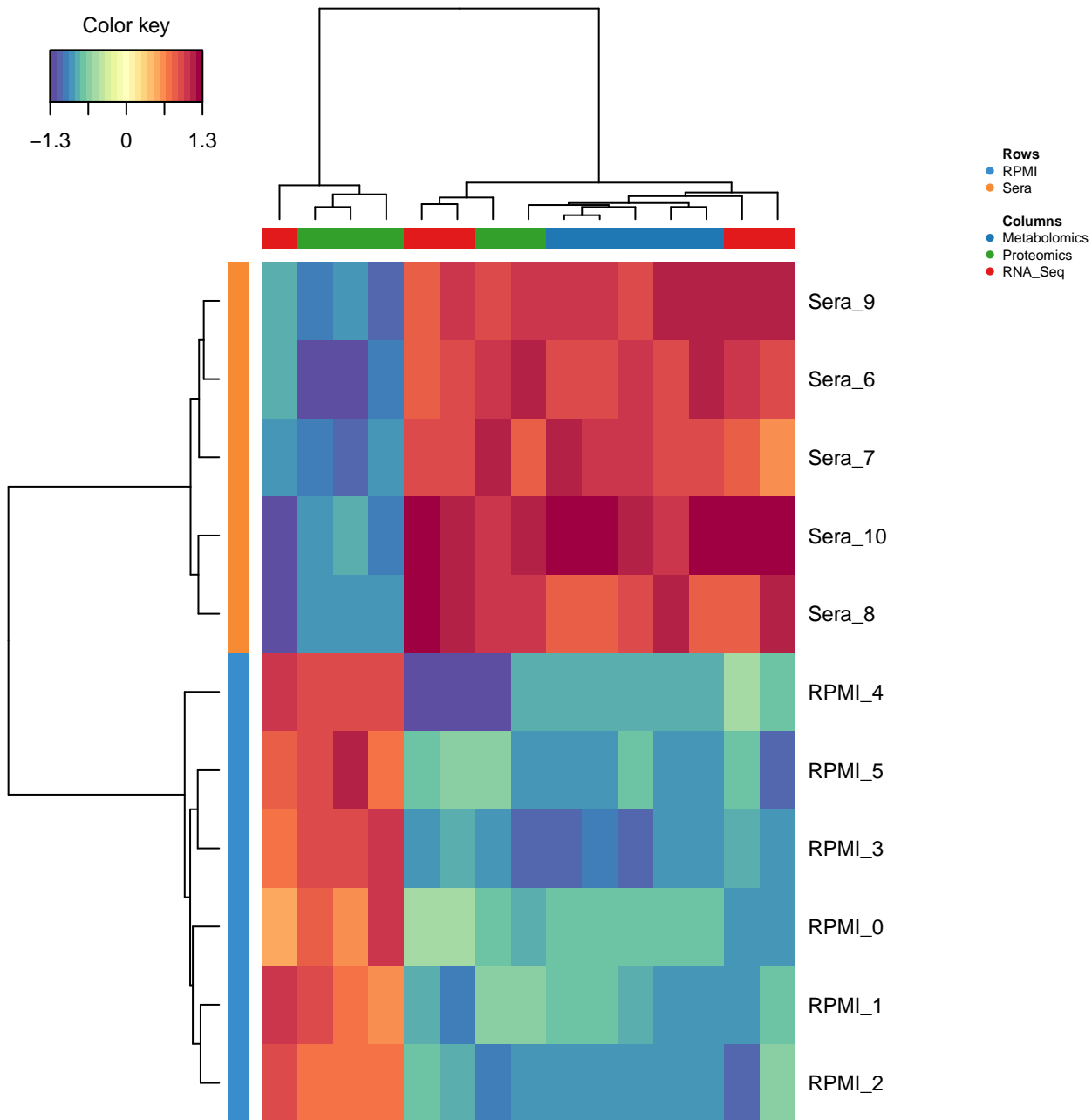
● Sera

Columns

● Metabolomics

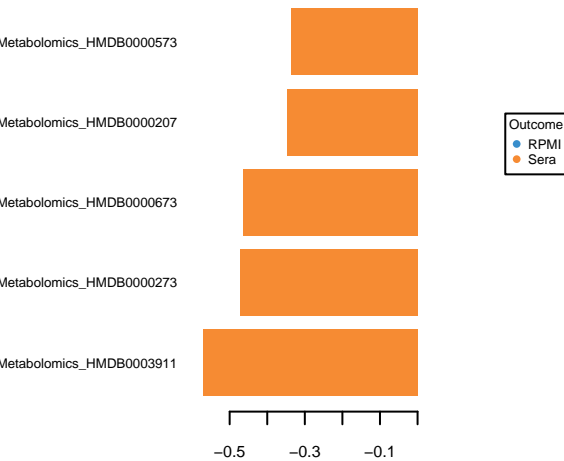
● Proteomics

● RNA_Seq

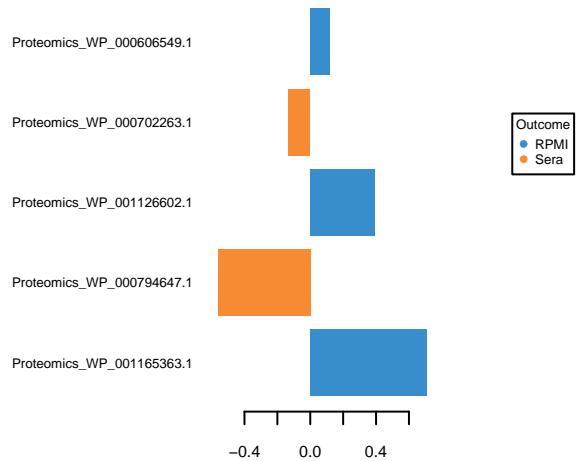


1 DIABLO max loadings

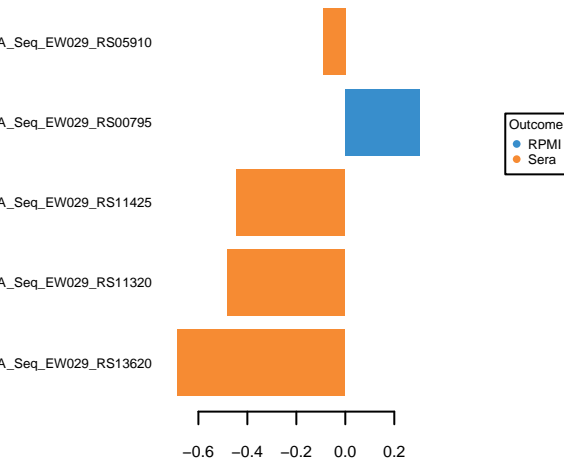
Contribution on comp 1
Block 'Metabolomics'



Contribution on comp 1
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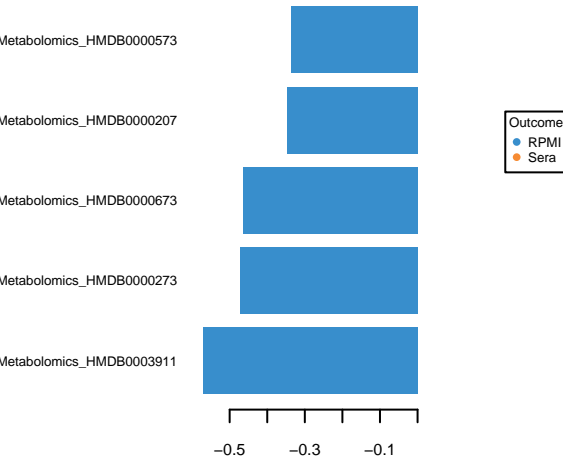


Contribution on comp 1
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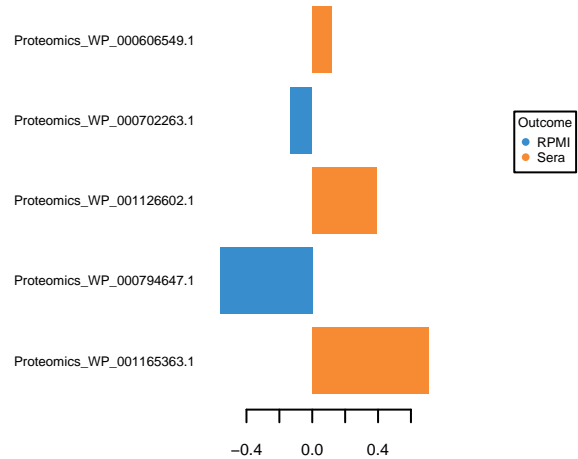


1 DIABLO min loadings

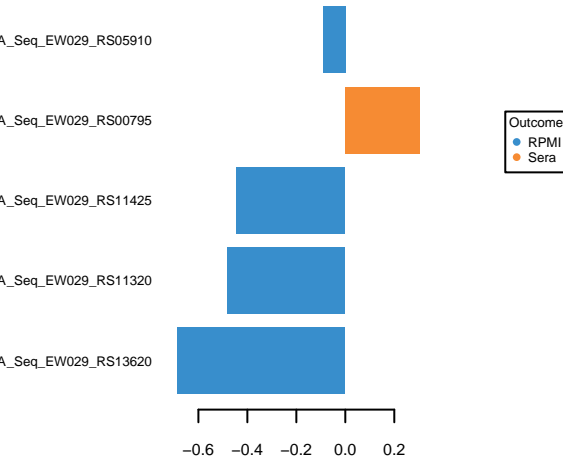
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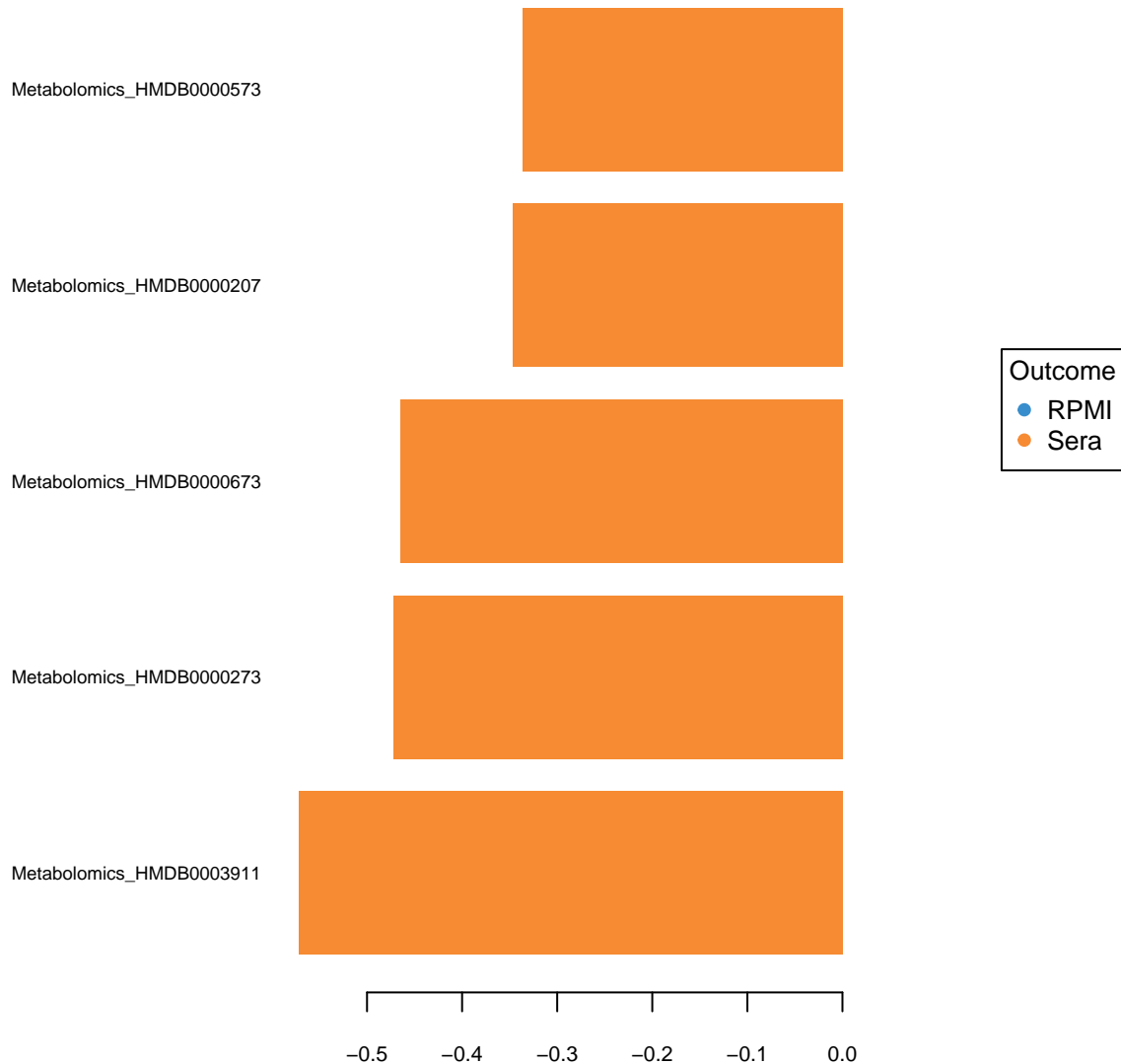
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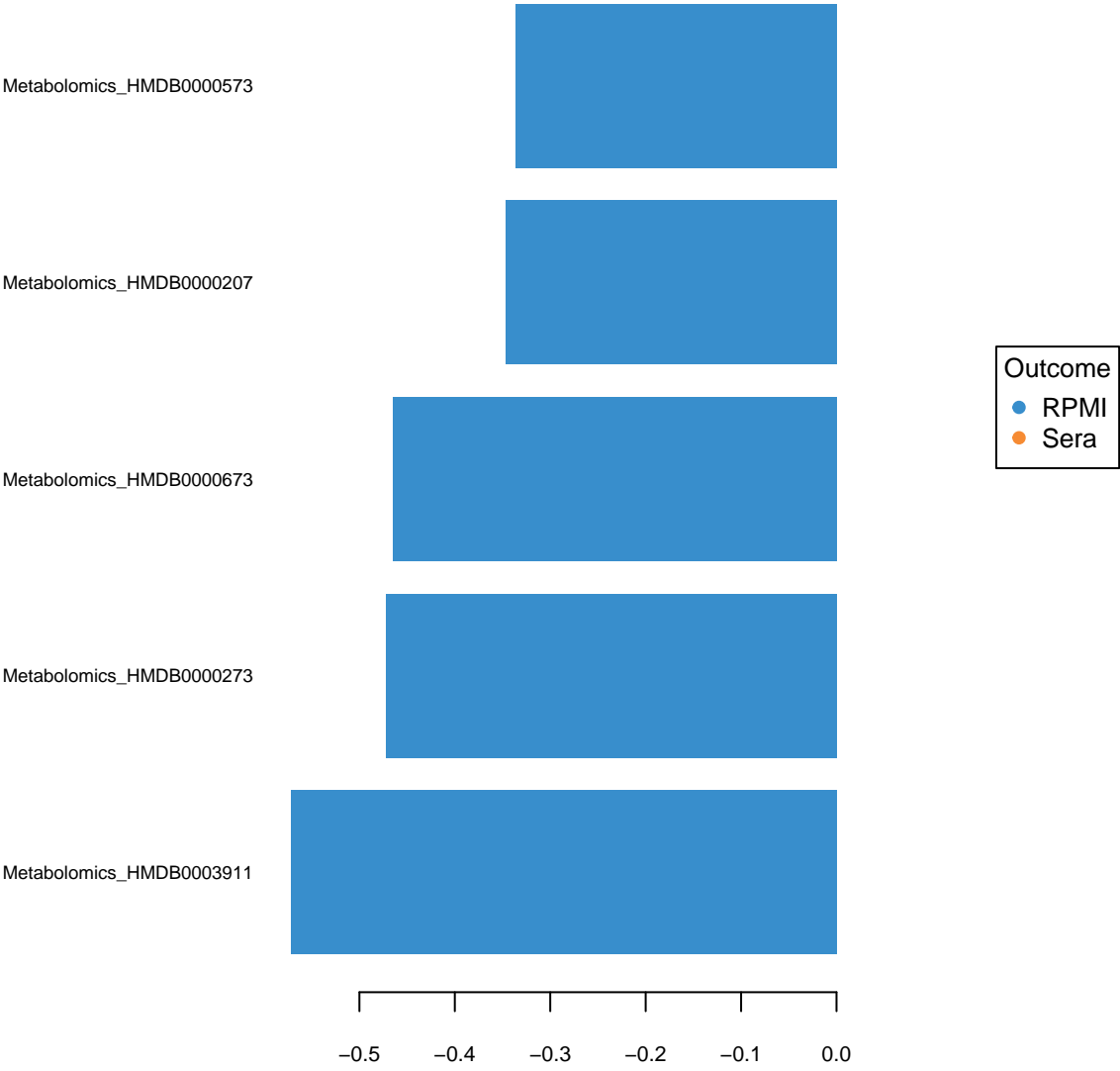
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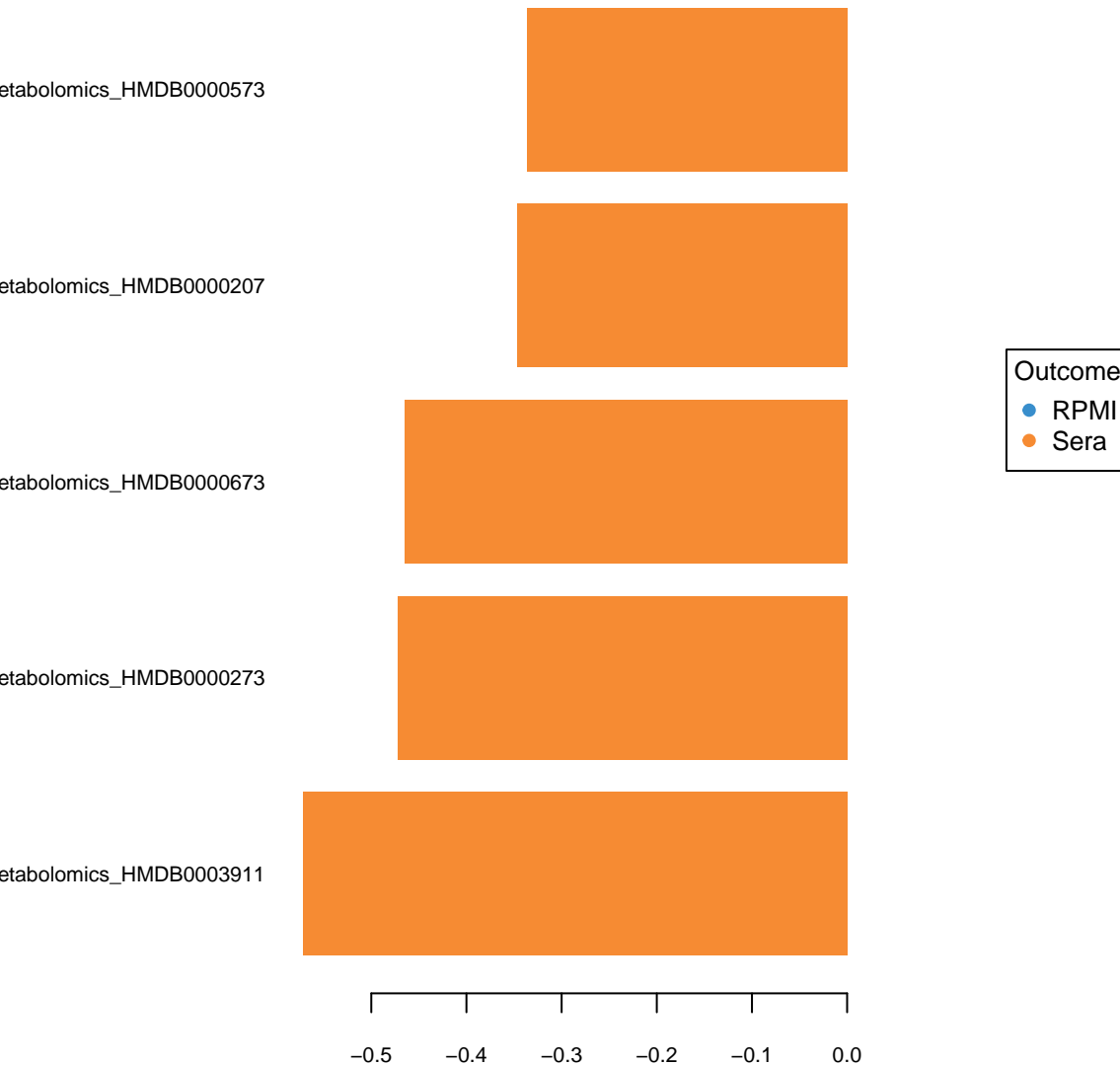
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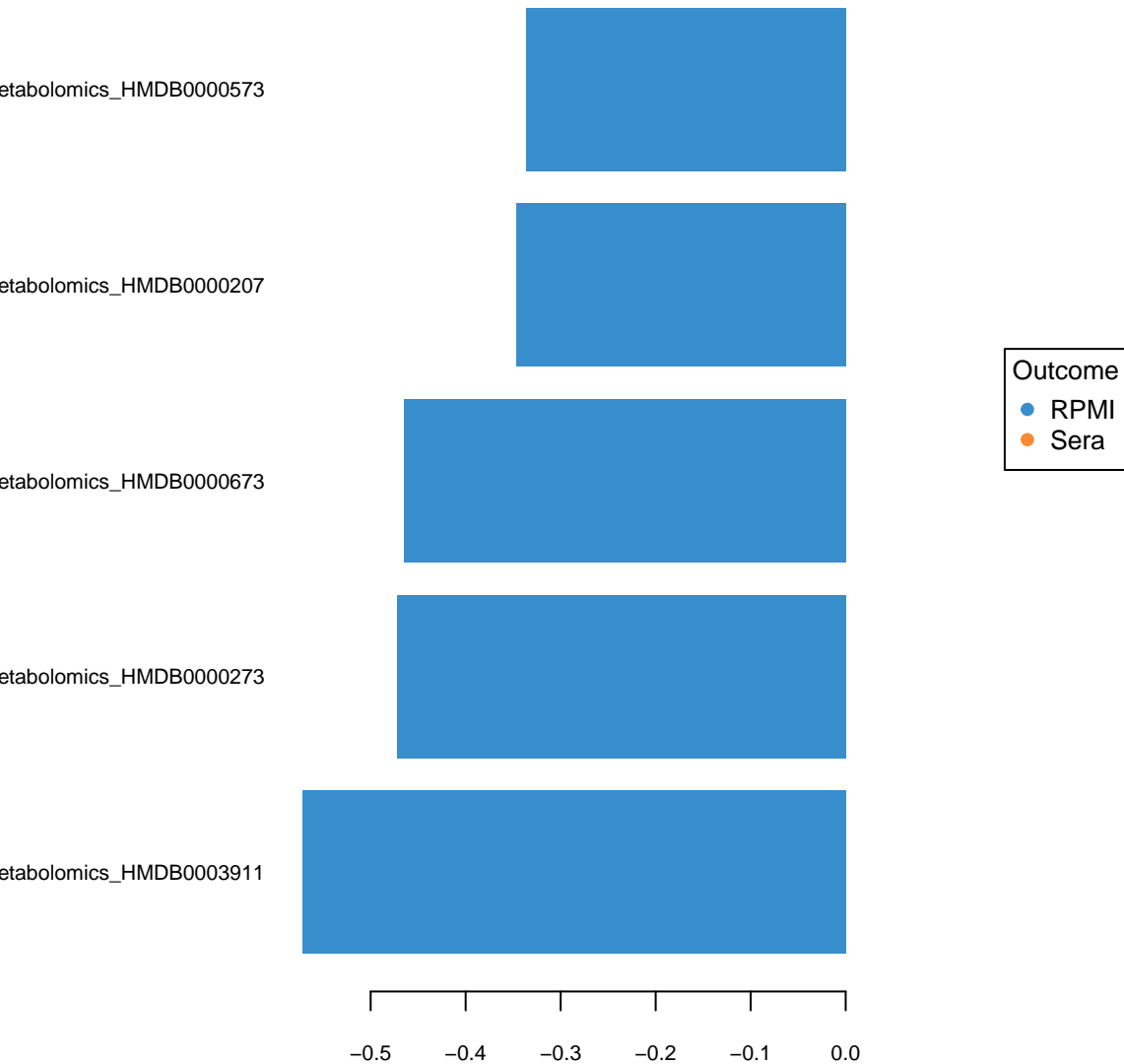
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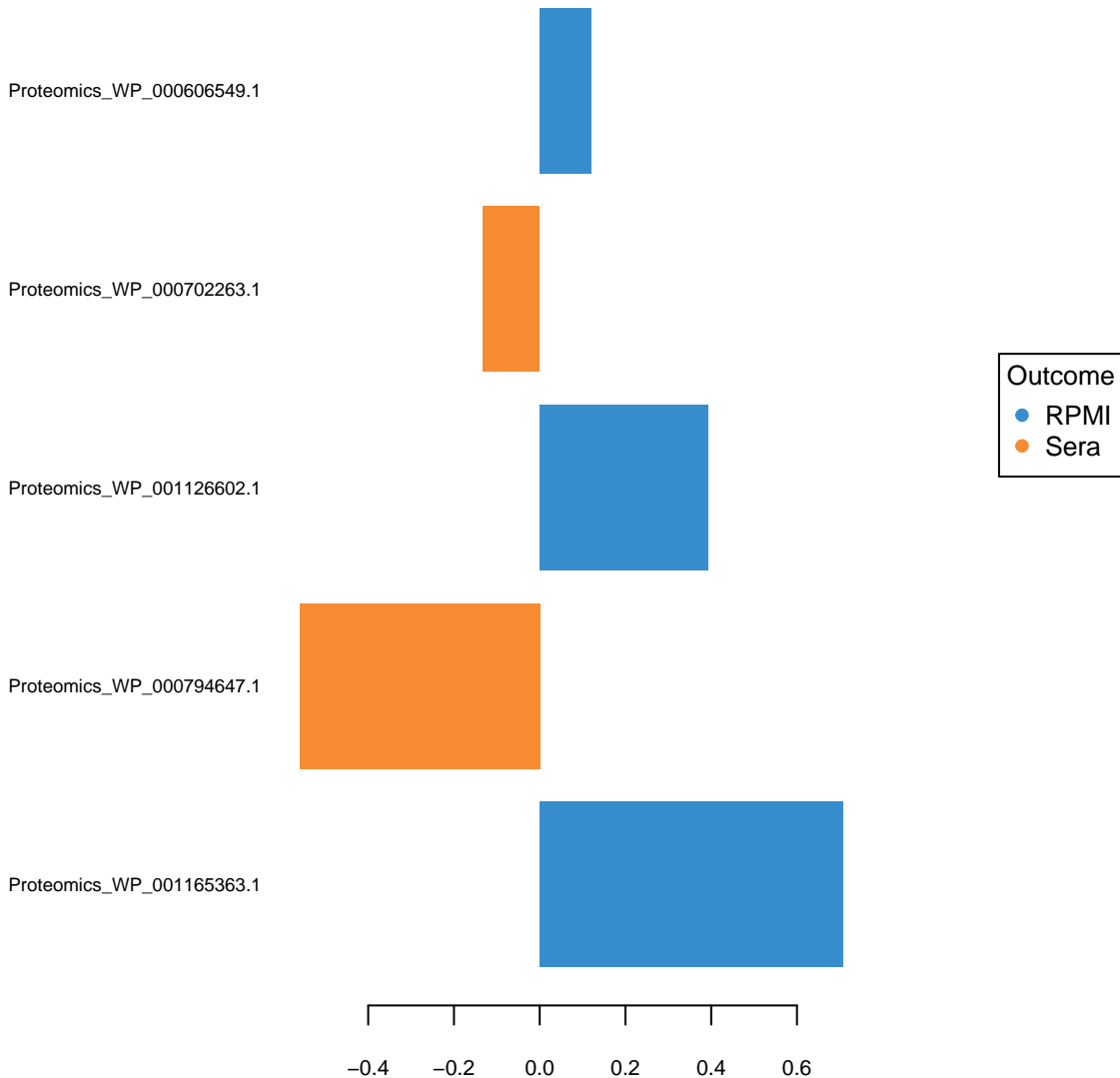
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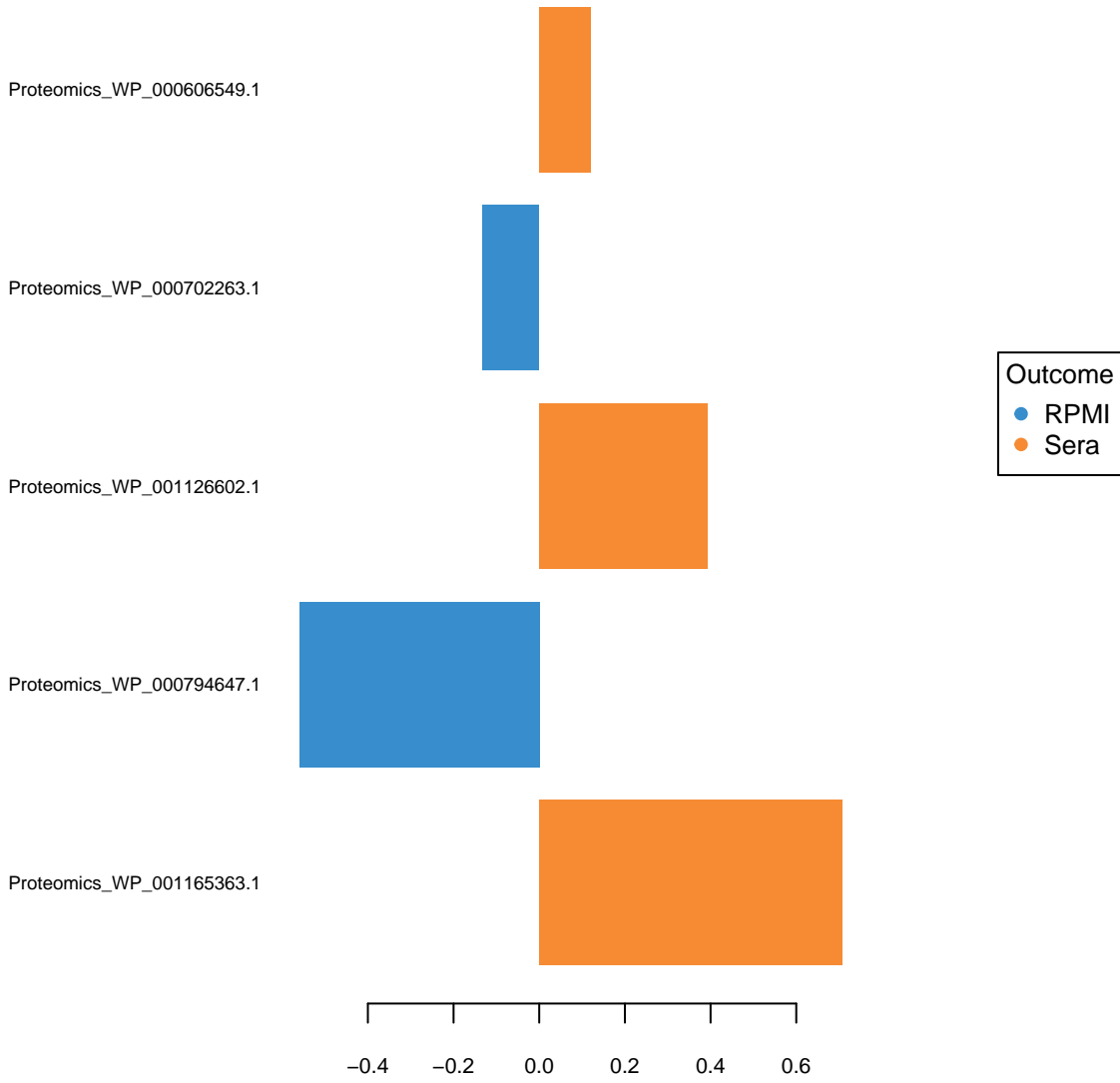
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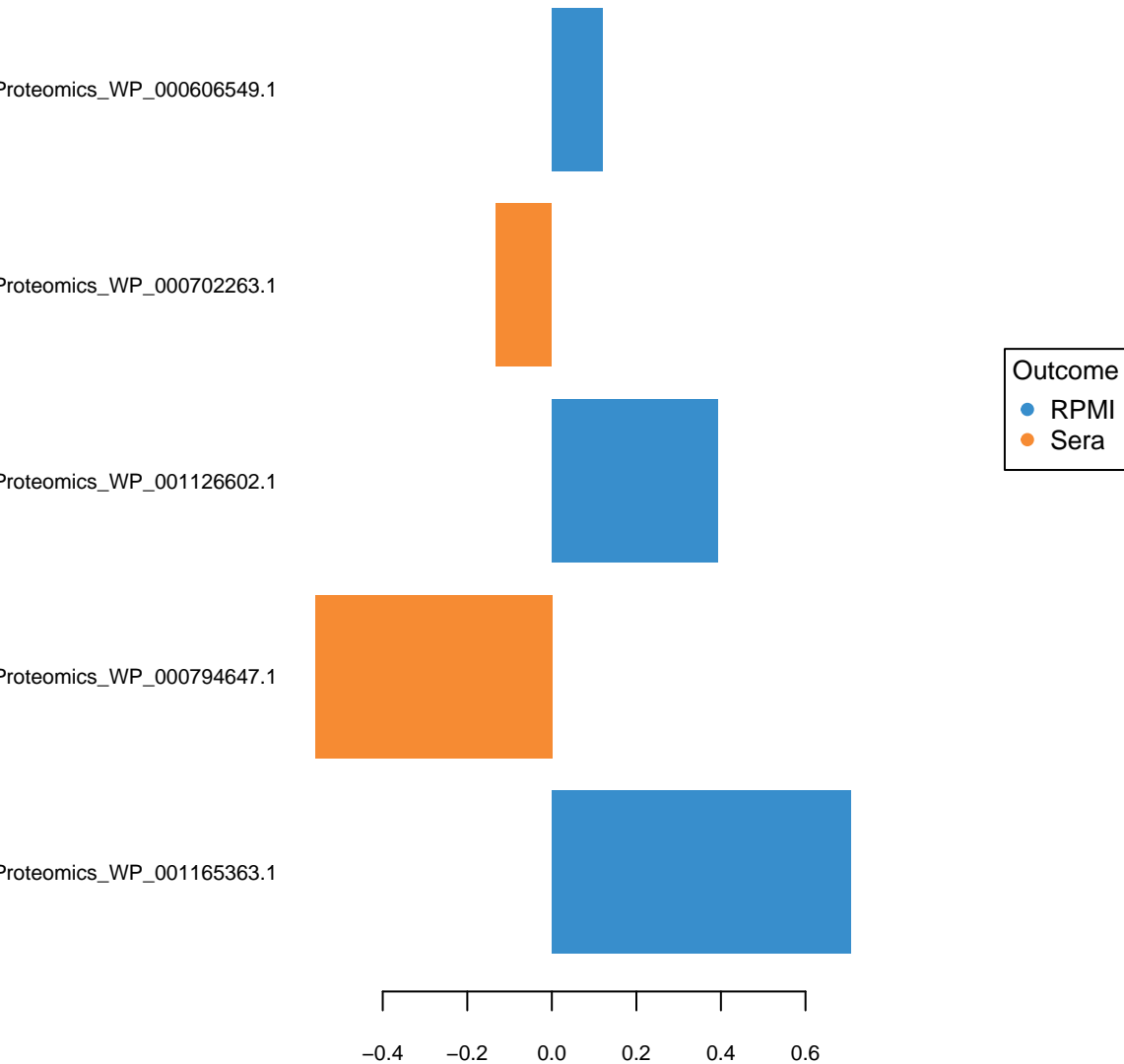
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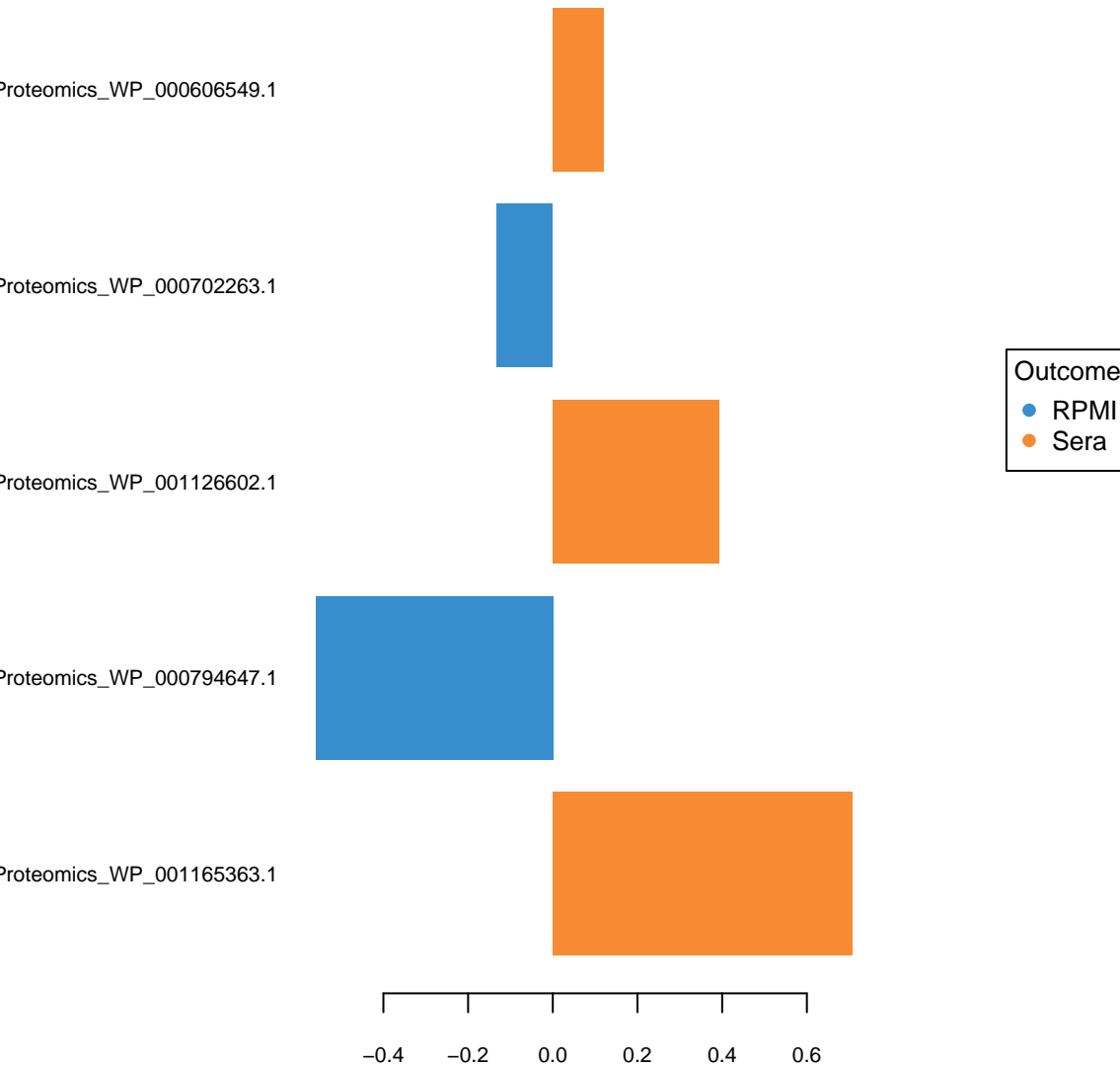
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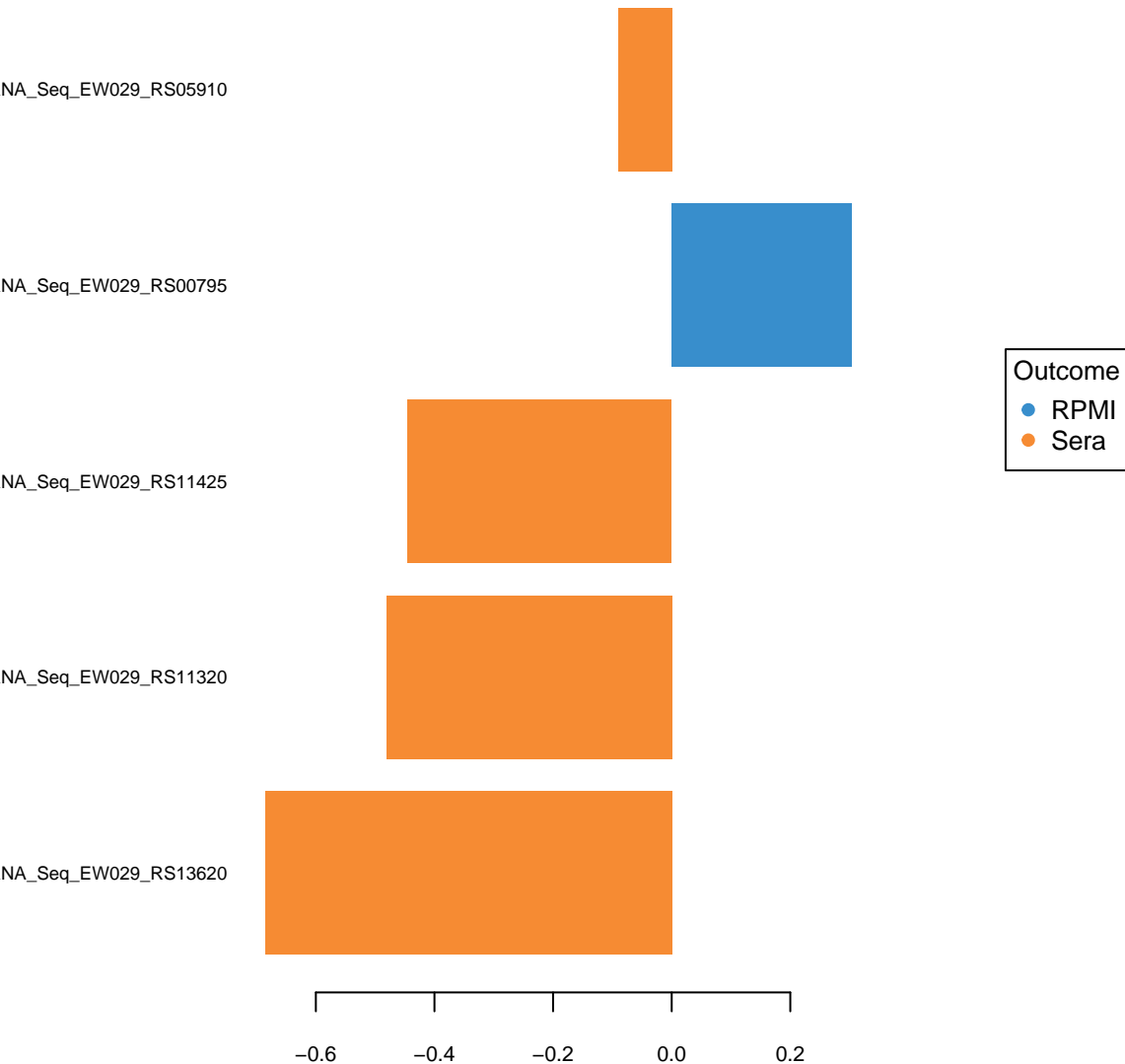
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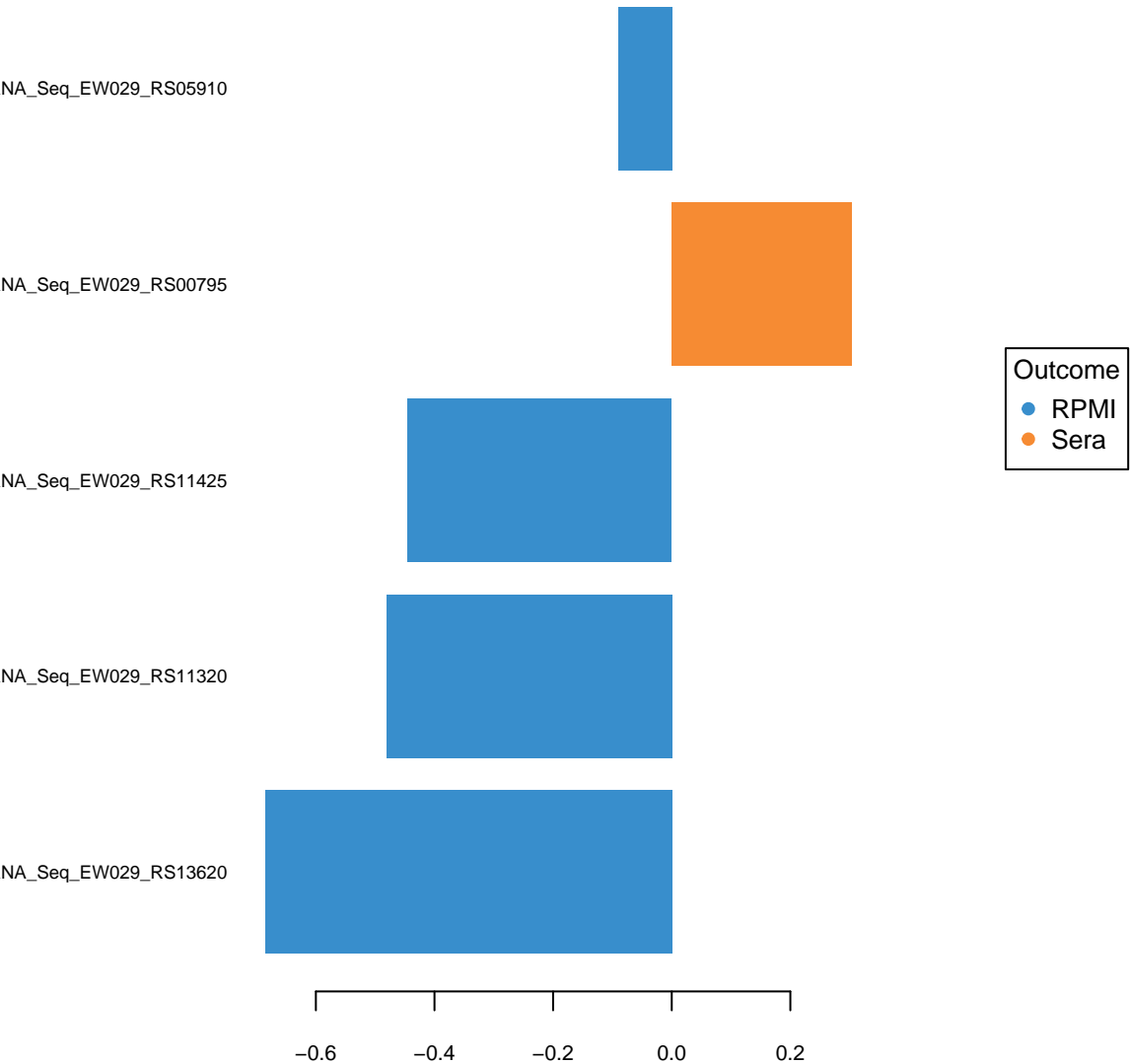
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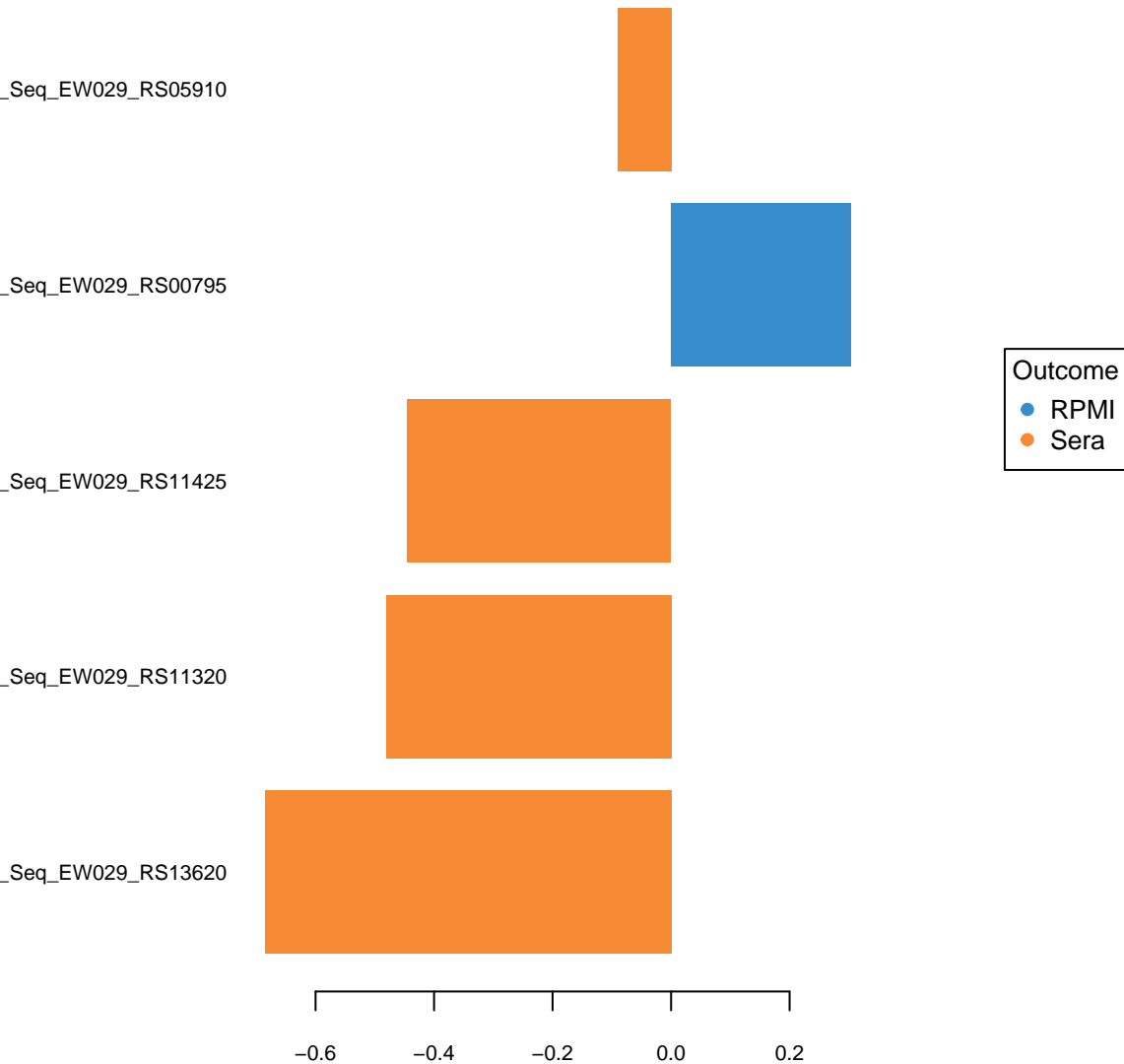
1 RNA_Seq DIABLO max load1



1 RNA_Seq DIABLO min load



Contribution on comp 1



Contribution on comp 1

