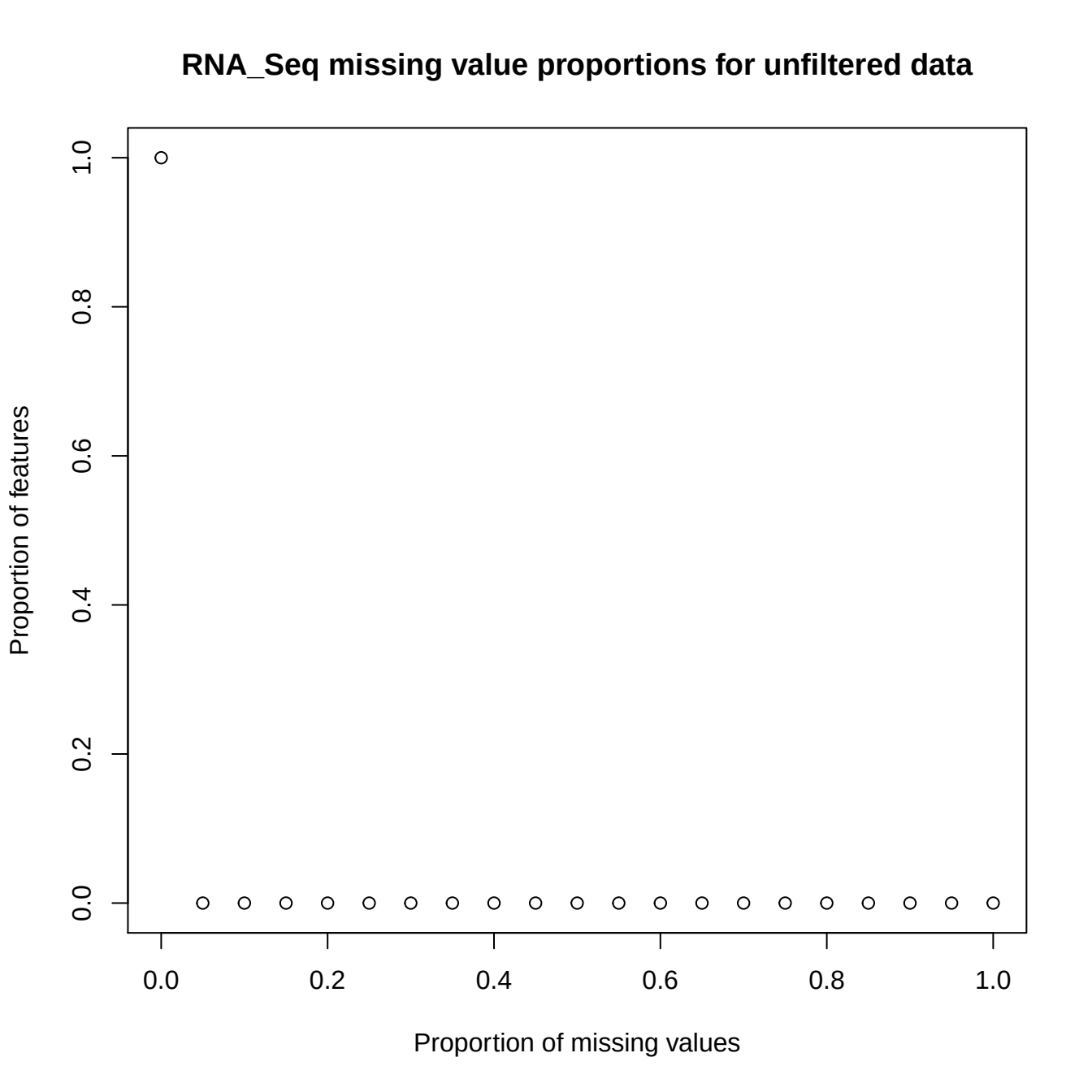
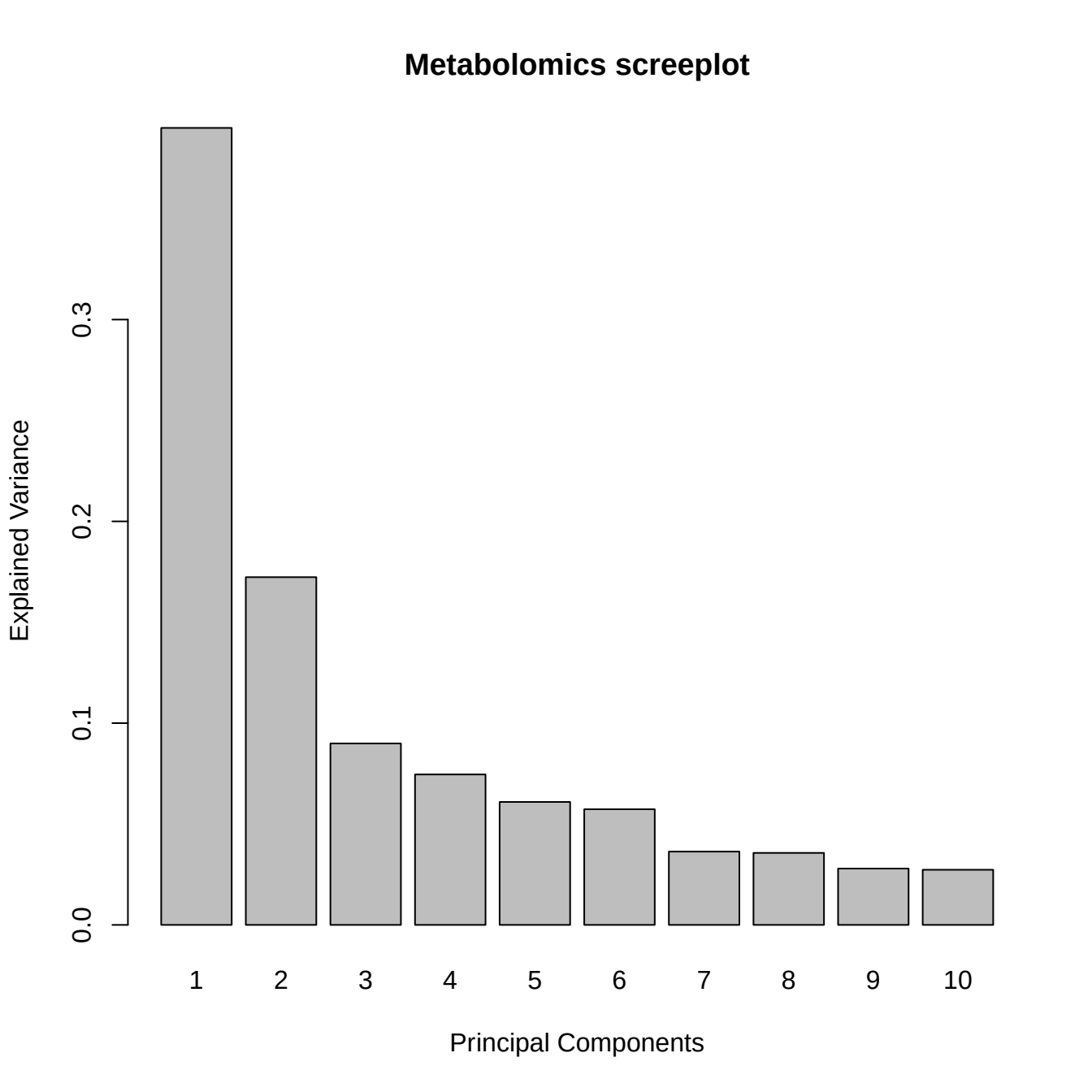
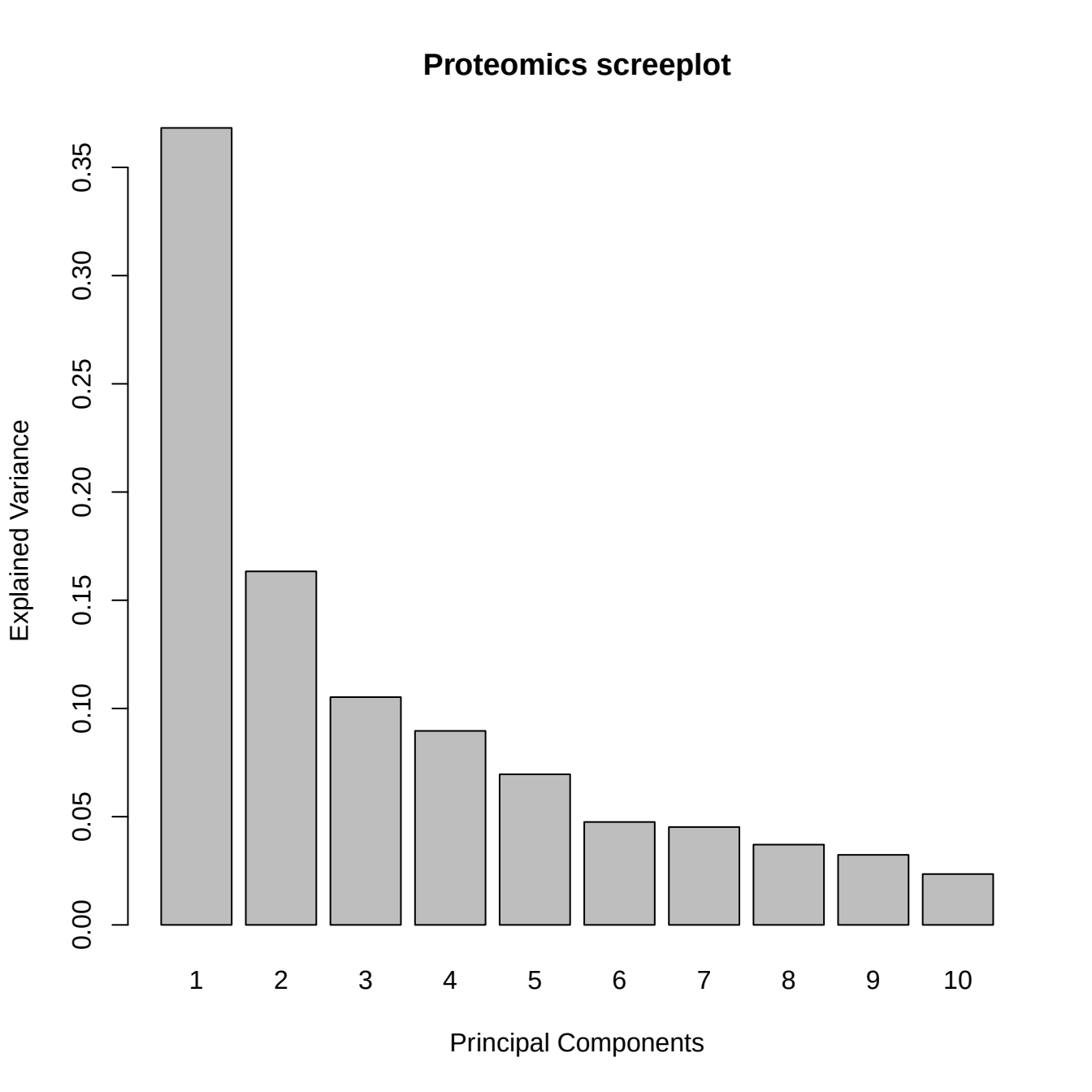
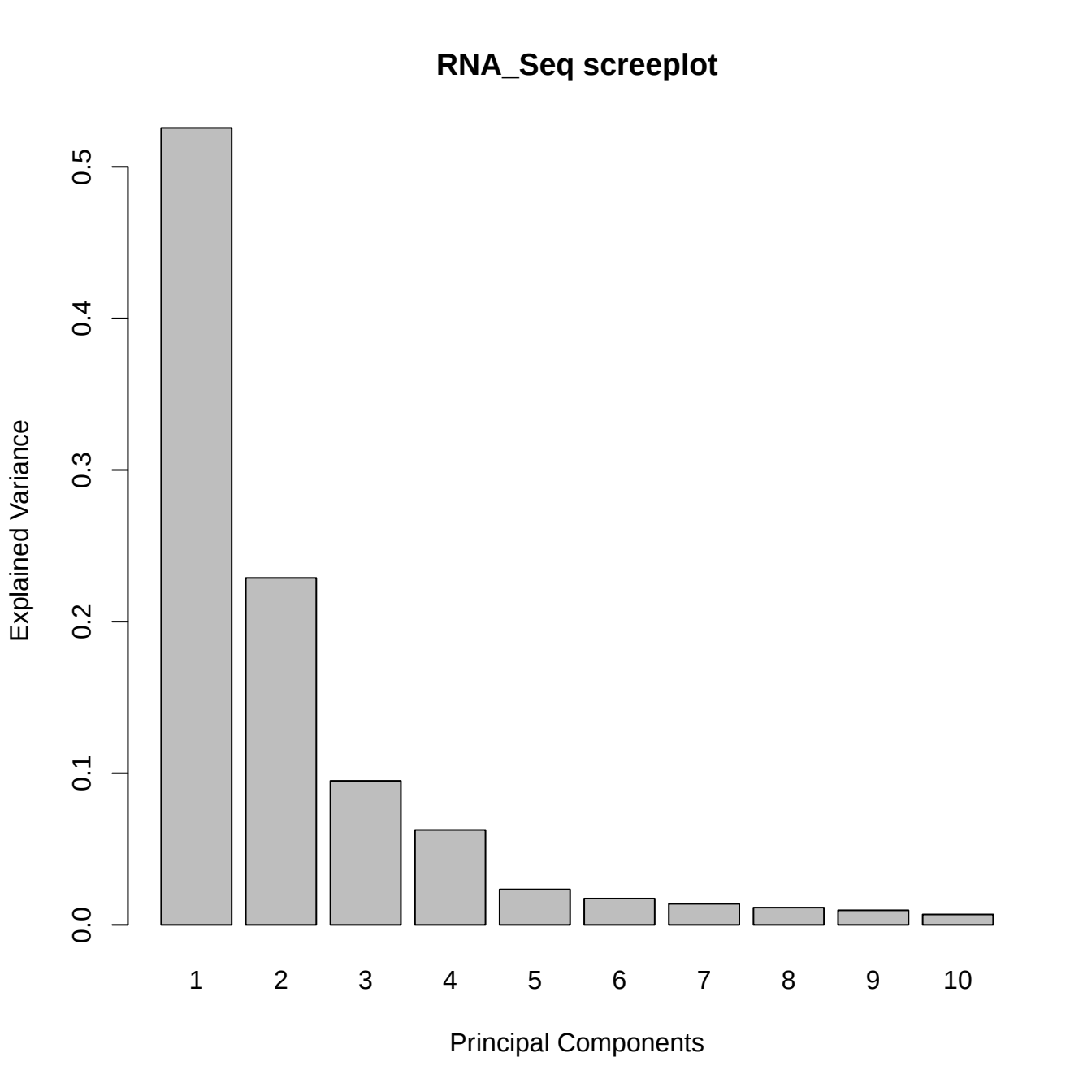
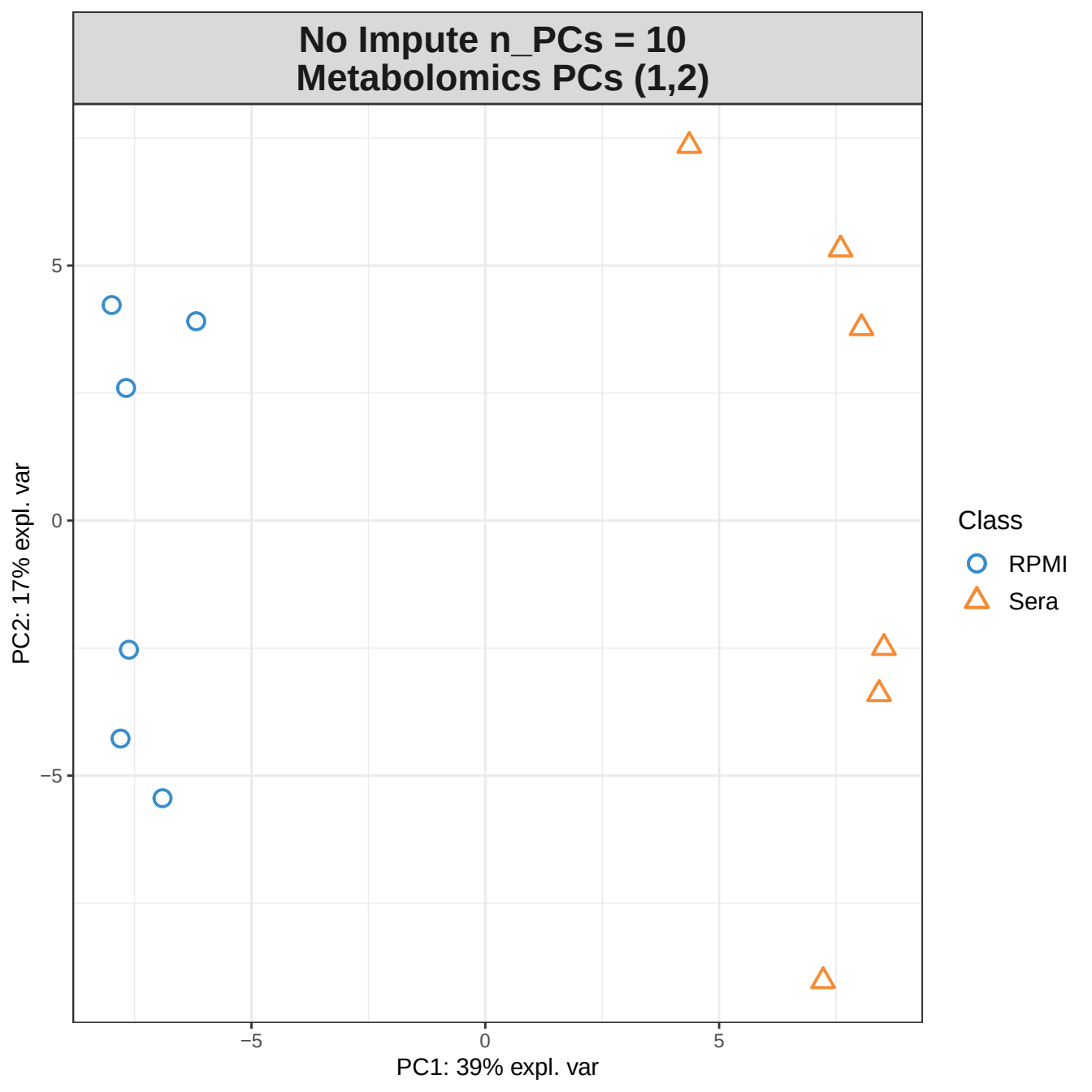
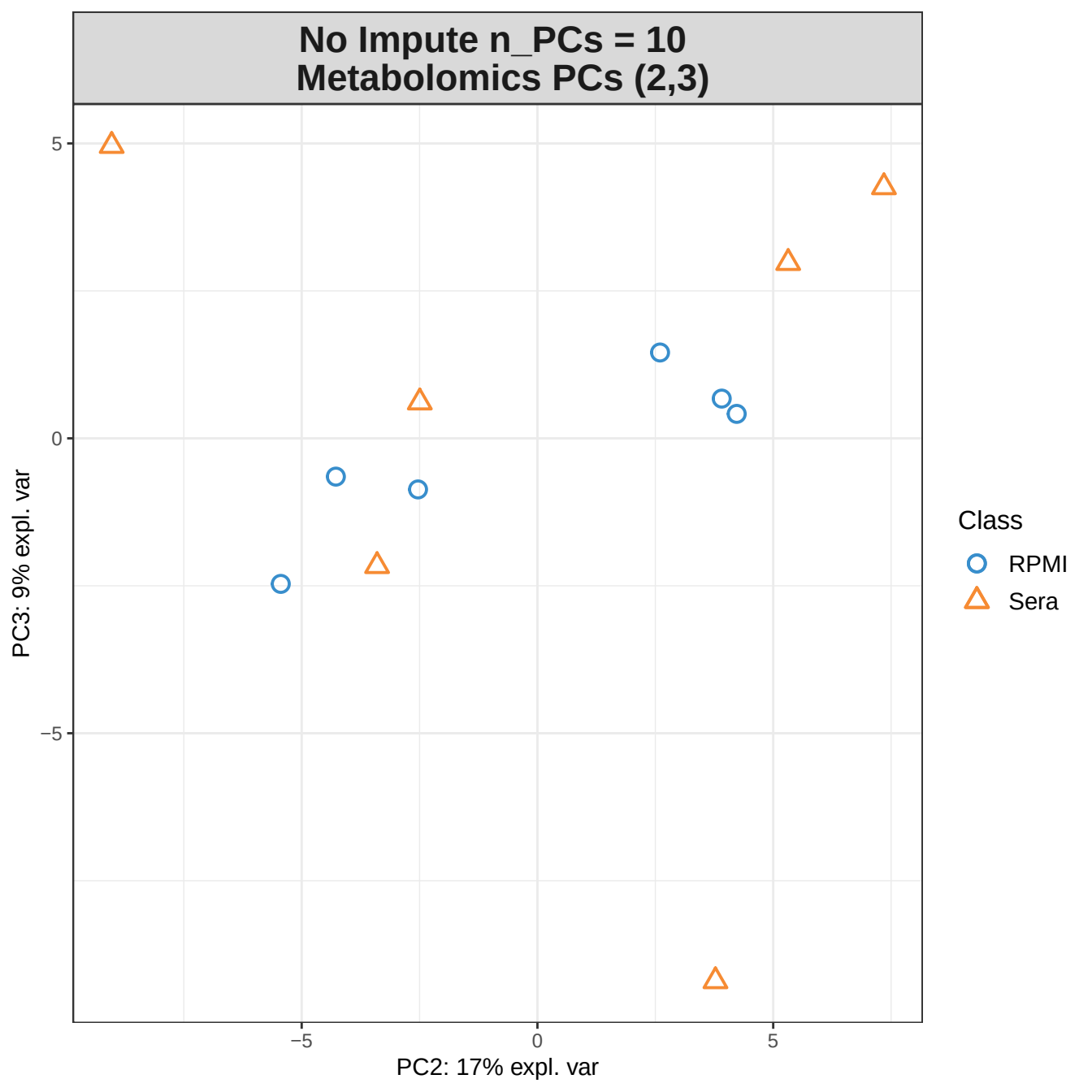

RNA_Seq missing value proportions for unfiltered data
Proportion of features
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.2
0.4
0.6
0.8
1.0
Proportion of missing values

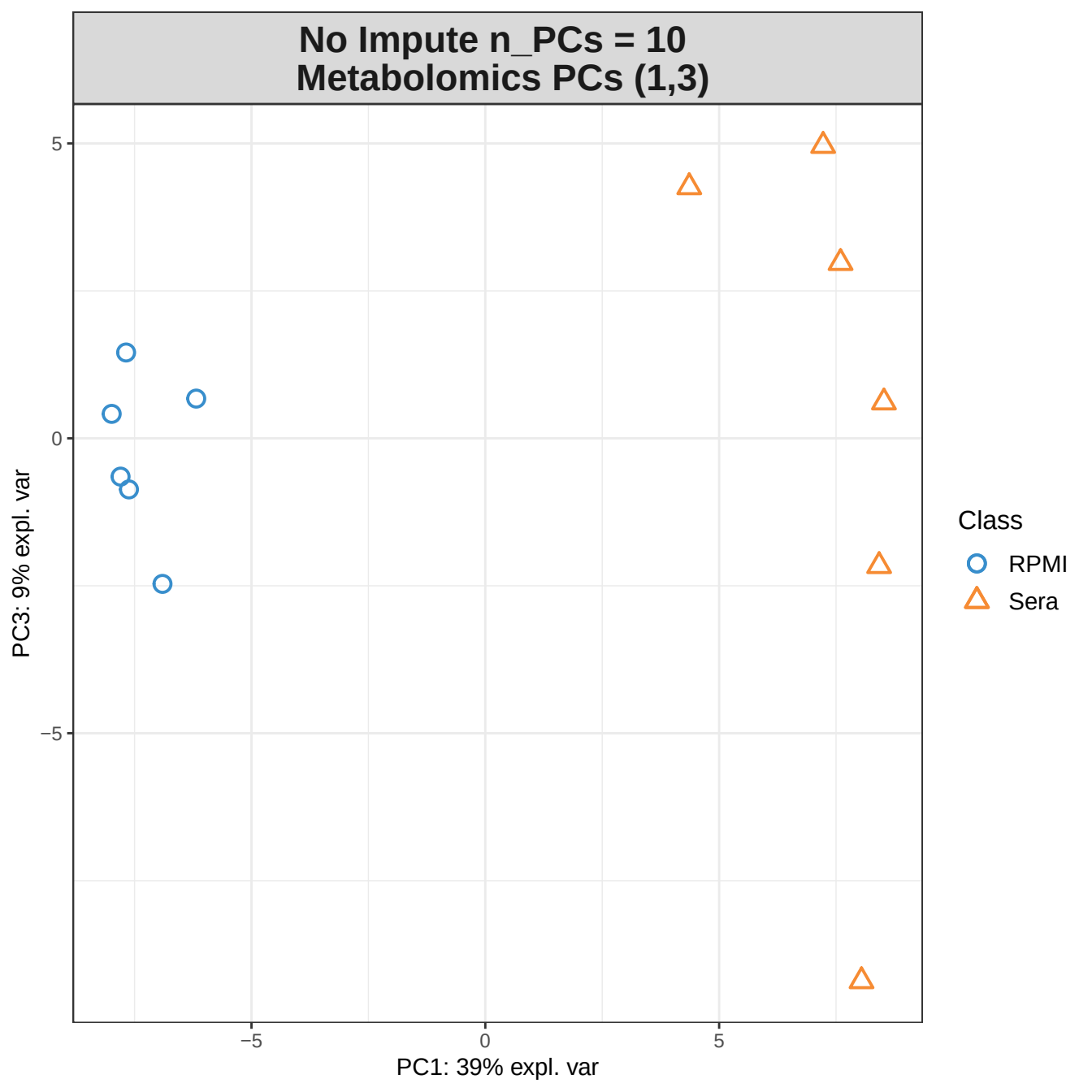

Metabolomics screeplot
Explained Variance
0.0
0.1
0.2
0.3
1
2
3
4
5
6
7
8
9
10
Principal Components

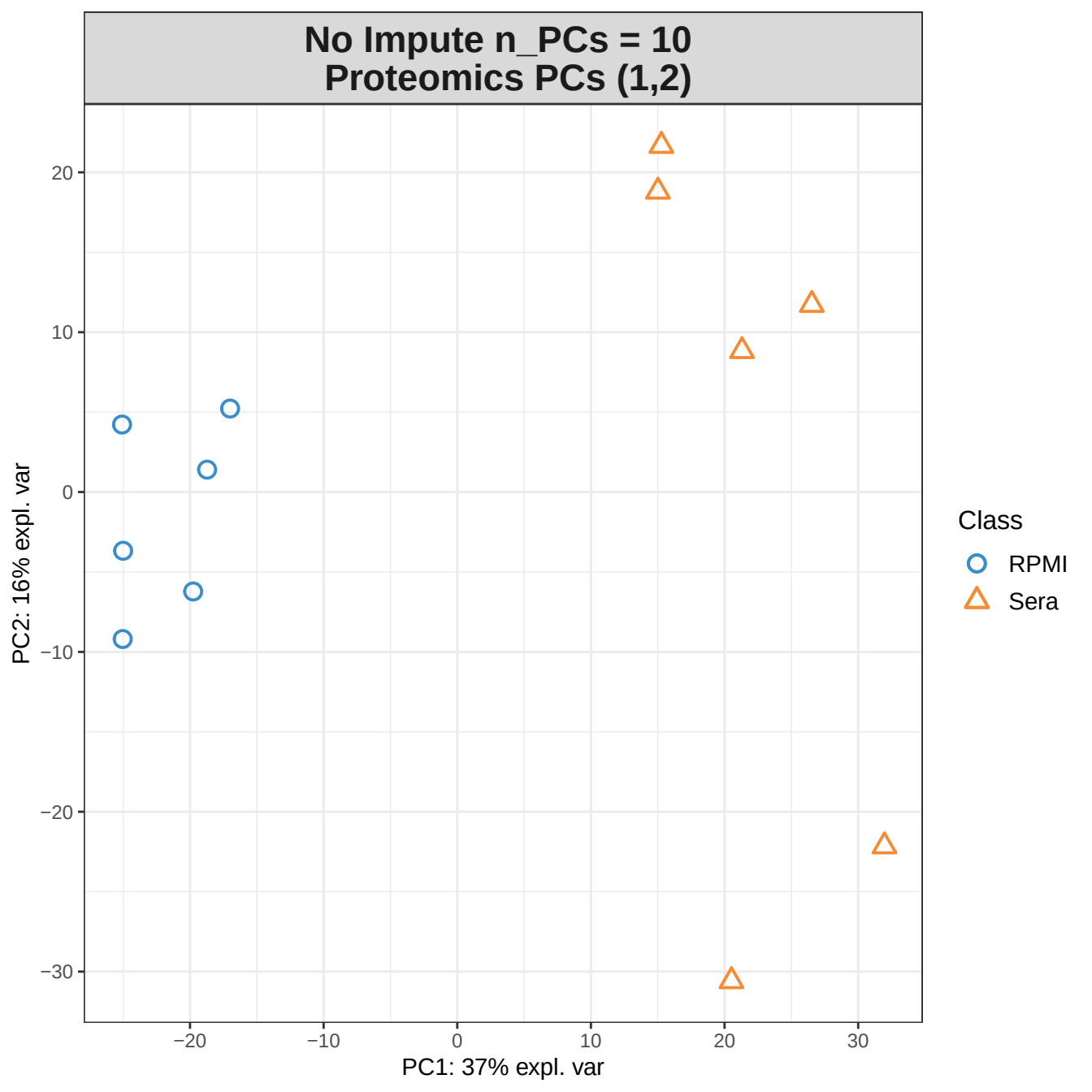

Proteomics screeplot
Explained Variance
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
1
2
3
4
5
6
7
8
9
10
Principal Components

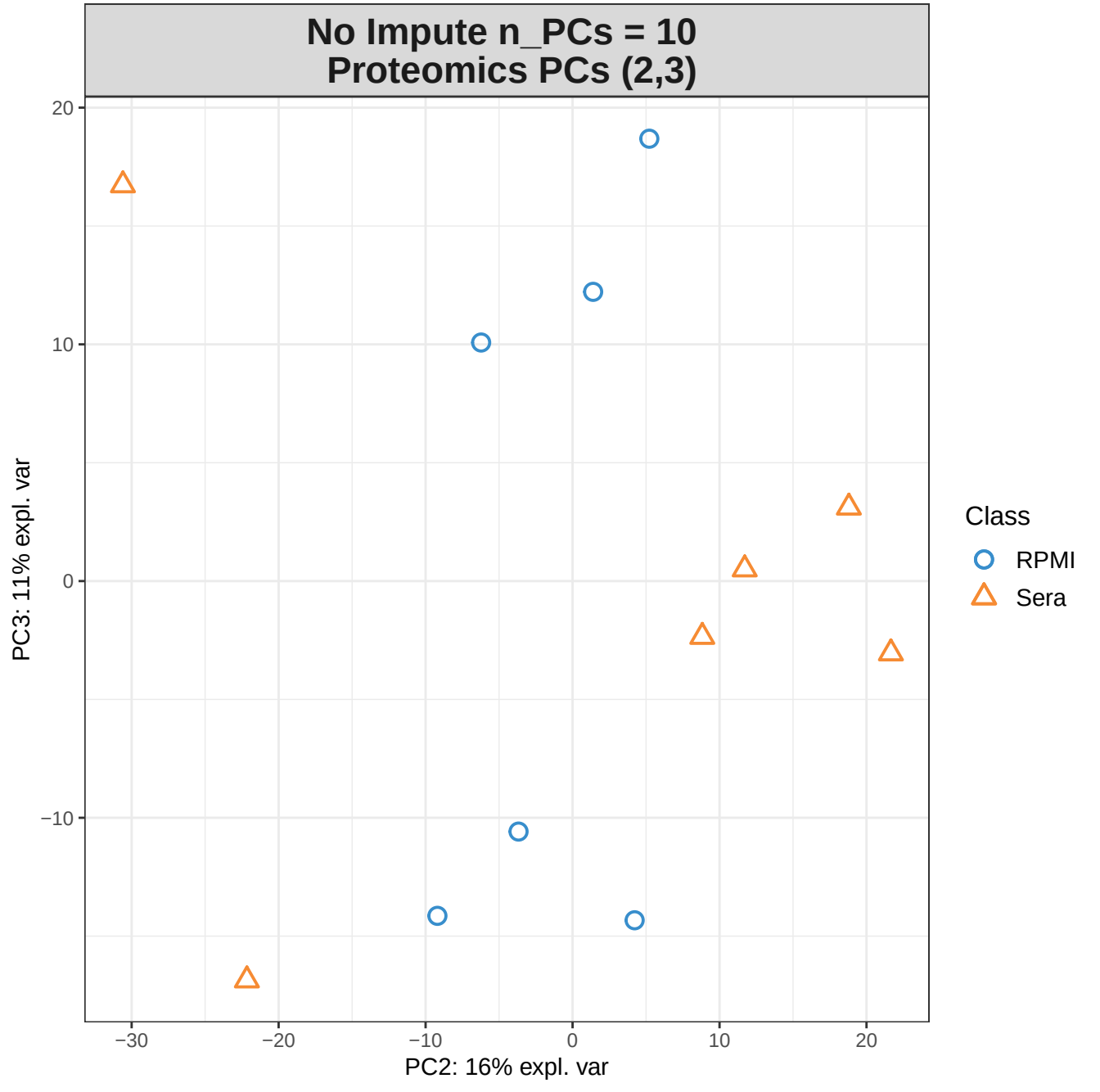

RNA_Seq screeplot
Explained Variance
0.0
0.1
0.2
0.3
0.4
0.5
1
2
3
4
5
6
7
8
9
10
Principal Components

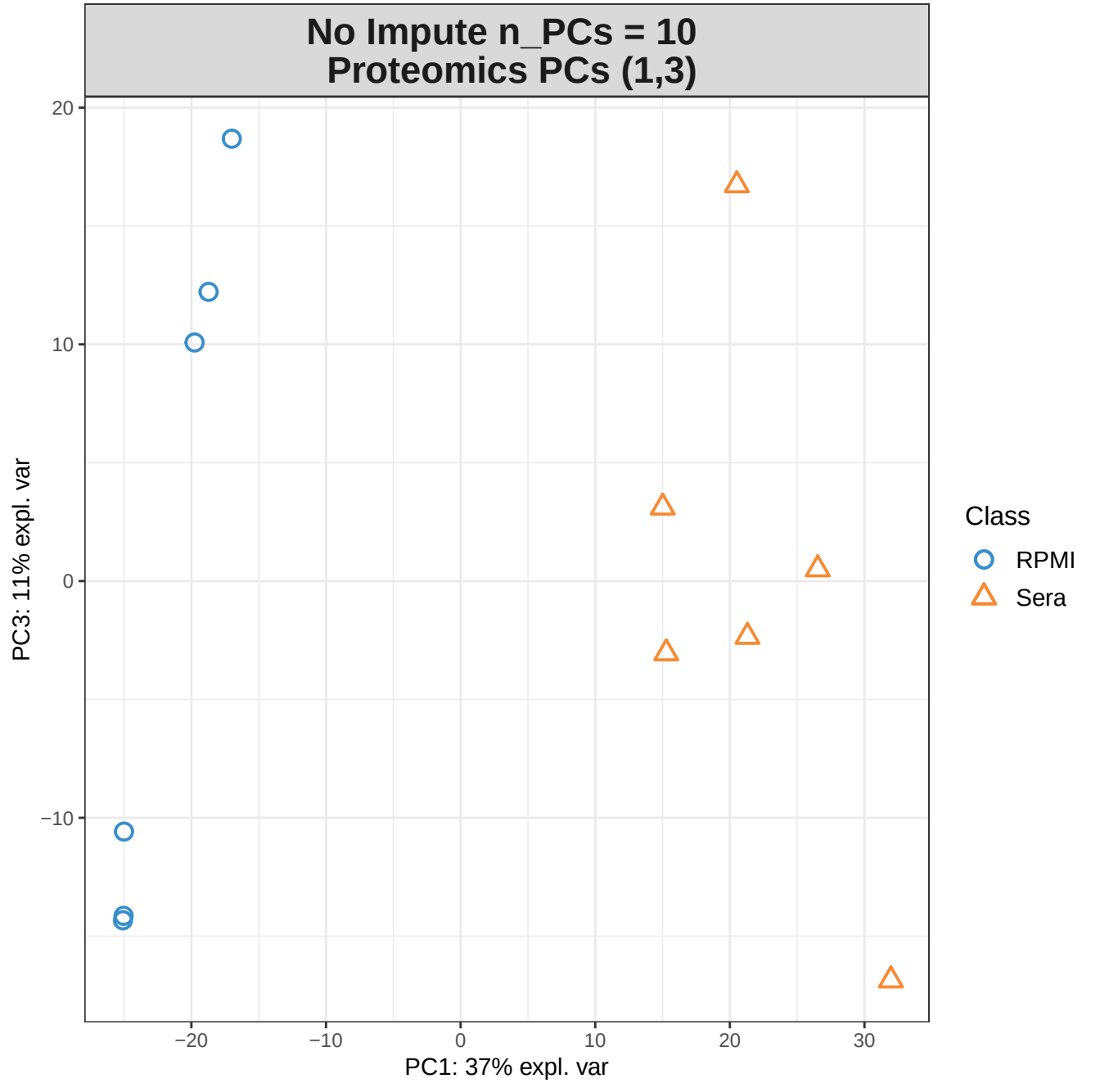

No Impute n_PCs = 10
Metabolomics PCs (1,2)
PC2: 17% expl. var
PC1: 39% expl. var
5
0
−5
−5
0
5
Class
RPMI
Sera

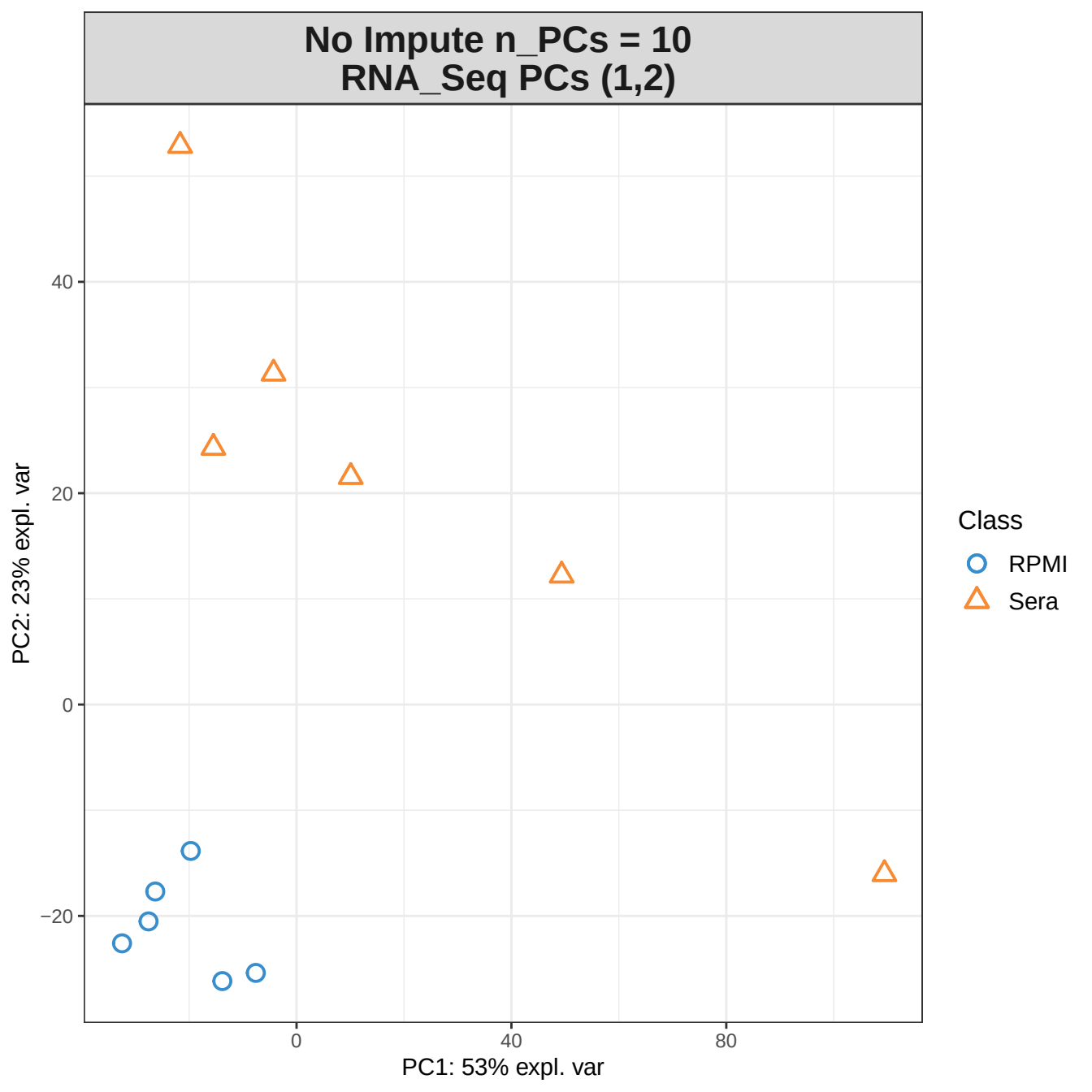

No Impute n_PCs = 10
Metabolomics PCs (2,3)
5
0
−5
PC3: 9% expl. var
−5
0
5
PC2: 17% expl. var
Class
RPMI
Sera

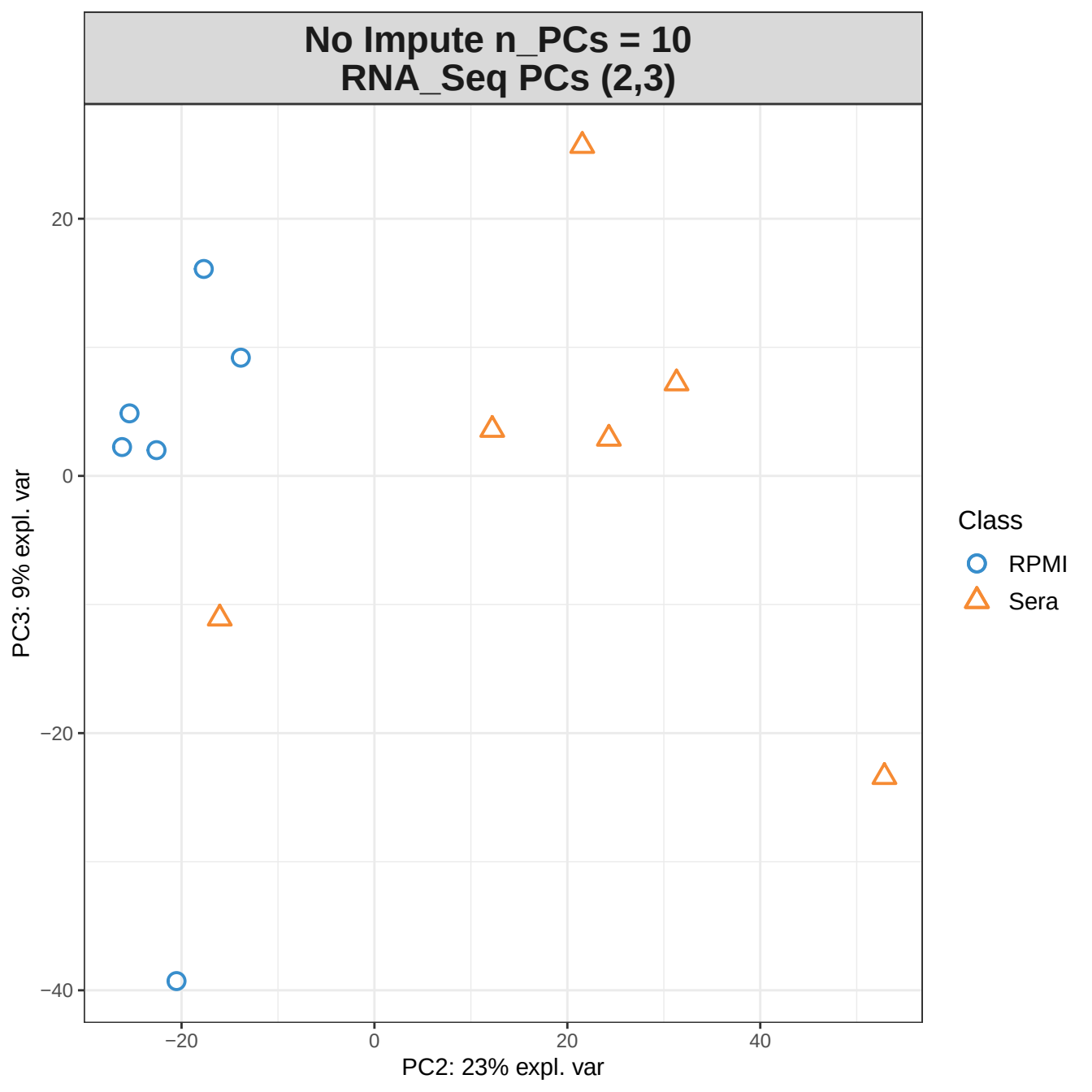

No Impute n_PCs = 10
Metabolomics PCs (1,3)
5
0
−5
PC3: 9% expl. var
−5
0
5
PC1: 39% expl. var
Class
RPMI
Sera

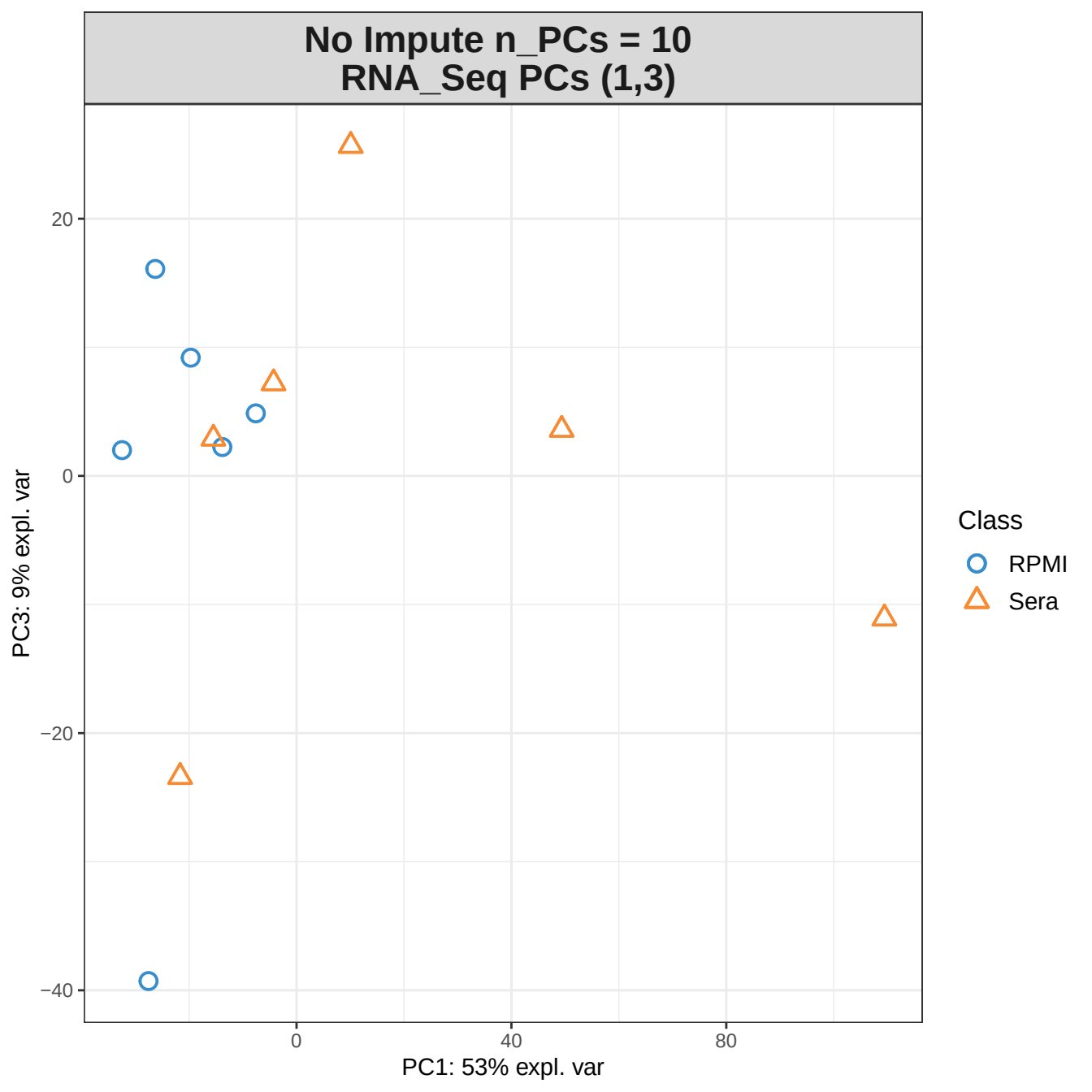

No Impute n_PCs = 10
Proteomics PCs (1,2)
PC2: 16% expl. var
PC1: 37% expl. var
20
10
0
−10
−20
−30
−20
−10
0
10
20
30
Class
RPMI
Sera

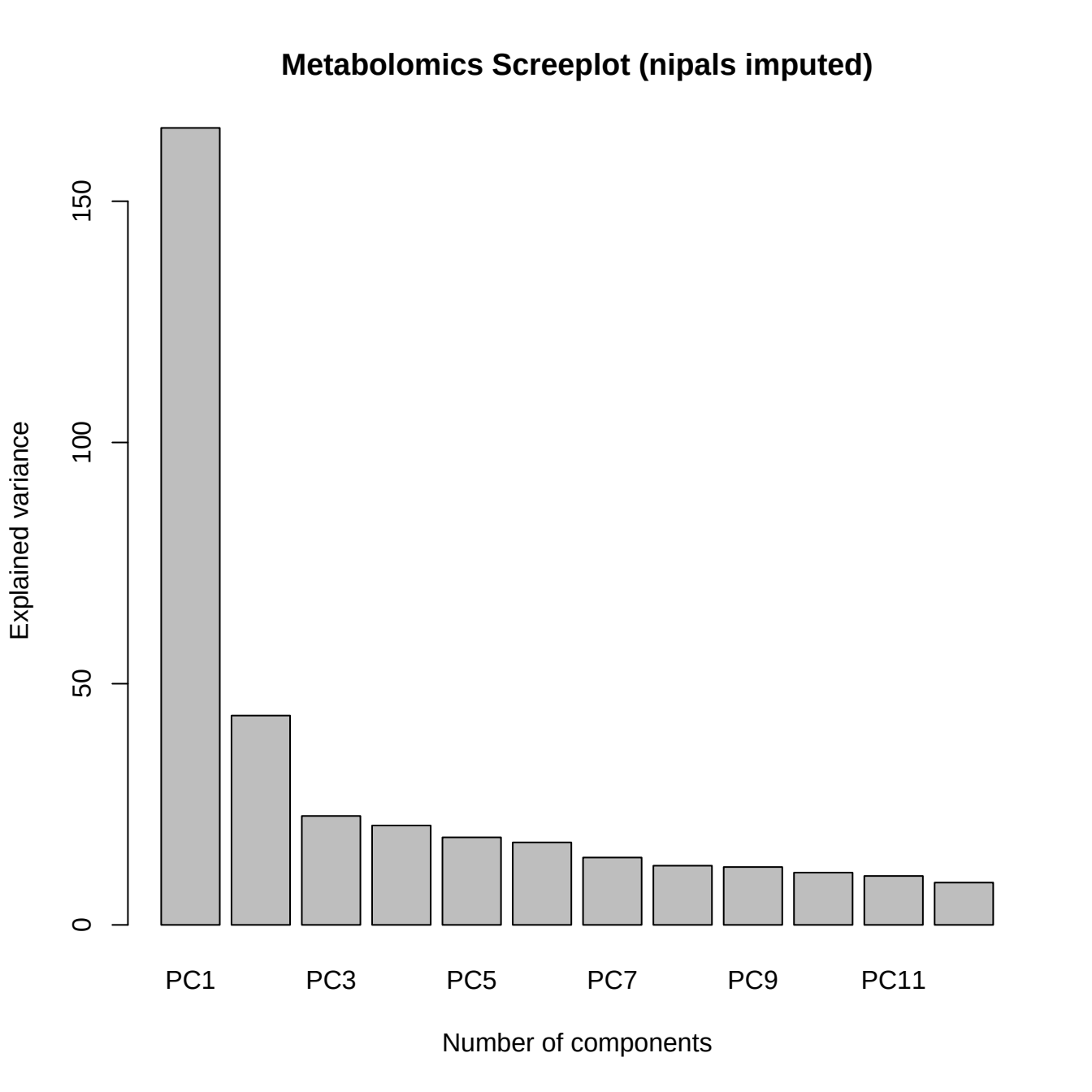

No Impute n_PCs = 10
Proteomics PCs (2,3)
20
10
0
−10
PC3: 11% expl. var
−30
−20
−10
0
10
20
PC2: 16% expl. var
Class
RPMI
Sera

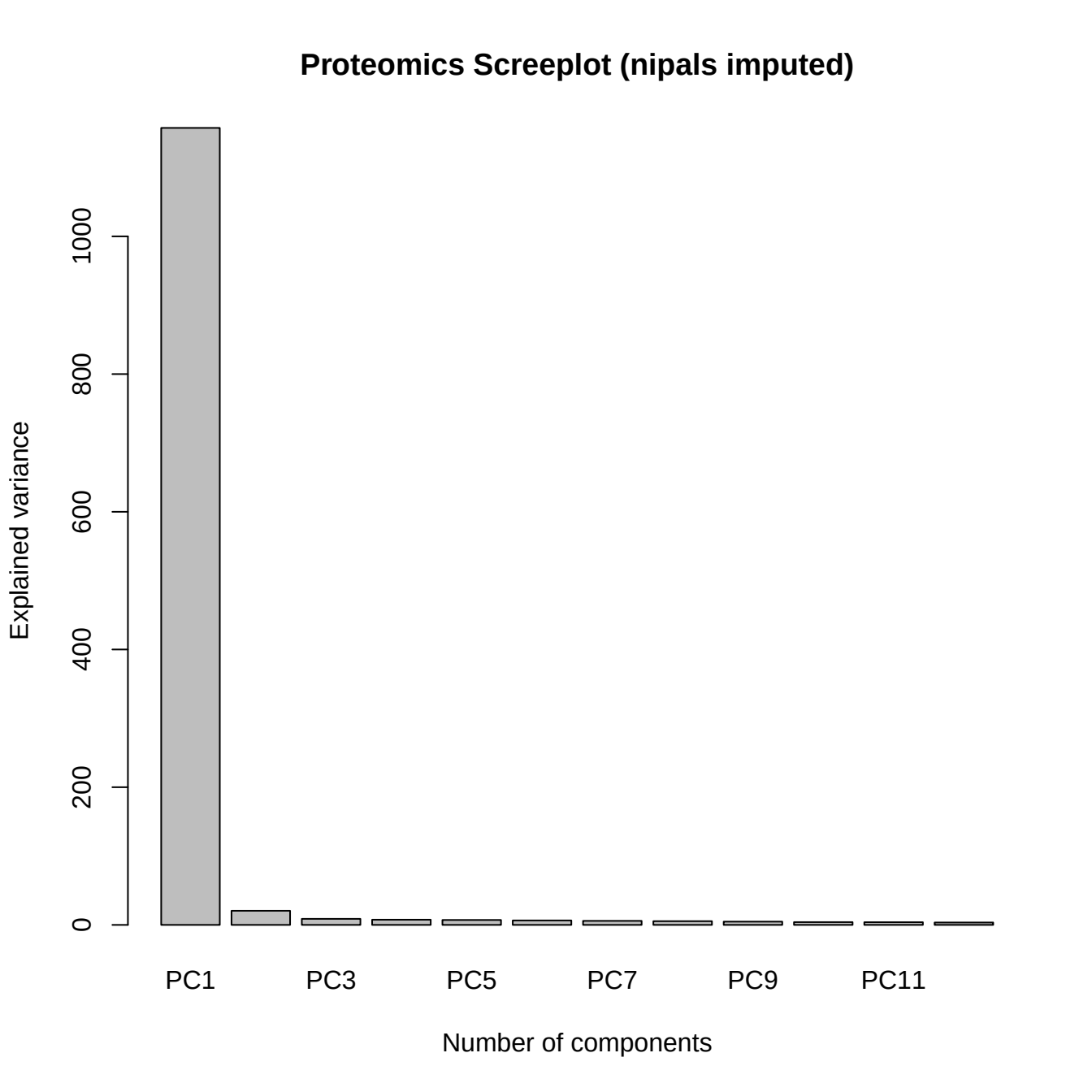

No Impute n_PCs = 10
Proteomics PCs (1,3)
PC3: 11% expl. var
PC1: 37% expl. var
20
10
0
−10
−20
−10
0
10
20
30
Class
RPMI
Sera

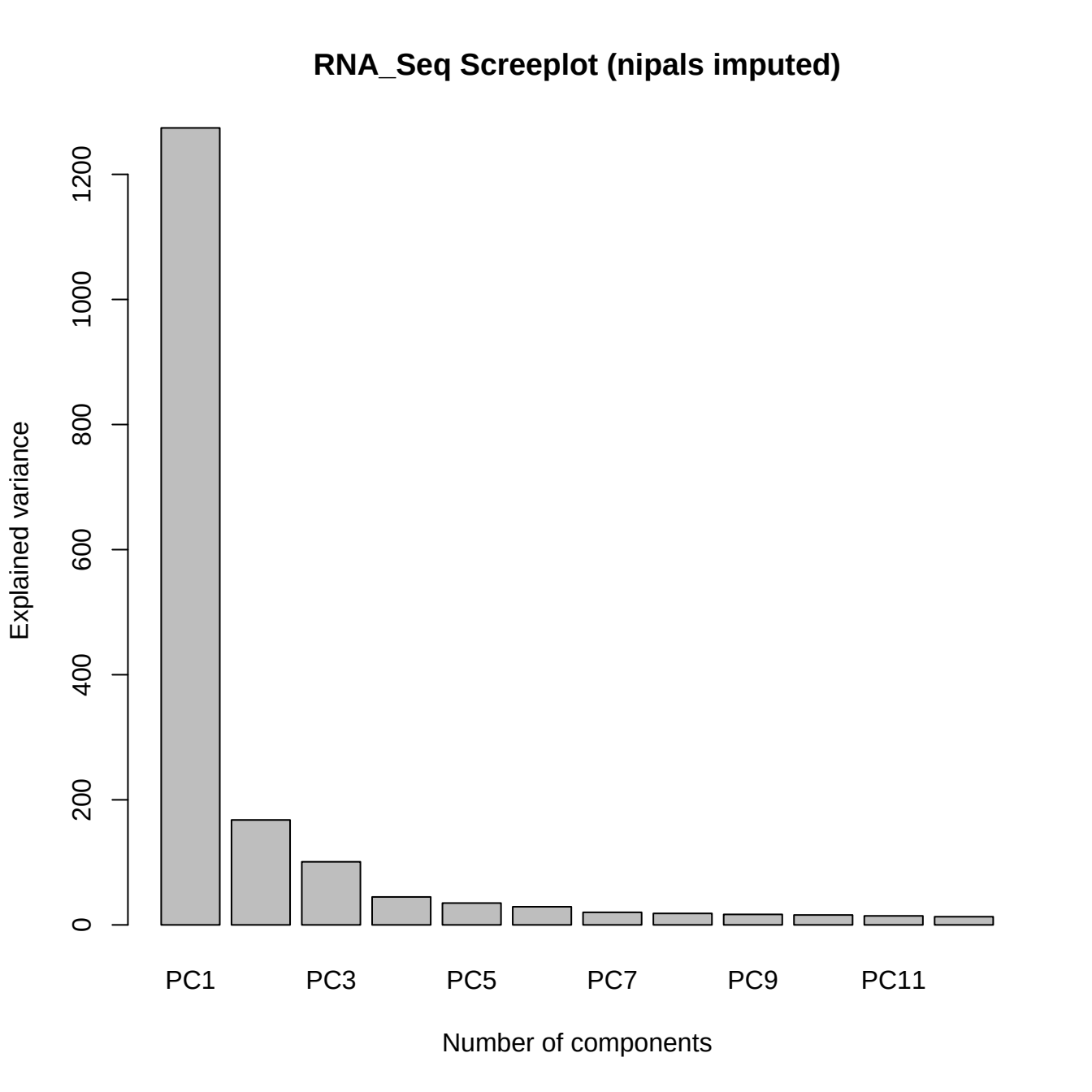

No Impute n_PCs = 10
RNA_Seq PCs (1,2)
PC2: 23% expl. var
PC1: 53% expl. var
40
20
0
−20
0
40
80
Class
RPMI
Sera

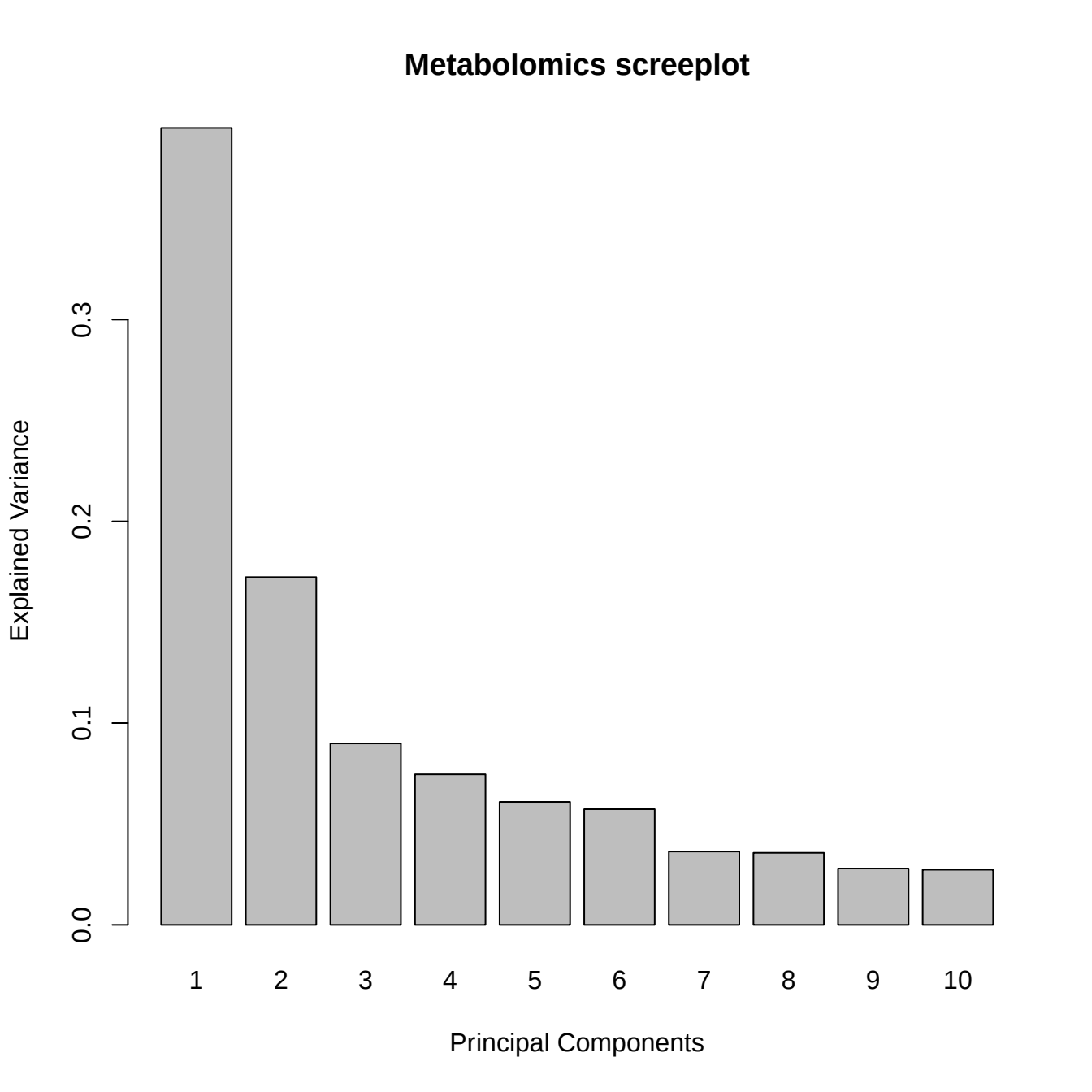

No Impute n_PCs = 10
RNA_Seq PCs (2,3)
20
0
−20
−40
PC3: 9% expl. var
−20
0
20
40
PC2: 23% expl. var
Class
RPMI
Sera

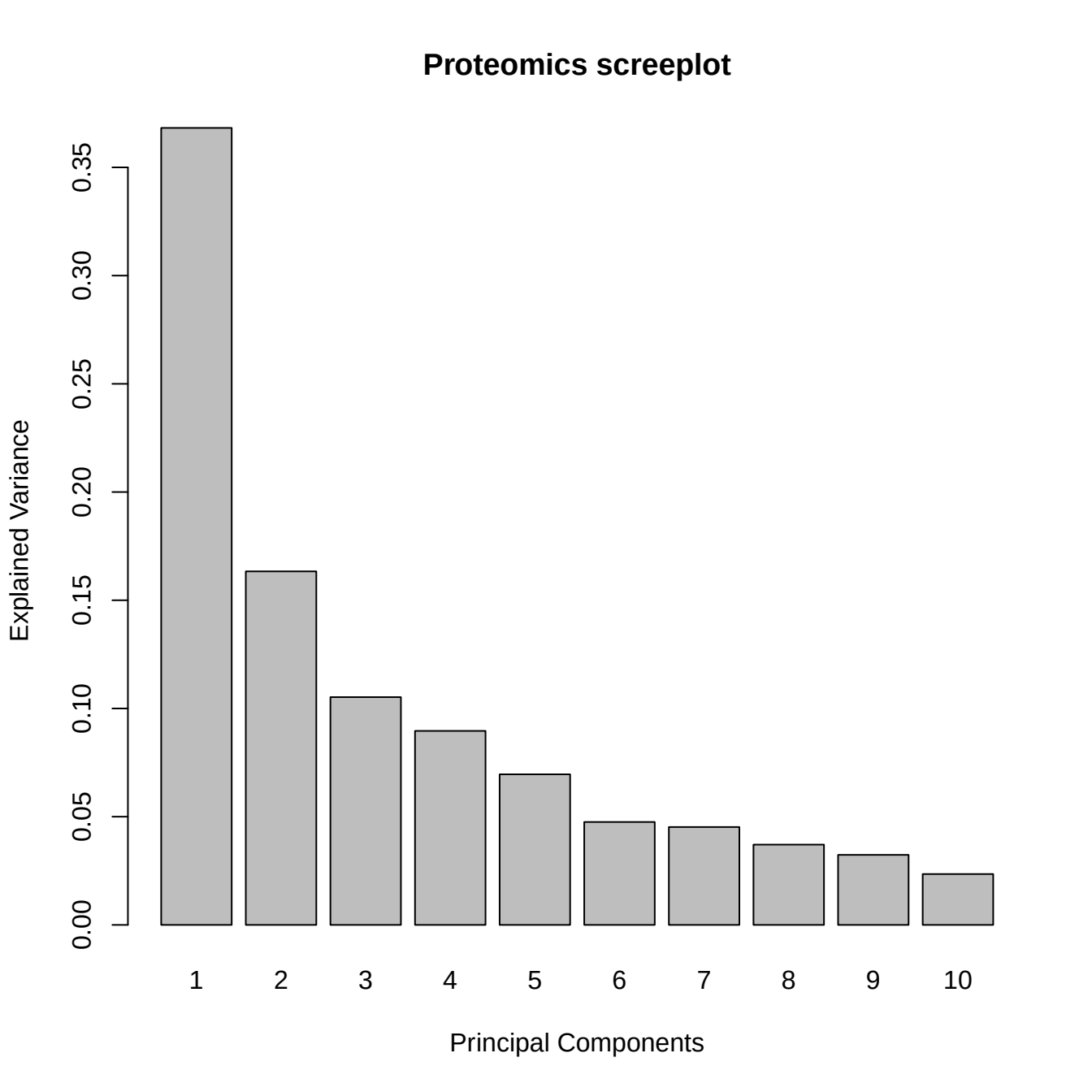

No Impute n_PCs = 10
RNA_Seq PCs (1,3)
20
0
−20
−40
PC3: 9% expl. var
0
40
80
PC1: 53% expl. var
Class
RPMI
Sera

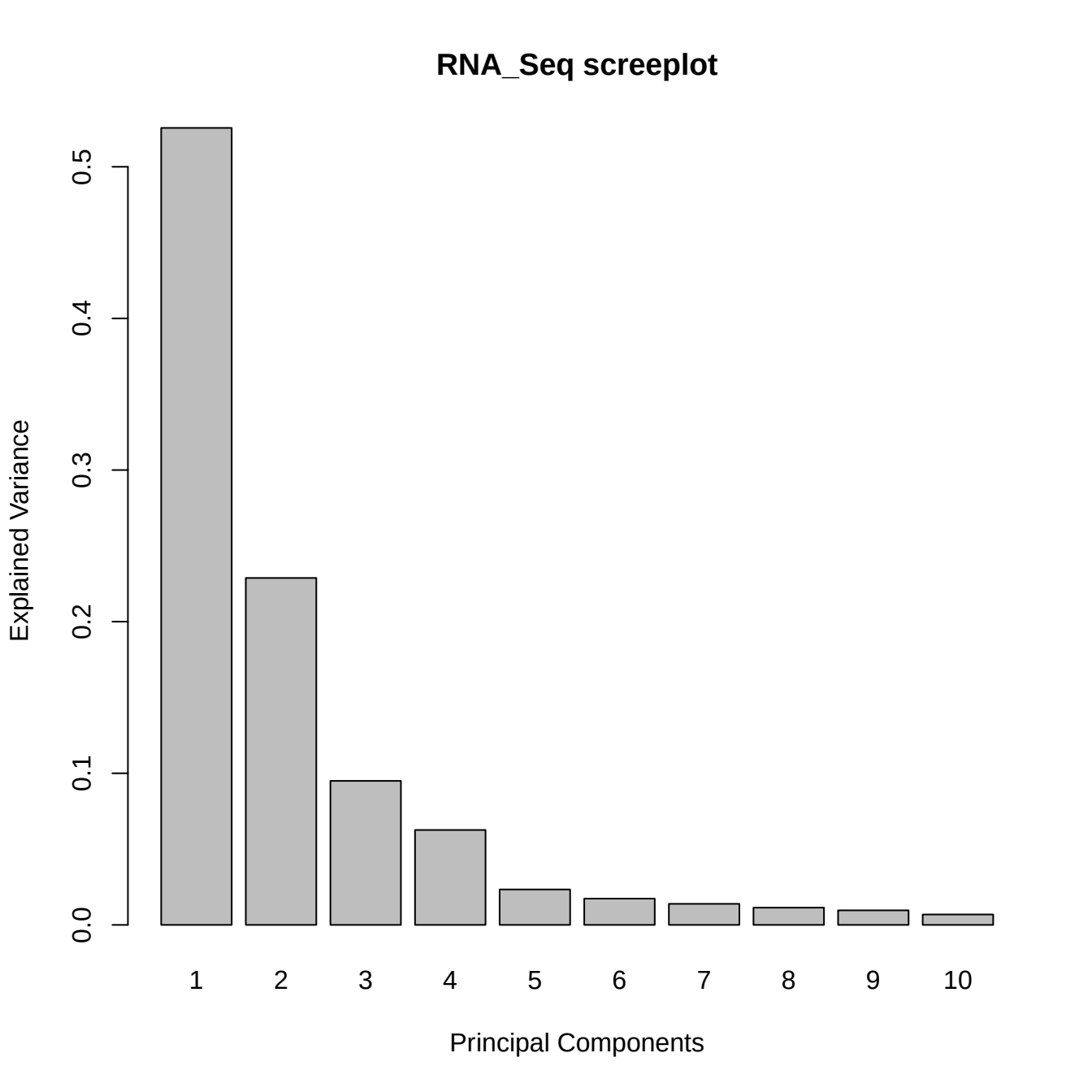

Metabolomics Screeplot (nipals imputed)
Explained variance
0
50
100
150
PC1
PC3
PC5
PC7
PC9
PC11
Number of components

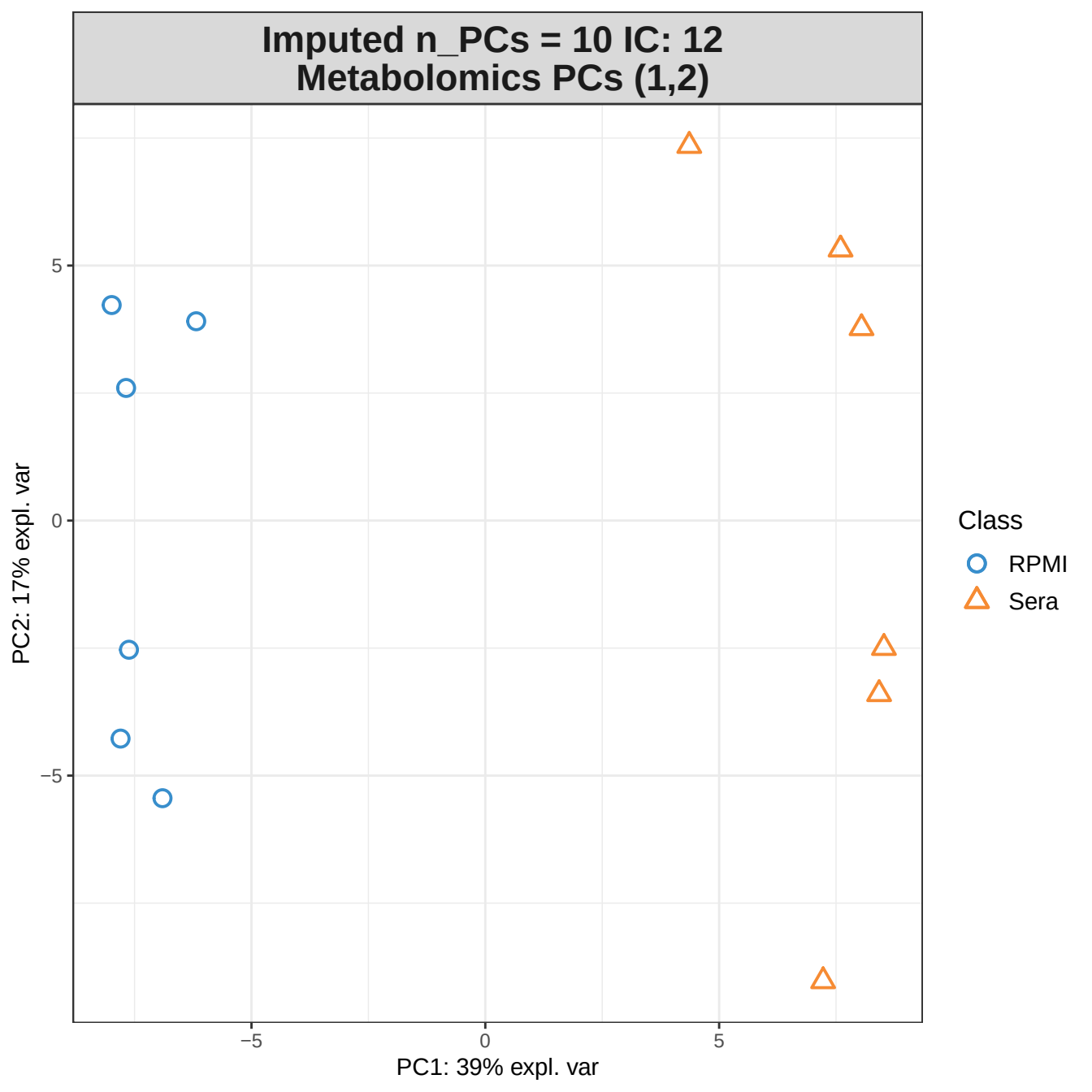

Proteomics Screeplot (nipals imputed)
Explained variance
0
200
400
600
800
1000
PC1
PC3
PC5
PC7
PC9
PC11
Number of components

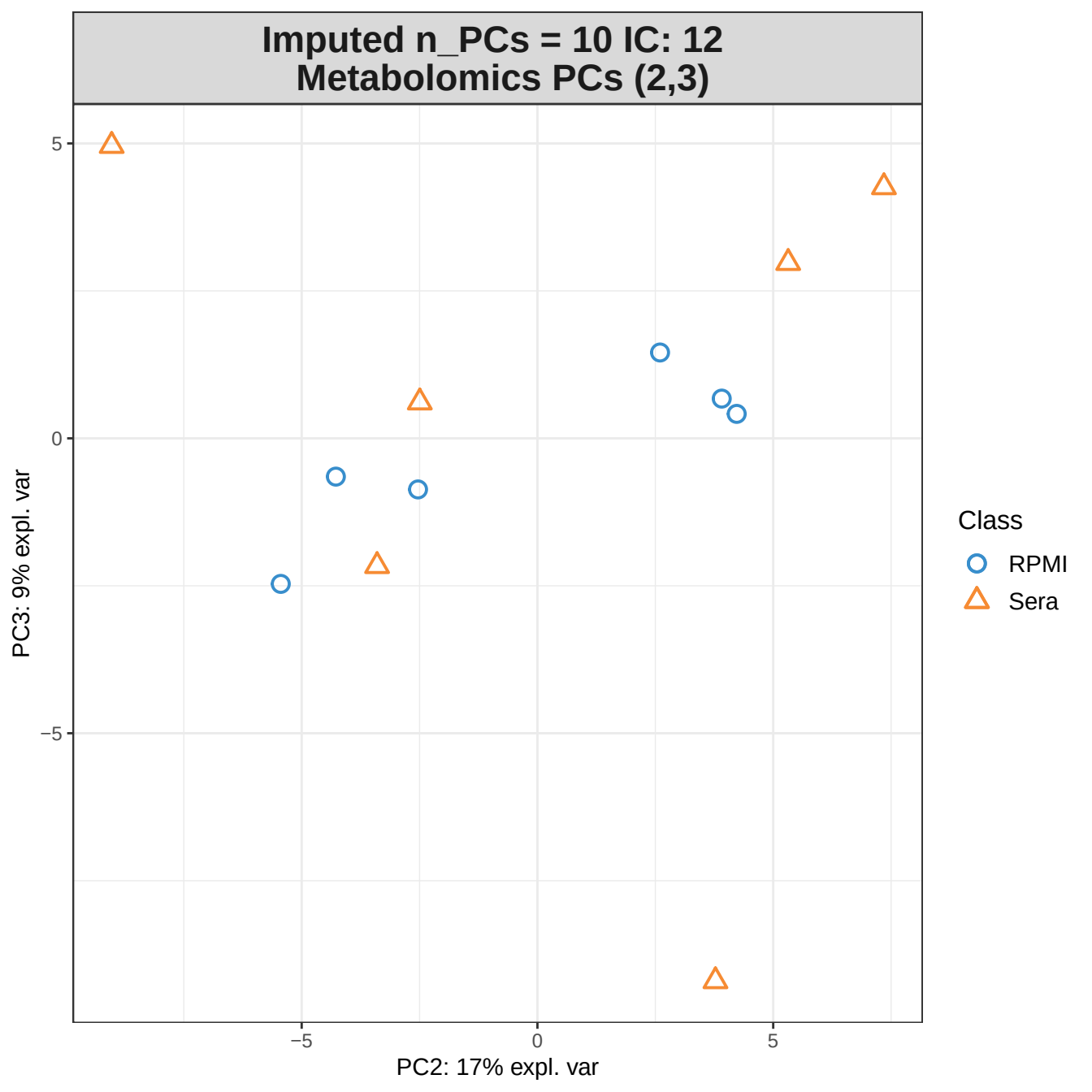

RNA_Seq Screeplot (nipals imputed)
Explained variance
0
200
400
600
800
1000
1200
PC1
PC3
PC5
PC7
PC9
PC11
Number of components

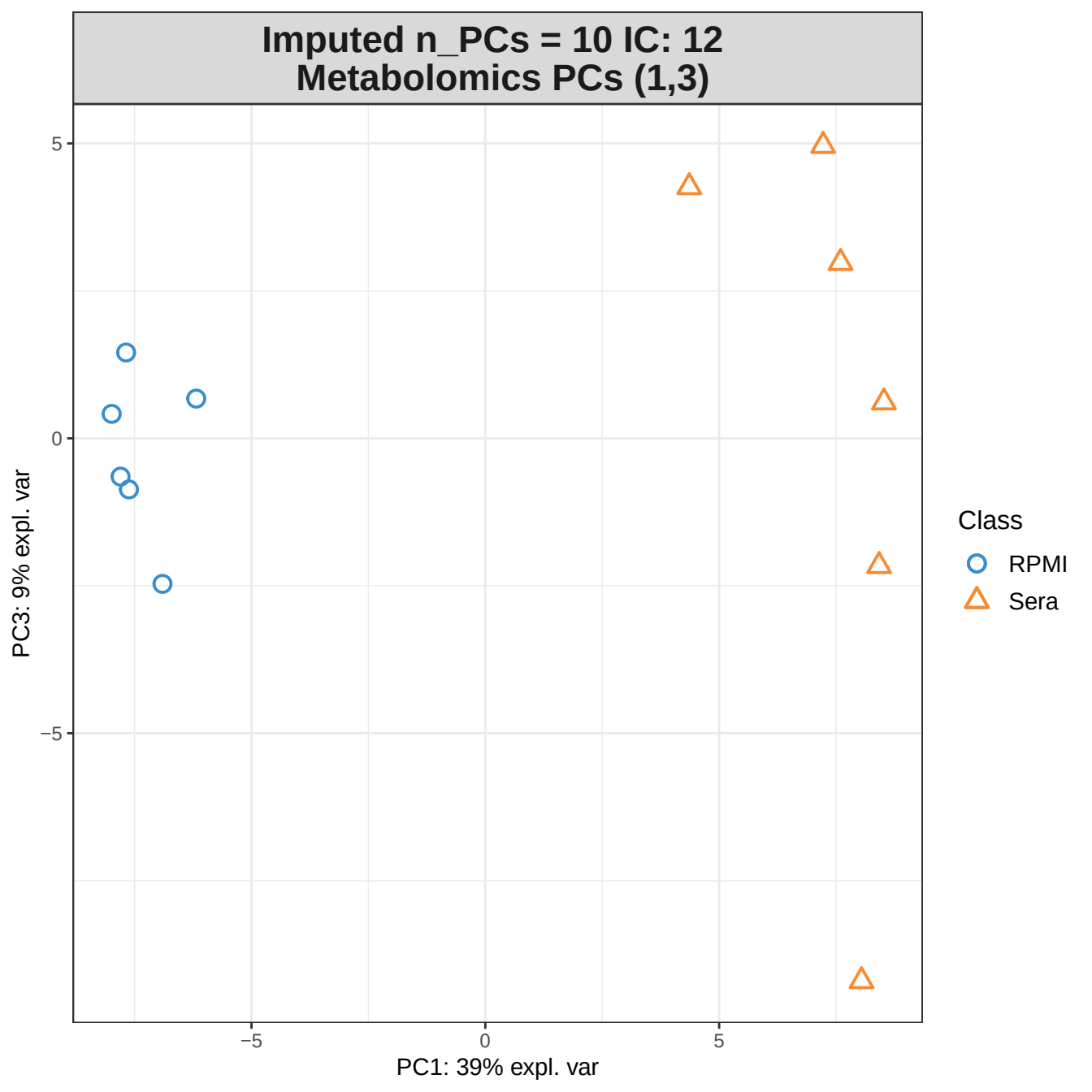

Metabolomics screeplot
Explained Variance
0.0
0.1
0.2
0.3
1
2
3
4
5
6
7
8
9
10
Principal Components

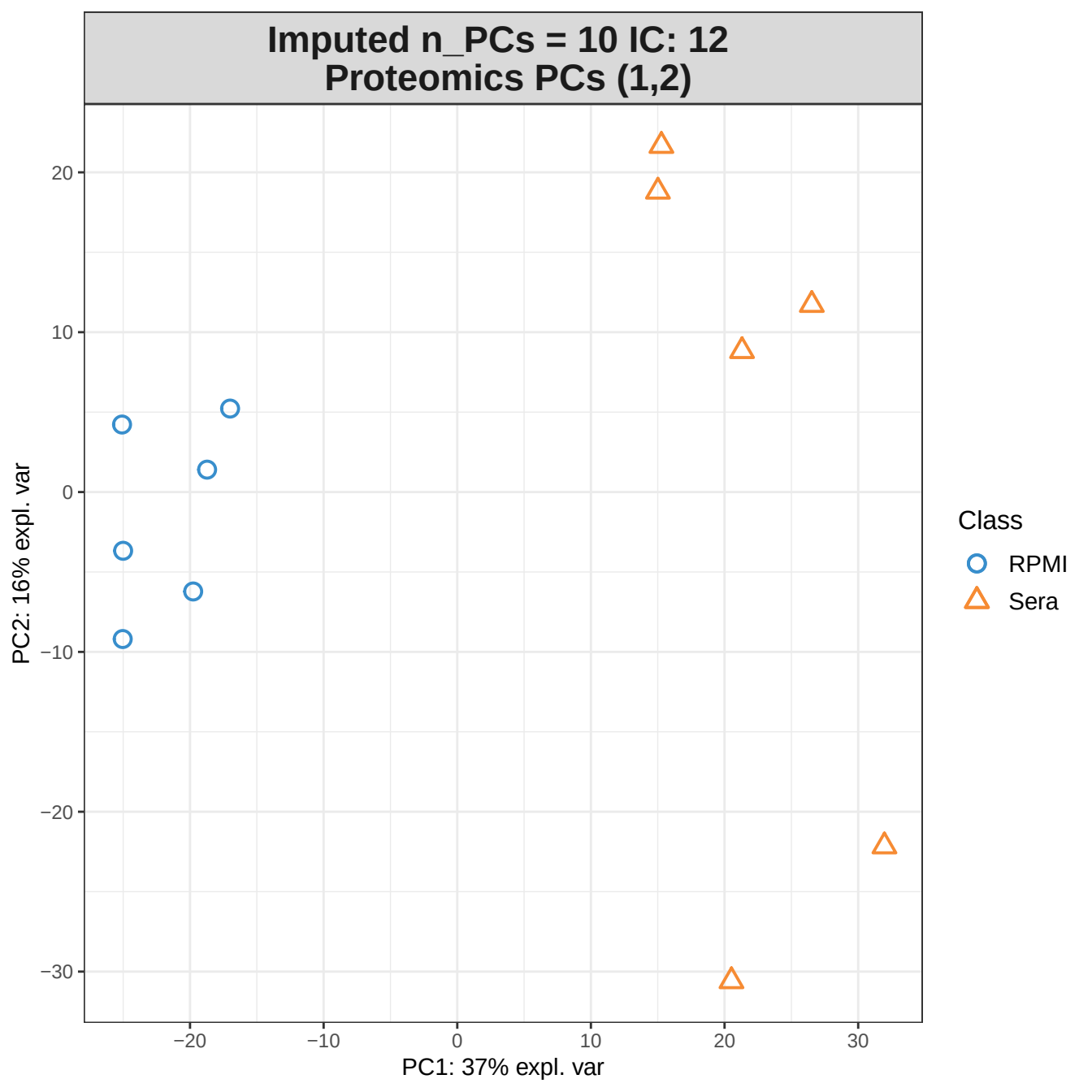

Proteomics screeplot
Explained Variance
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
1
2
3
4
5
6
7
8
9
10
Principal Components

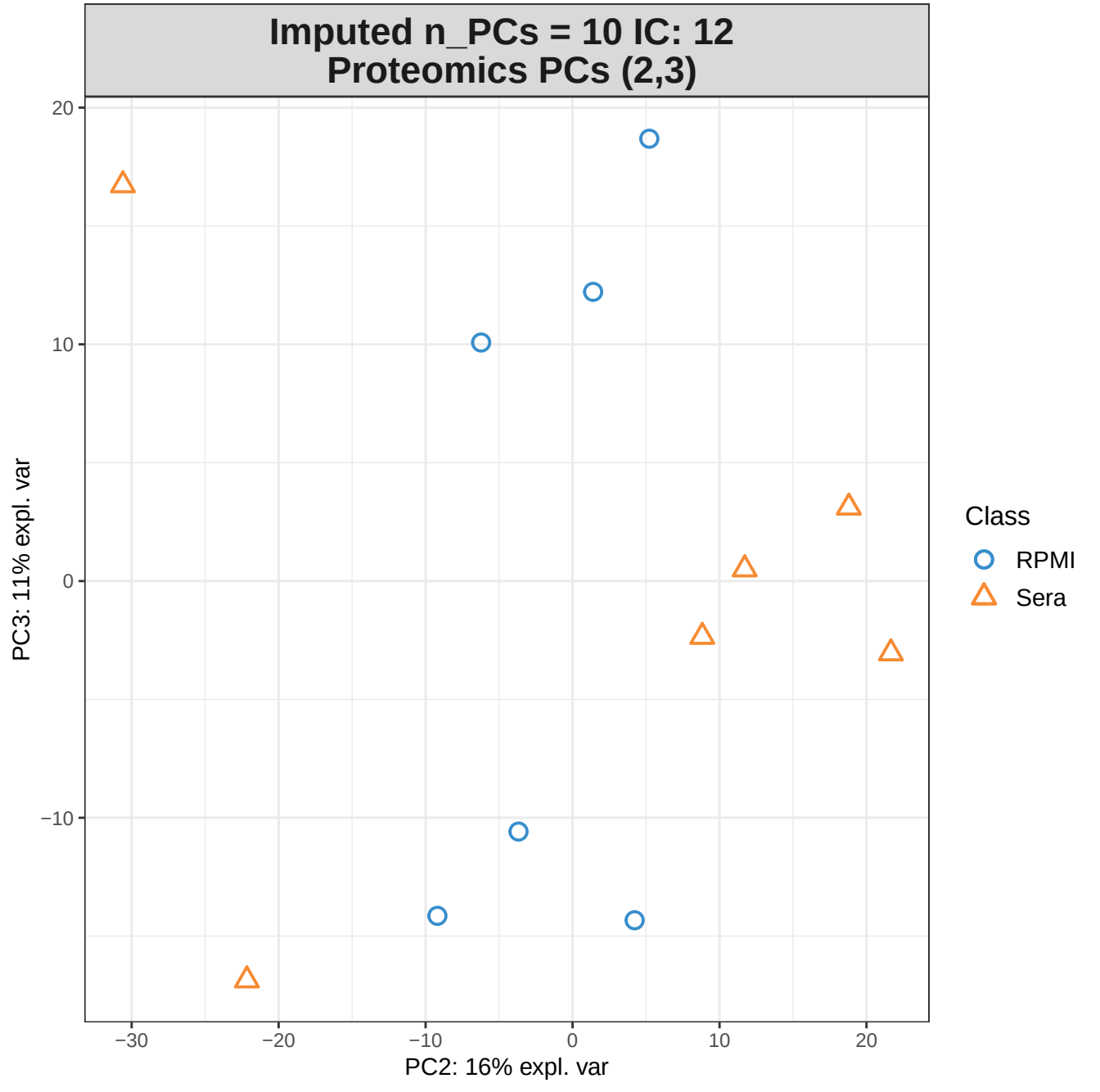

RNA_Seq screeplot
Explained Variance
0.0
0.1
0.2
0.3
0.4
0.5
1
2
3
4
5
6
7
8
9
10
Principal Components

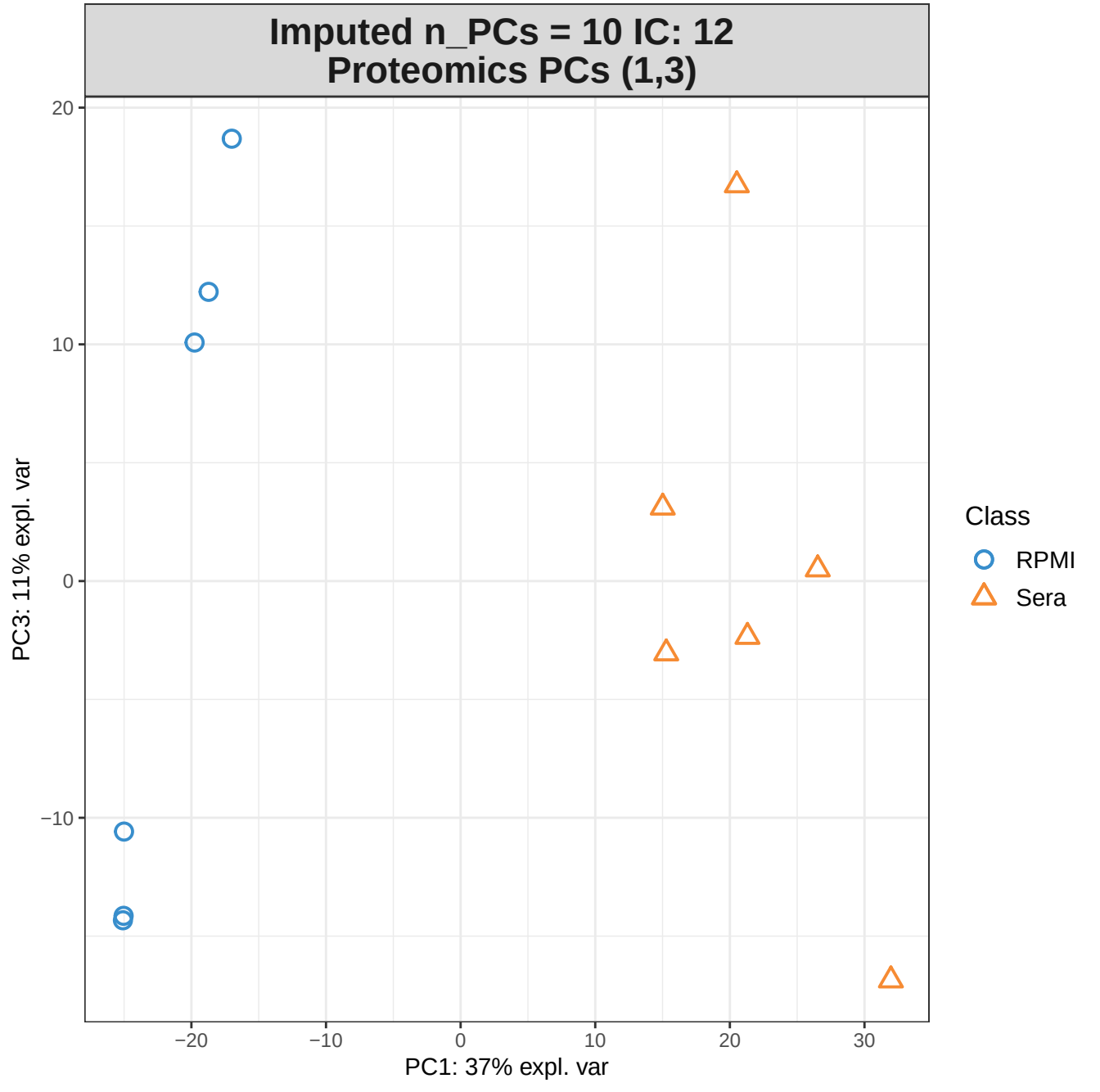

Imputed n_PCs = 10 IC: 12
Metabolomics PCs (1,2)
PC2: 17% expl. var
PC1: 39% expl. var
5
0
−5
−5
0
5
Class
RPMI
Sera

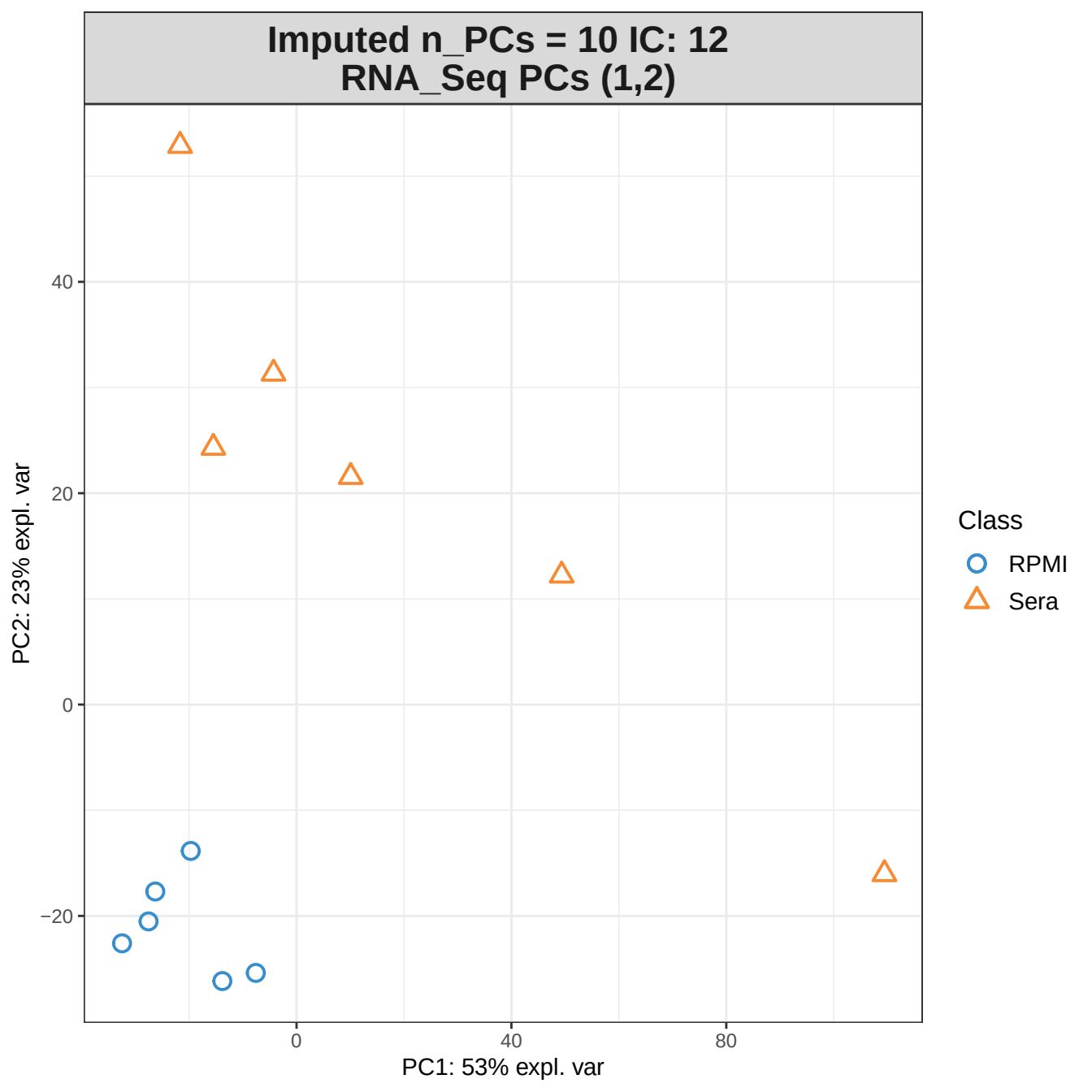

Imputed n_PCs = 10 IC: 12
Metabolomics PCs (2,3)
5
0
−5
PC3: 9% expl. var
−5
0
5
PC2: 17% expl. var
Class
RPMI
Sera

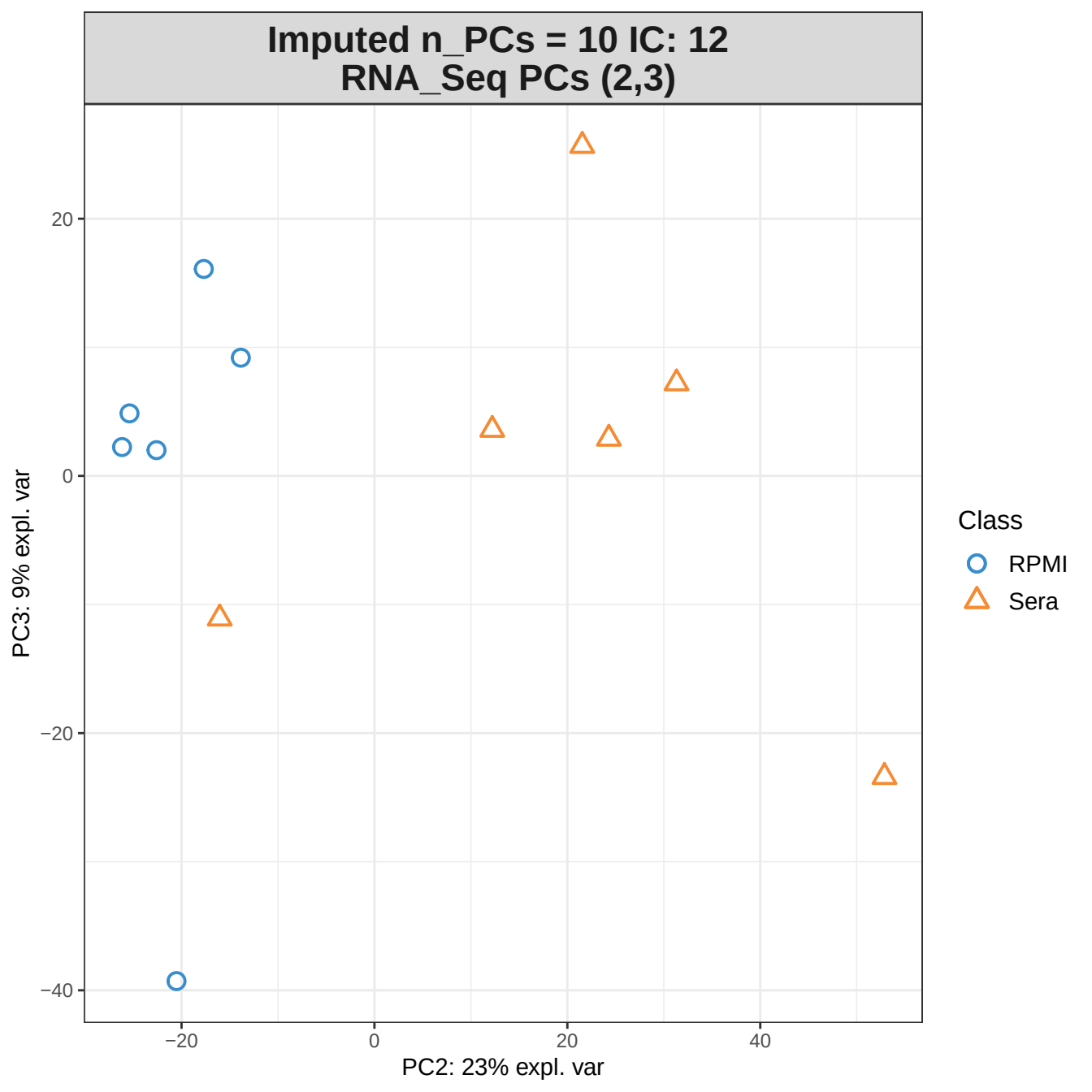

Imputed n_PCs = 10 IC: 12
Metabolomics PCs (1,3)
PC3: 9% expl. var
PC1: 39% expl. var
5
0
−5
−5
0
5
Class
RPMI
Sera

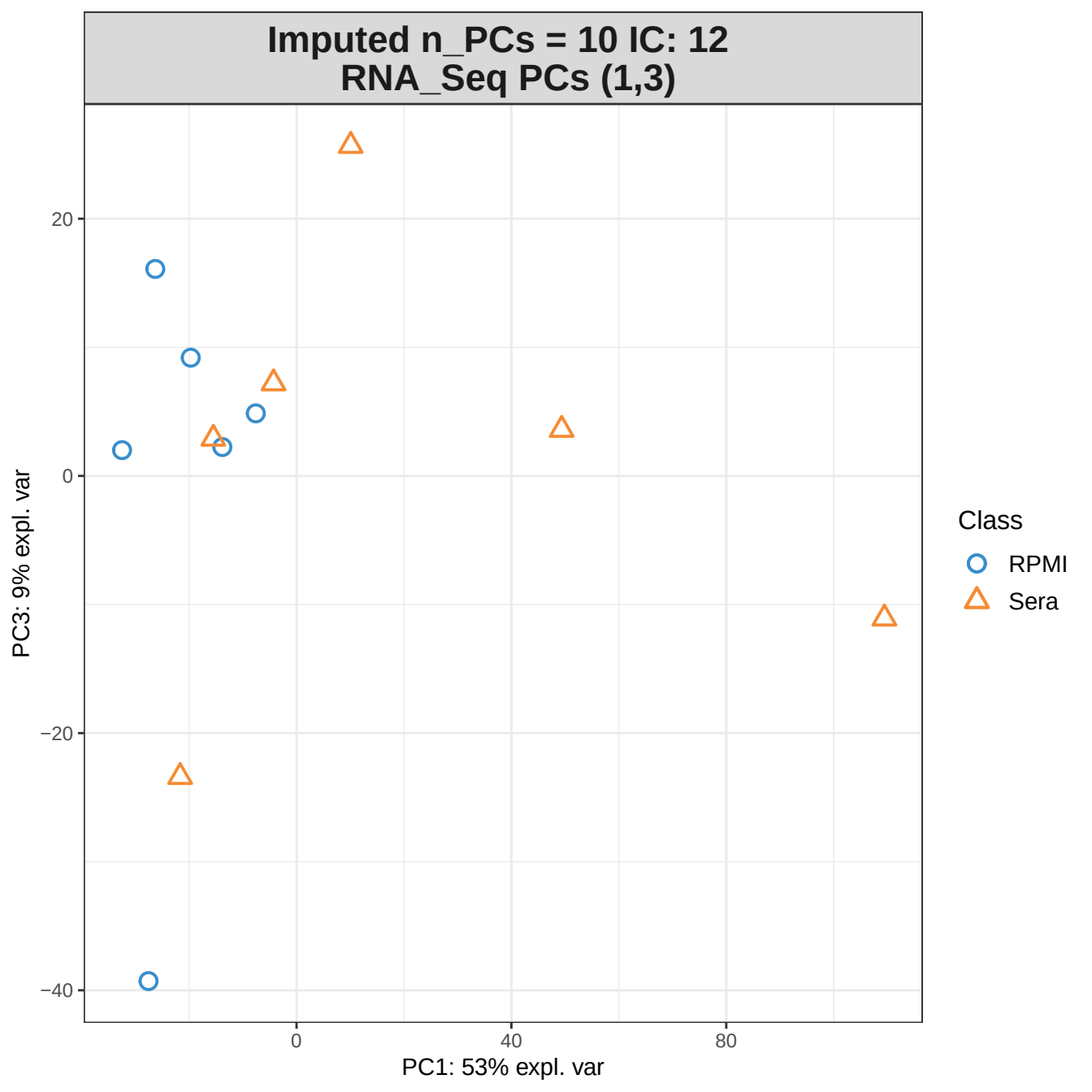

Imputed n_PCs = 10 IC: 12
Proteomics PCs (1,2)
PC2: 16% expl. var
PC1: 37% expl. var
20
10
0
−10
−20
−30
−20
−10
0
10
20
30
Class
RPMI
Sera

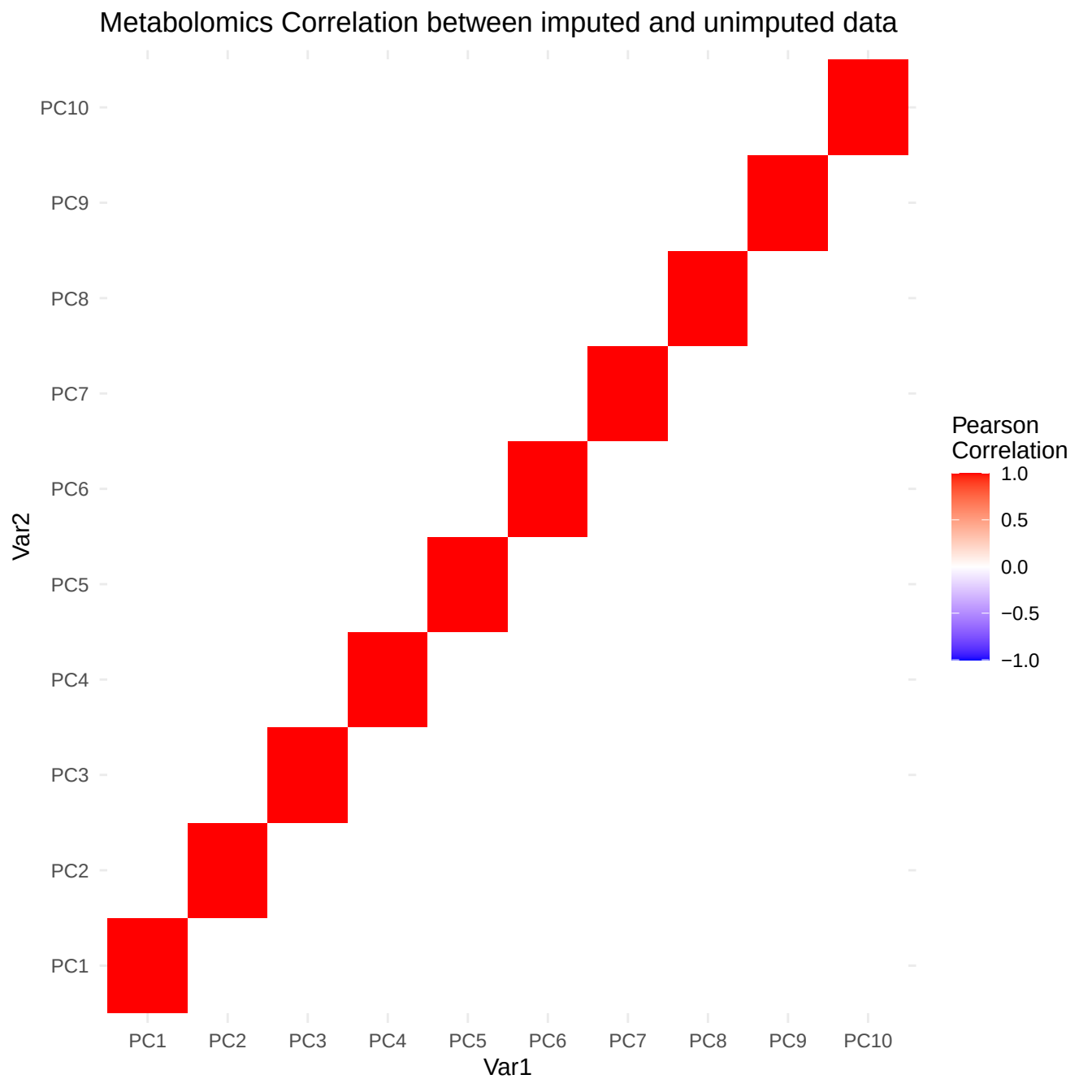

Imputed n_PCs = 10 IC: 12
Proteomics PCs (2,3)
PC3: 11% expl. var
PC2: 16% expl. var
20
10
0
−10
−30
−20
−10
0
10
20
Class
RPMI
Sera

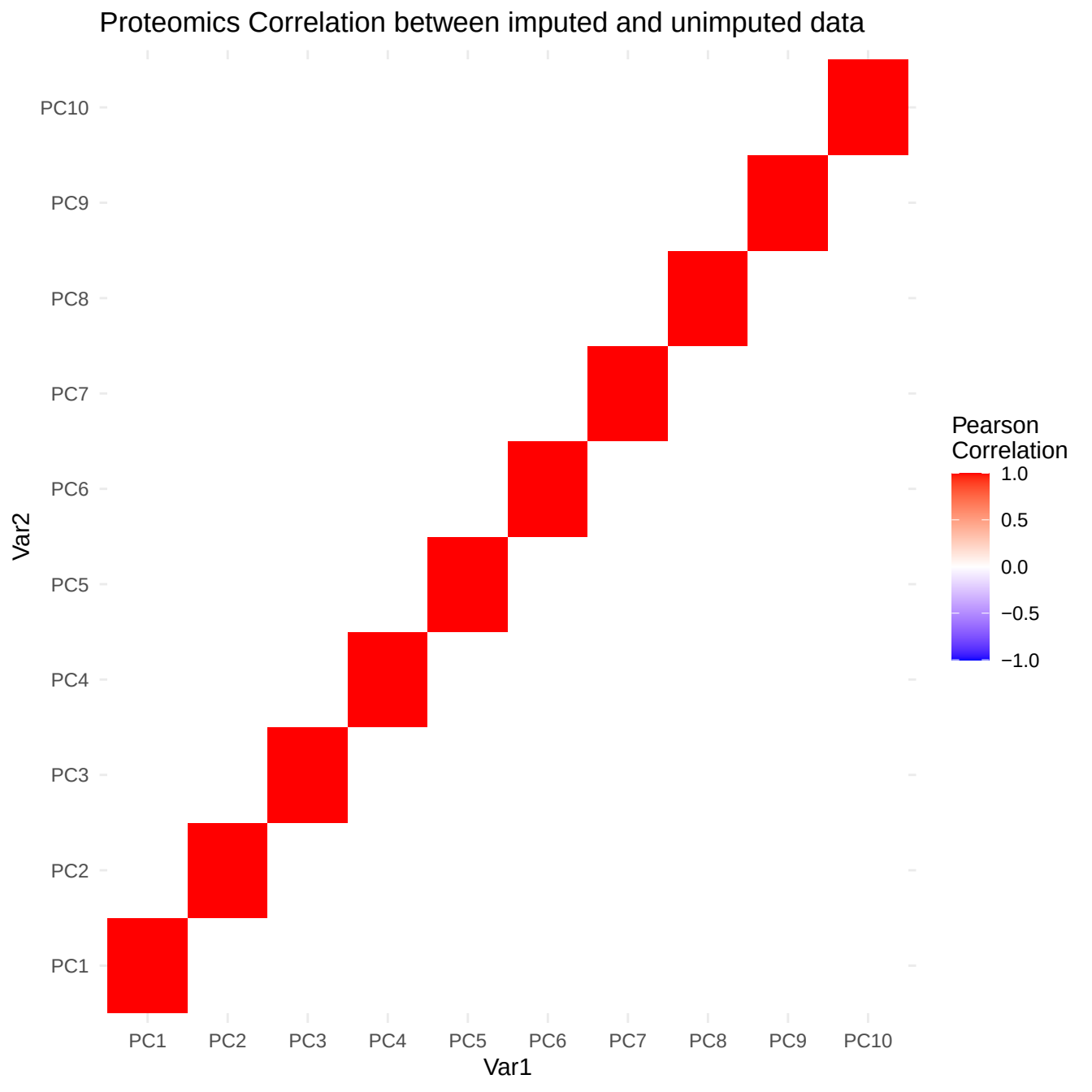

Imputed n_PCs = 10 IC: 12
Proteomics PCs (1,3)
20
10
0
−10
PC3: 11% expl. var
−20
−10
0
10
20
30
PC1: 37% expl. var
Class
RPMI
Sera

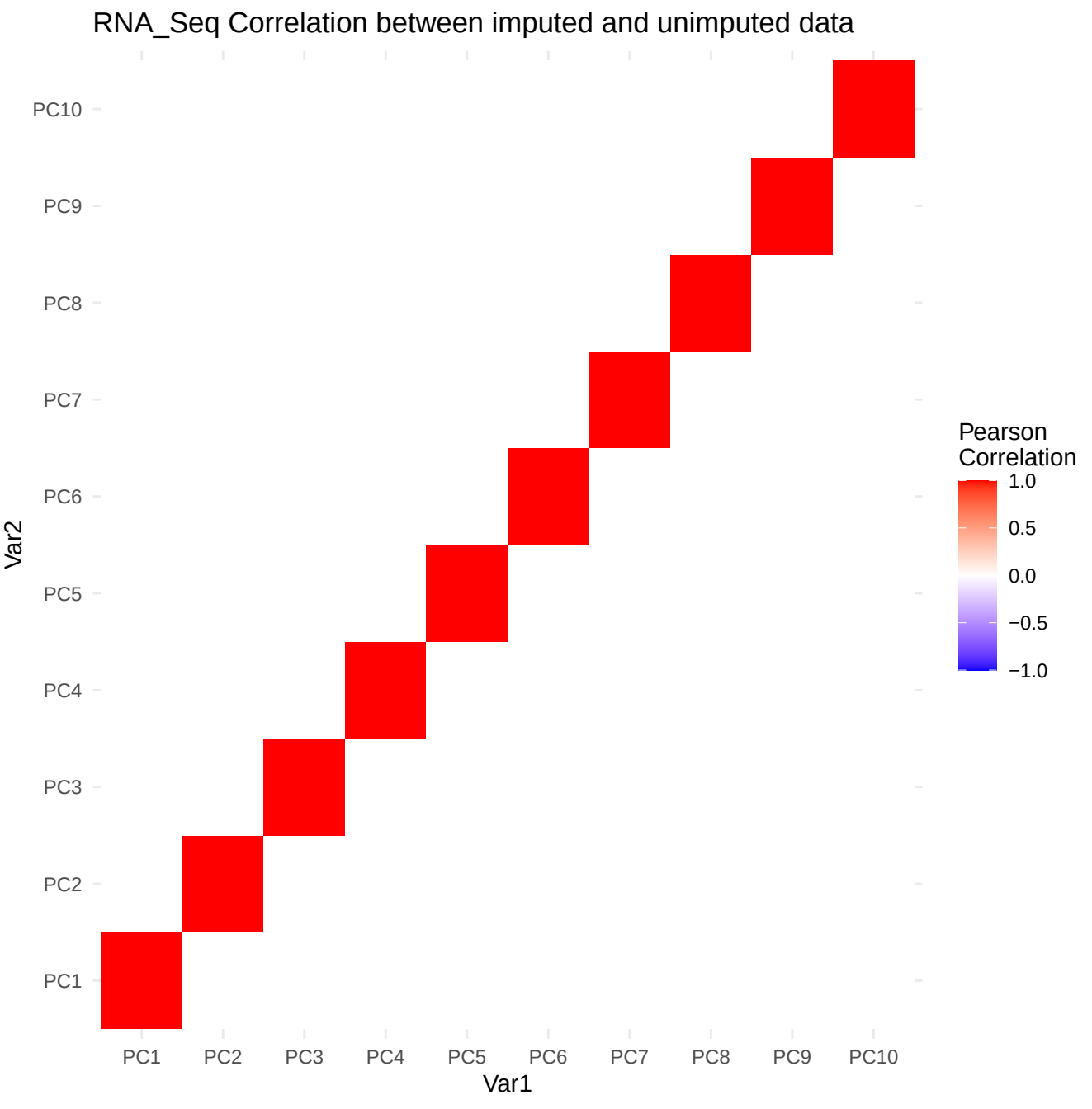

Imputed n_PCs = 10 IC: 12
RNA_Seq PCs (1,2)
PC2: 23% expl. var
PC1: 53% expl. var
40
20
0
−20
0
40
80
Class
RPMI
Sera

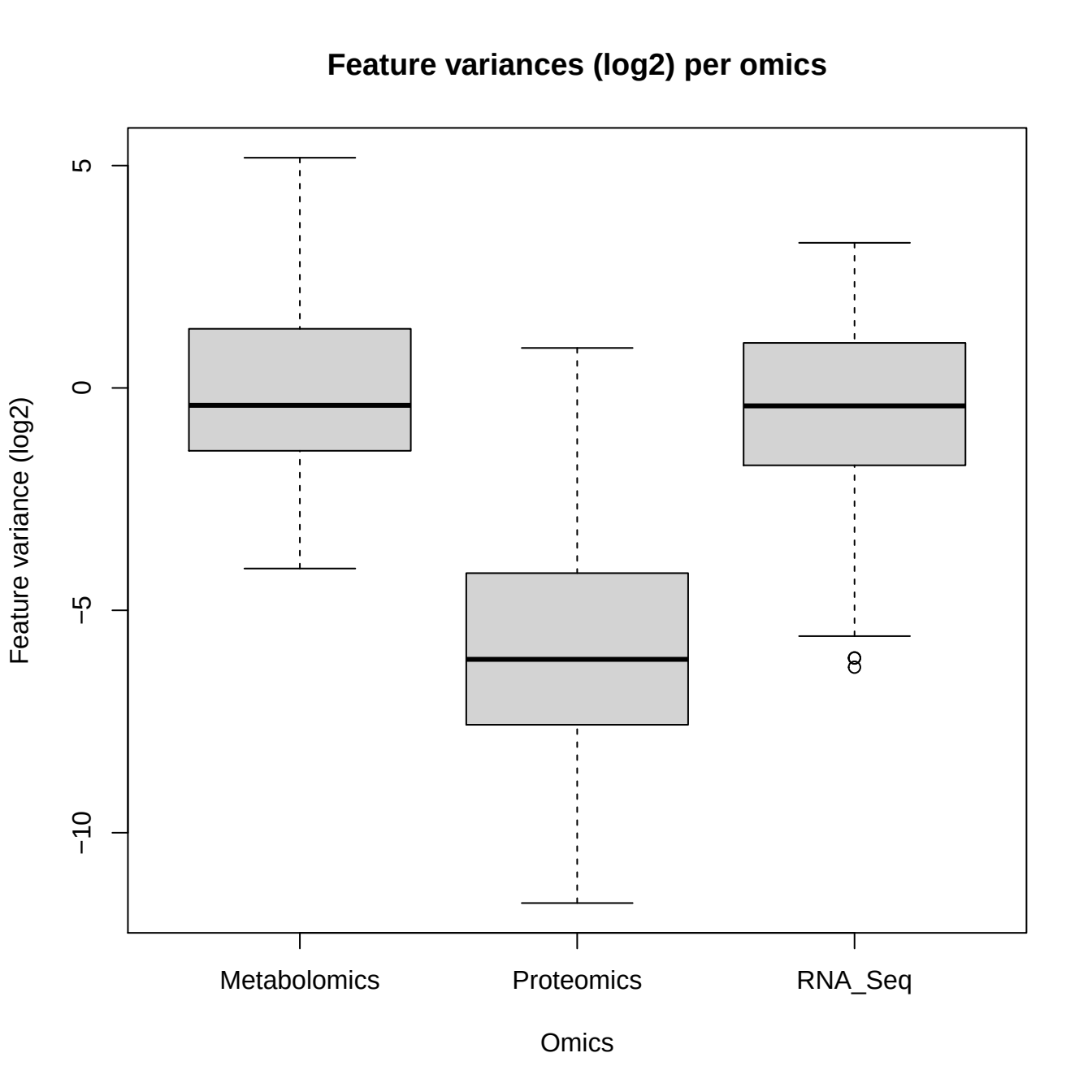

Imputed n_PCs = 10 IC: 12
RNA_Seq PCs (2,3)
20
0
−20
−40
PC3: 9% expl. var
−20
0
20
40
PC2: 23% expl. var
Class
RPMI
Sera

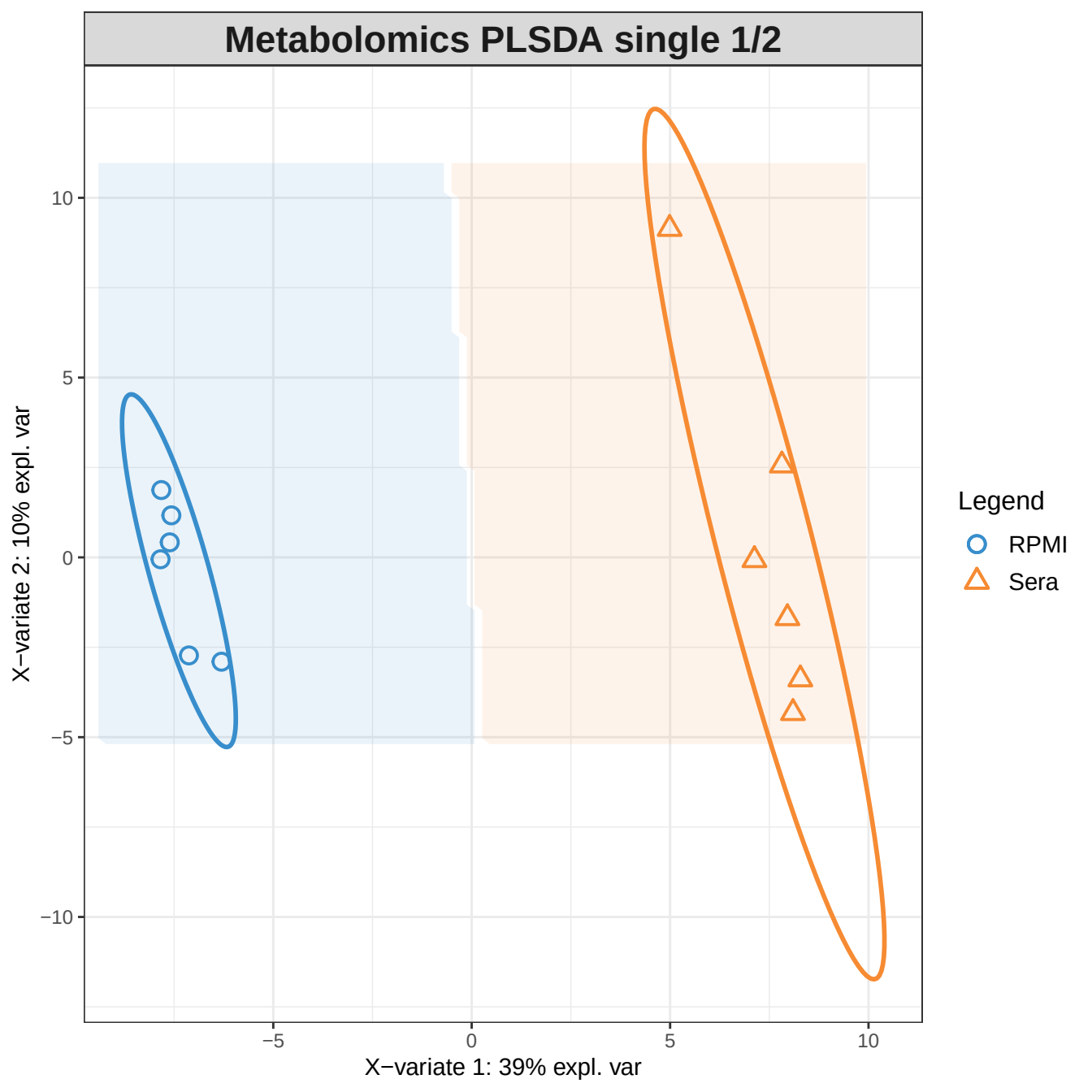

Imputed n_PCs = 10 IC: 12
RNA_Seq PCs (1,3)
20
0
−20
−40
PC3: 9% expl. var
0
40
80
PC1: 53% expl. var
Class
RPMI
Sera

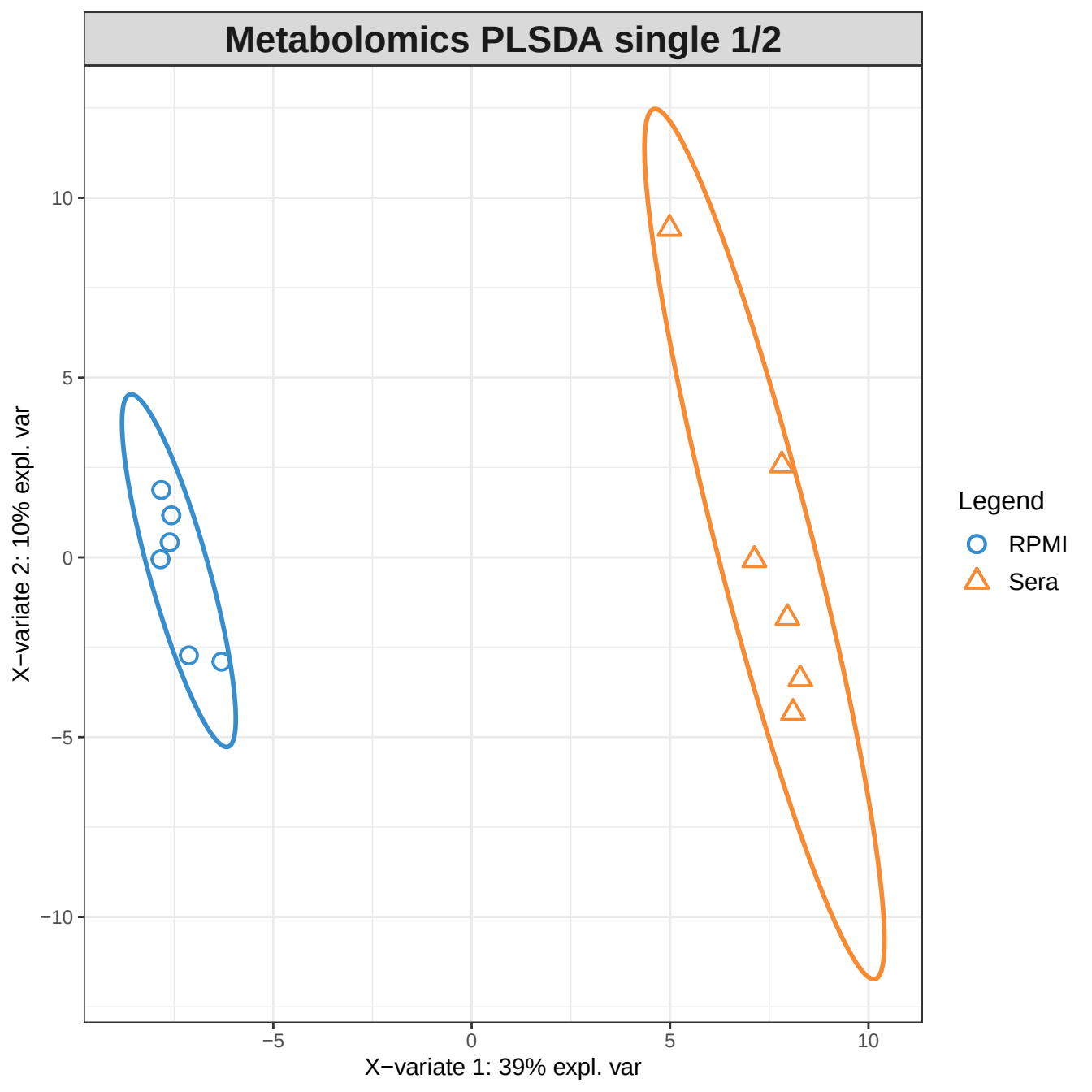

Metabolomics Correlation between imputed and unimputed data
PC10
PC9
PC8
PC7
PC6
PC5
PC4
PC3
PC2
PC1
Var2
PC1
PC2
PC3
PC4
PC5
PC6
PC7
PC8
PC9
PC10
Var1
Pearson Correlation
1.0
0.5
0.0
−0.5
−1.0

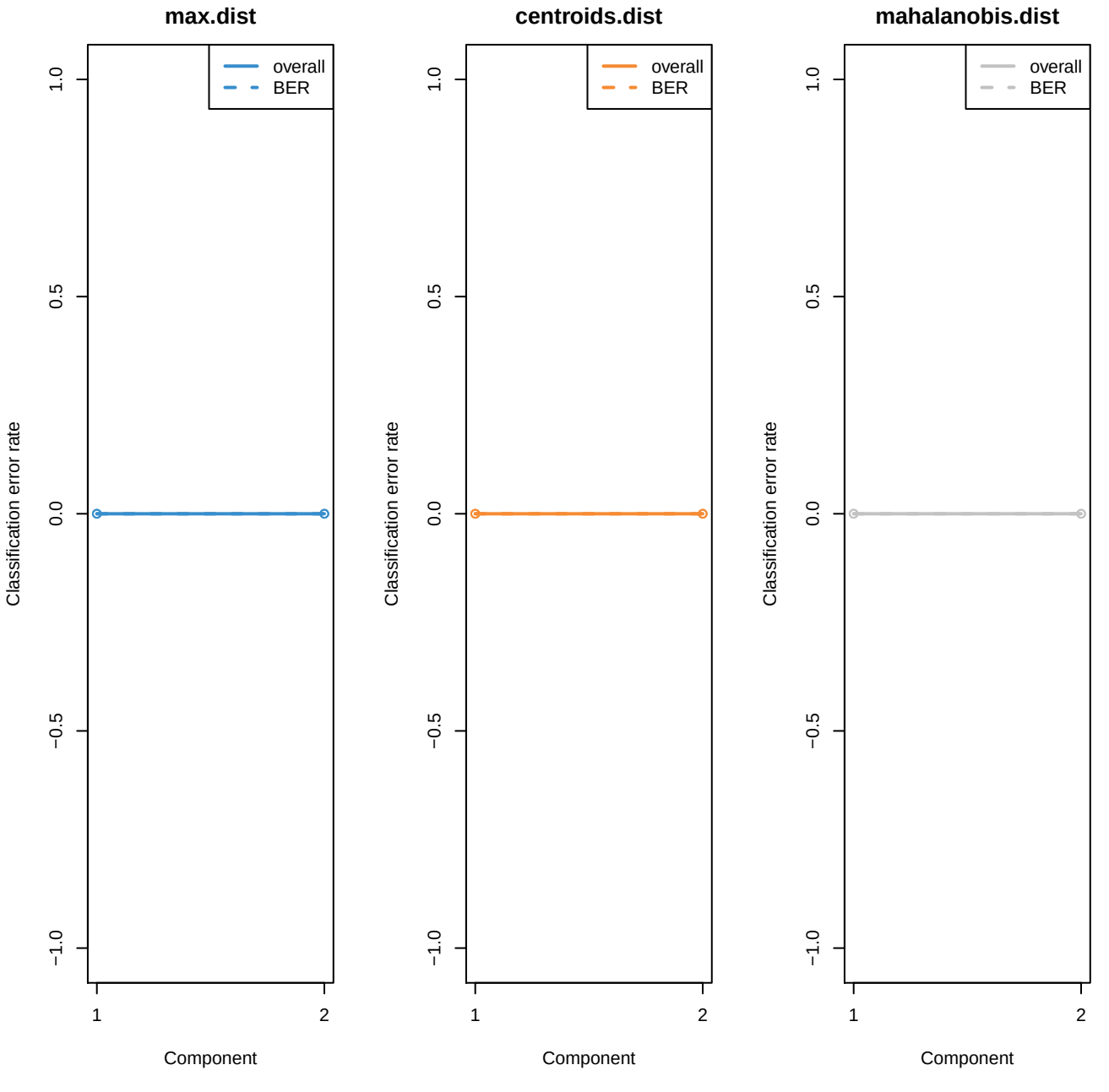

Proteomics Correlation between imputed and unimputed data
PC10
PC9
PC8
PC7
PC6
PC5
PC4
PC3
PC2
PC1
Var2
PC1
PC2
PC3
PC4
PC5
PC6
PC7
PC8
PC9
PC10
Var1
Pearson Correlation
1.0
0.5
0.0
−0.5
−1.0

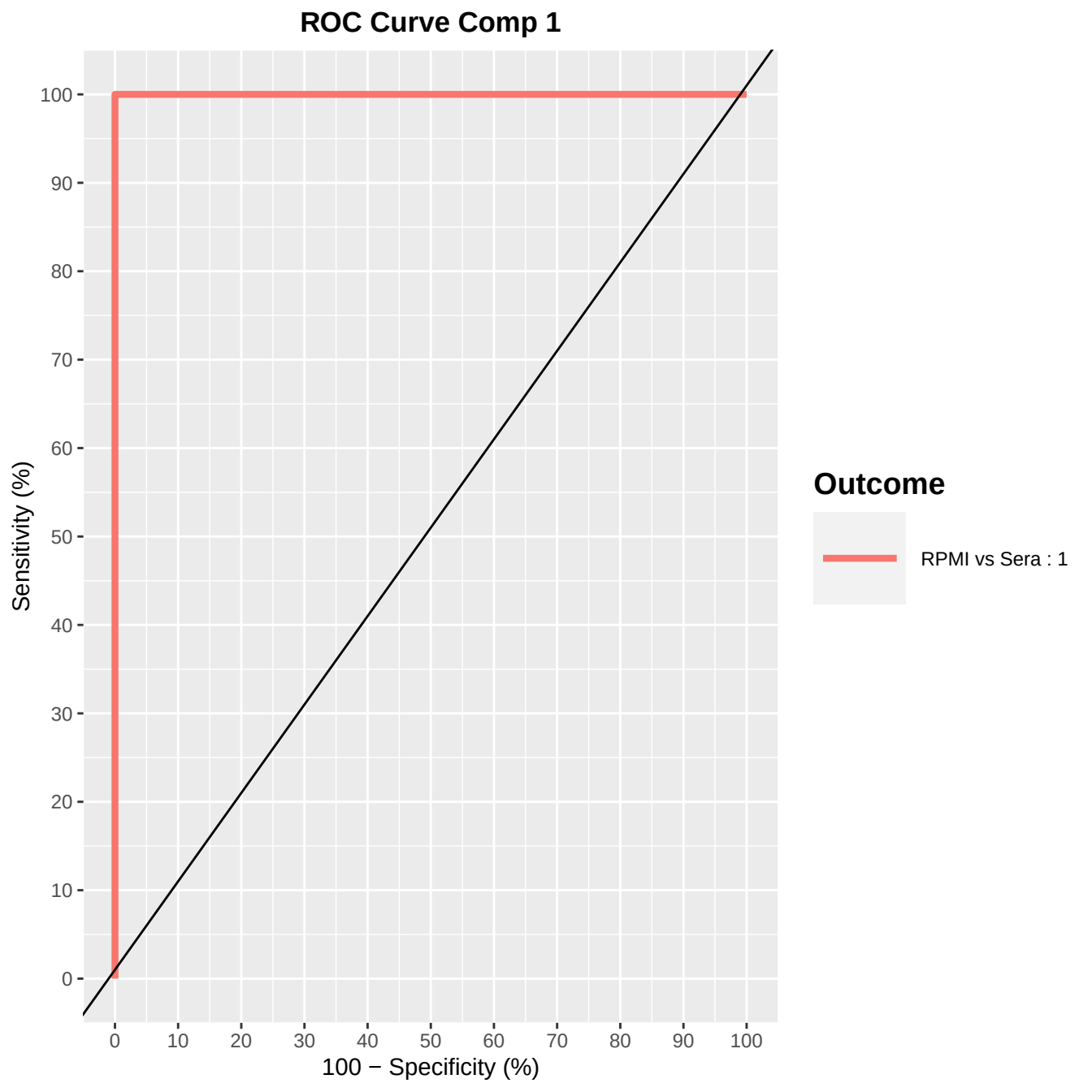

RNA_Seq Correlation between imputed and unimputed data
PC10
PC9
PC8
PC7
PC6
PC5
PC4
PC3
PC2
PC1
Var2
PC1
PC2
PC3
PC4
PC5
PC6
PC7
PC8
PC9
PC10
Var1
Pearson Correlation
1.0
0.5
0.0
−0.5
−1.0

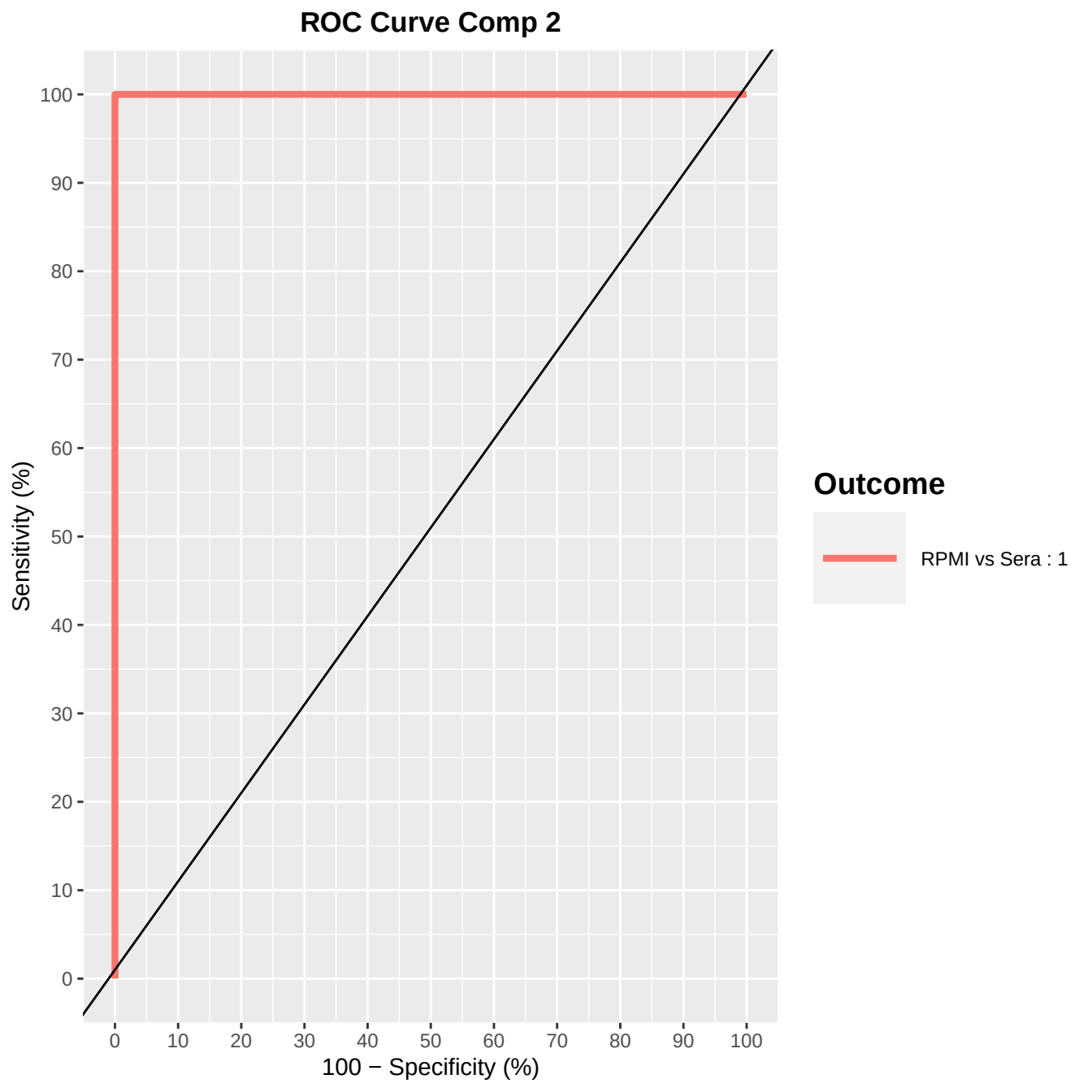

Feature variances (log2) per omics
Feature variance (log2)
5
0
−5
−10
Metabolomics
Proteomics
RNA_Seq
Omics

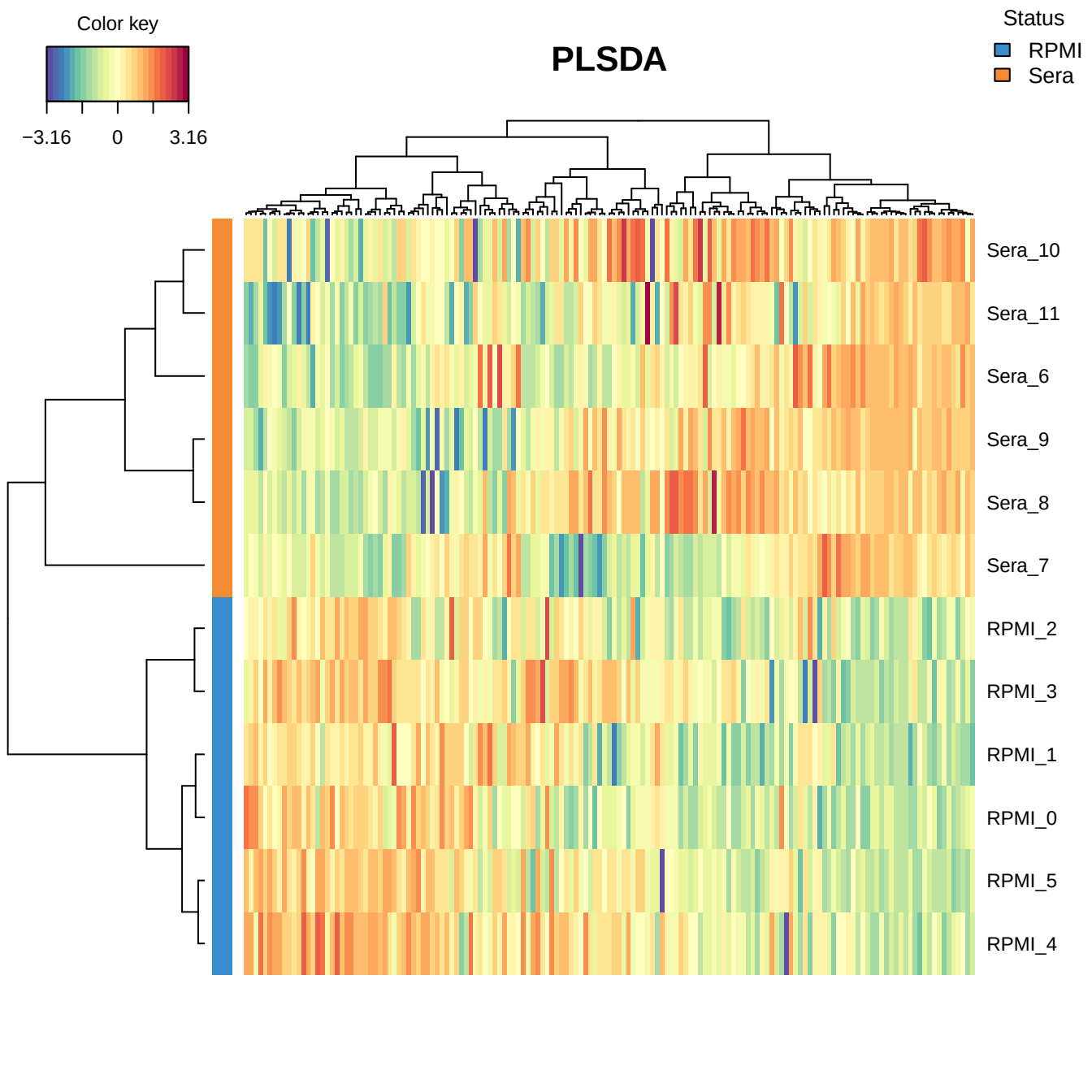

Metabolomics PLSDA single 1/2
10
5
0
−5
−10
X−variate 2: 10% expl. var
−5
0
5
10
X−variate 1: 39% expl. var
Legend
RPMI
Sera

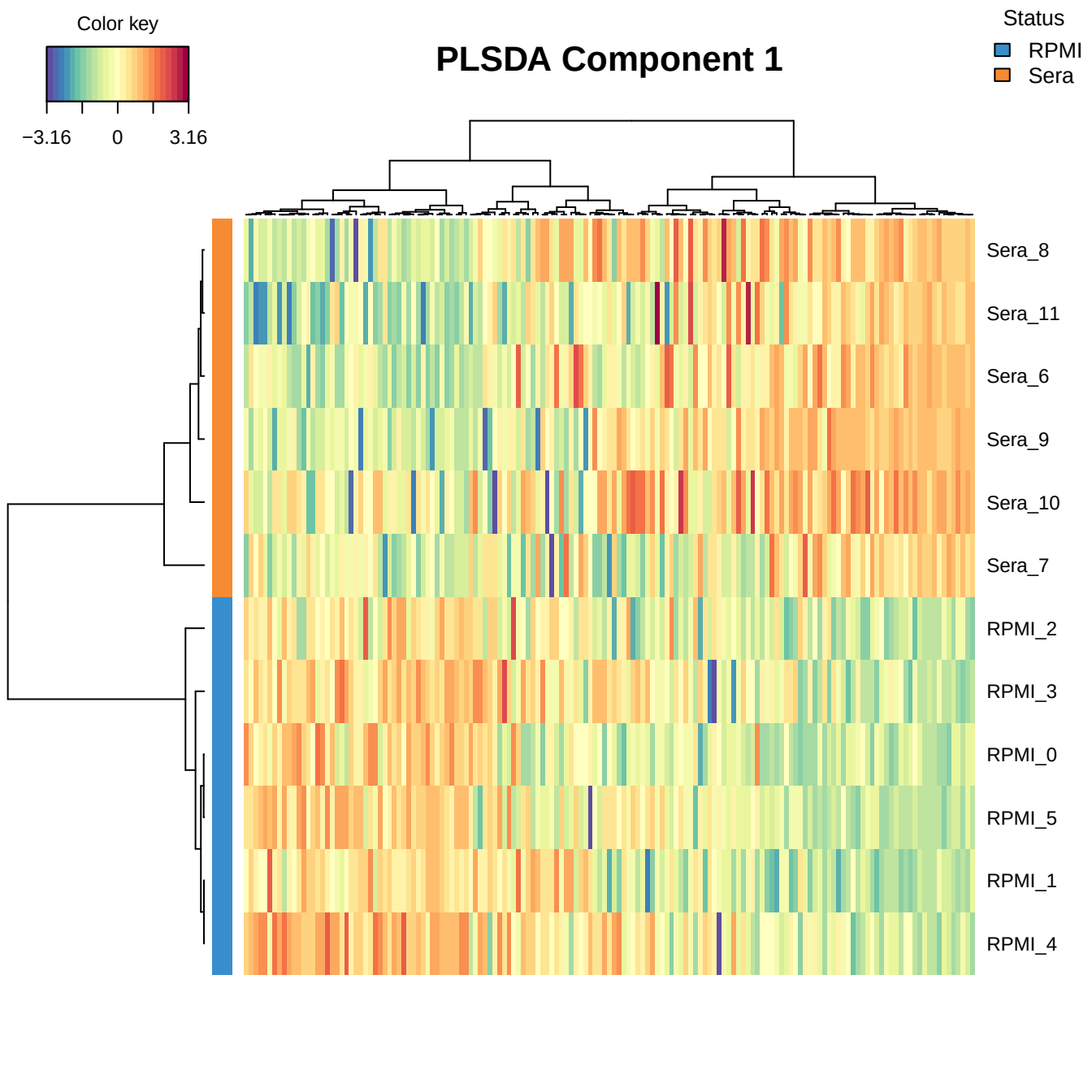

Metabolomics PLSDA single 1/2
10
5
0
−5
−10
X−variate 2: 10% expl. var
−5
0
5
10
X−variate 1: 39% expl. var
Legend
RPMI
Sera


max.dist
centroids.dist
mahalanobis.dist
overall
BER
Classification error rate
1.0
0.5
0.0
−0.5
−1.0
1
2
Component

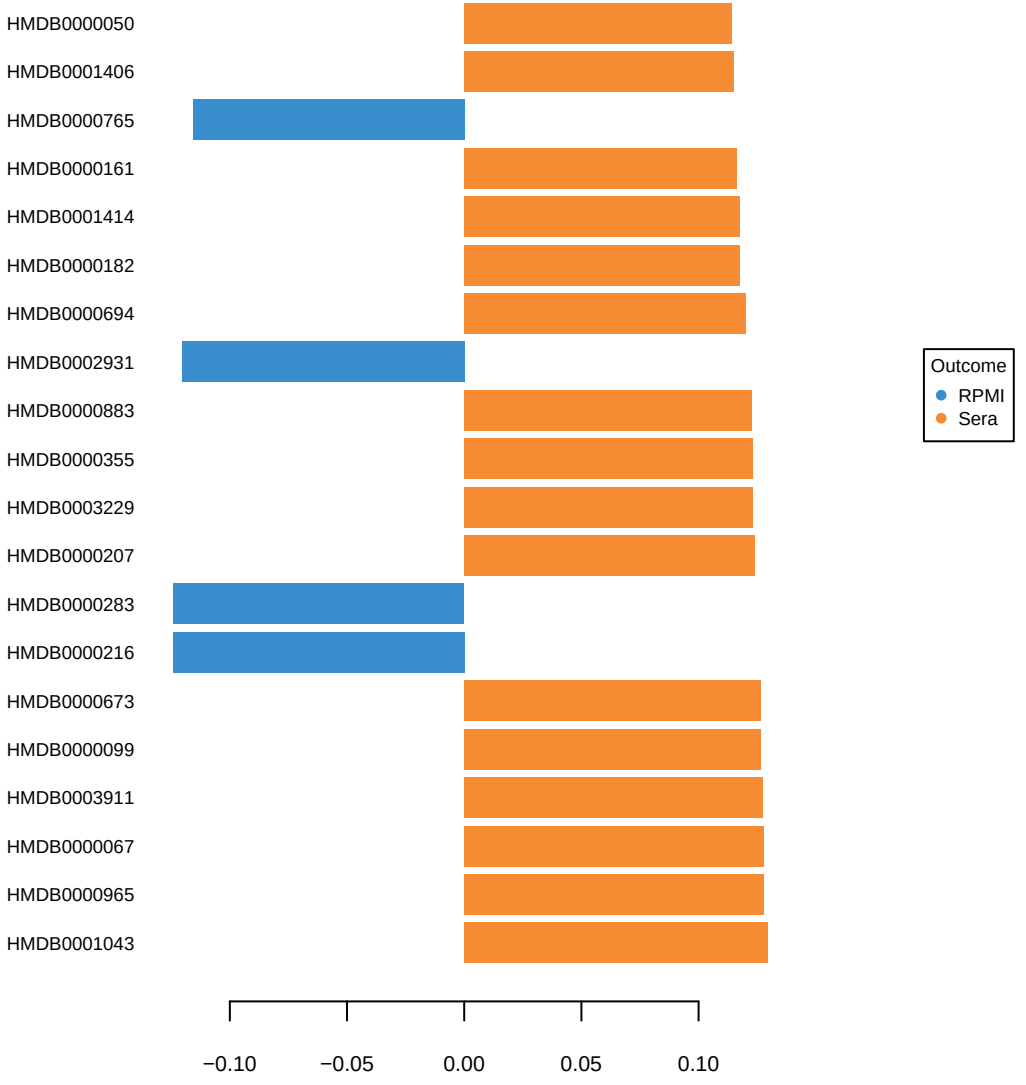

ROC Curve Comp 1
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1


ROC Curve Comp 2
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1

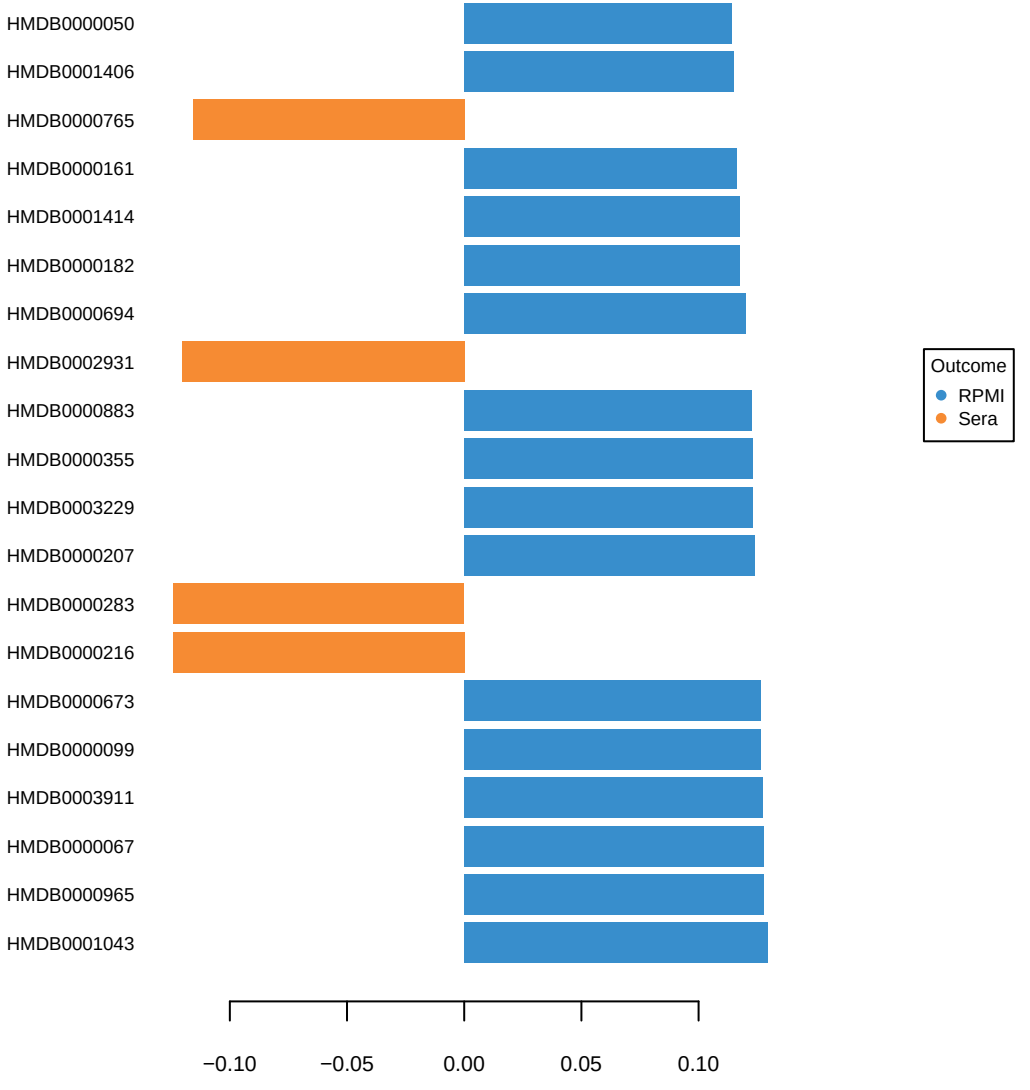

Color key
−3.16
0
3.16
PLSDA
Status
RPMI
Sera
Sera_10
Sera_11
Sera_6
Sera_9
Sera_8
Sera_7
RPMI_2
RPMI_3
RPMI_1
RPMI_0
RPMI_5
RPMI_4

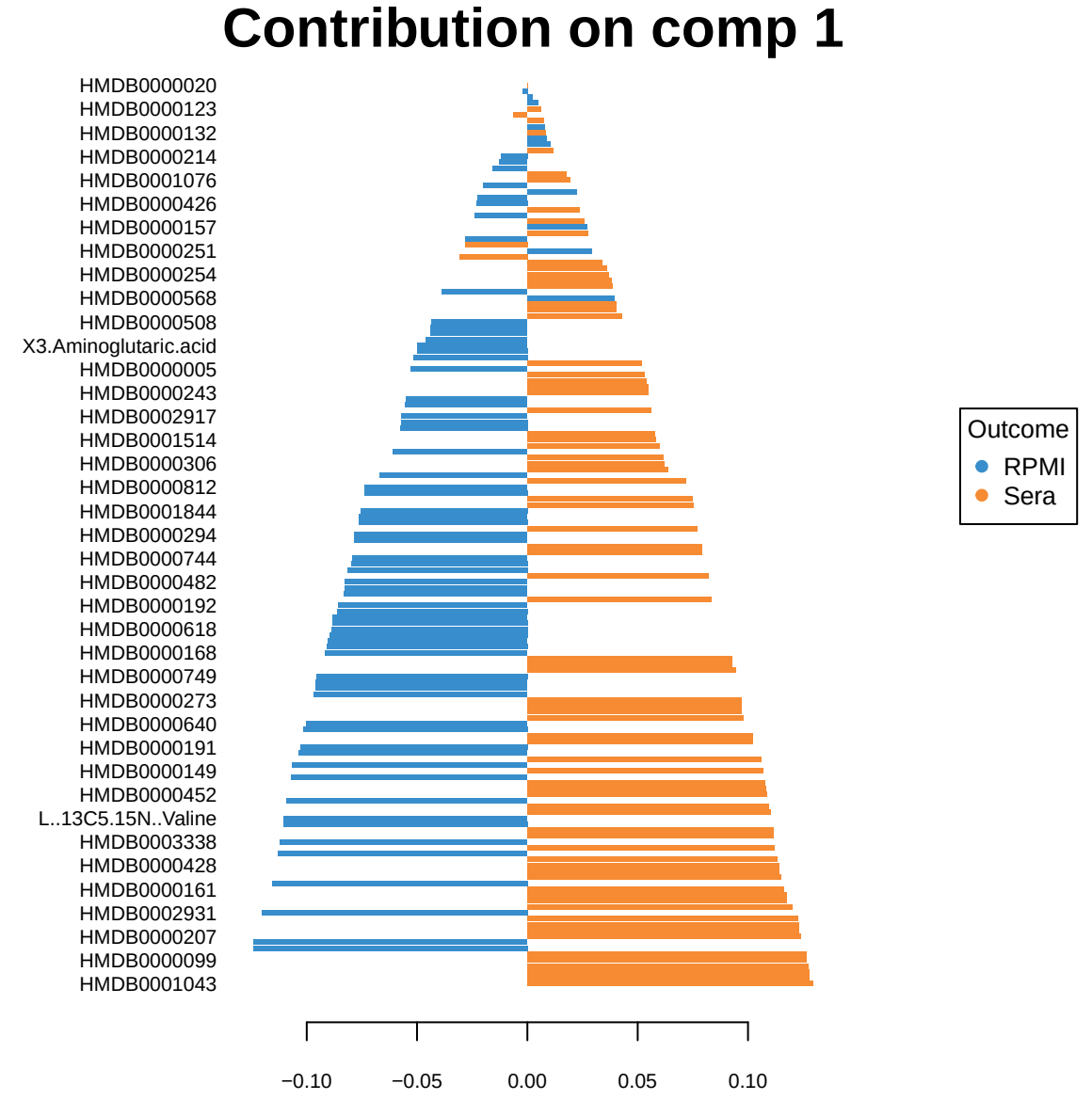

Color key
−3.16
0
3.16
PLSDA Component 1
Status
RPMI
Sera
Sera_8
Sera_11
Sera_6
Sera_9
Sera_10
Sera_7
RPMI_2
RPMI_3
RPMI_0
RPMI_5
RPMI_1
RPMI_4

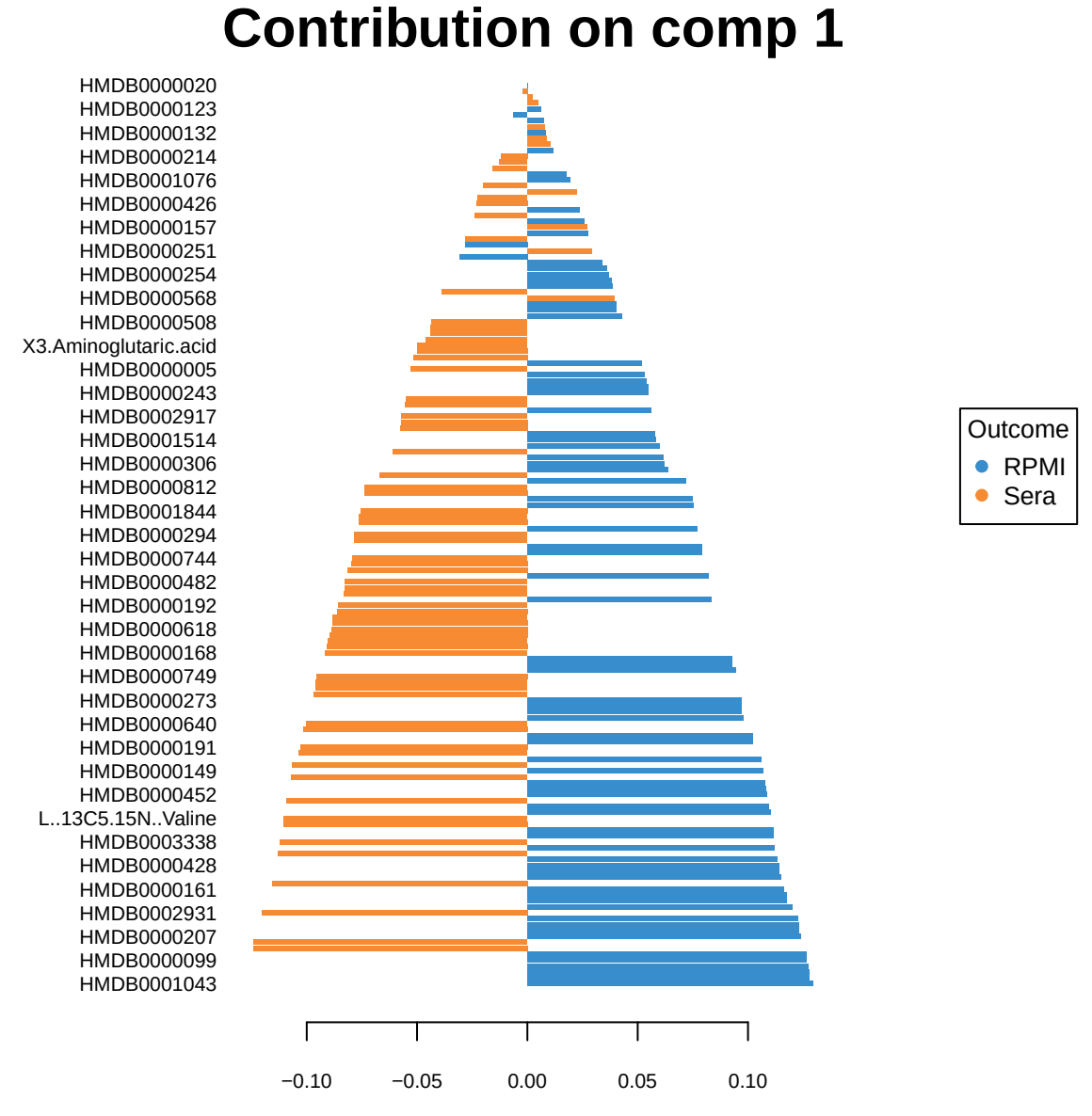
Metabolomics 1 PLSDA max loa

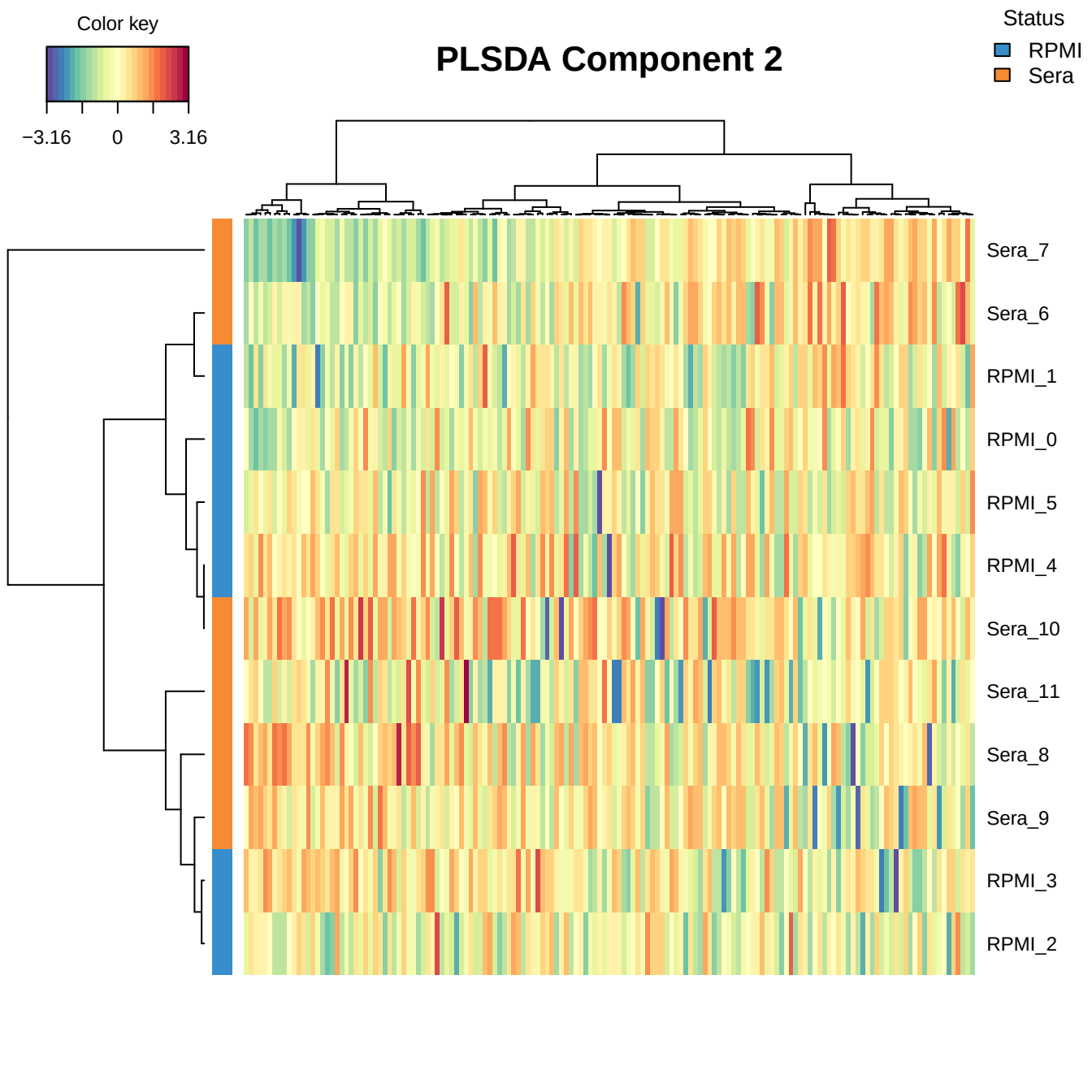


Metabolomics 1 PLSDA min loac

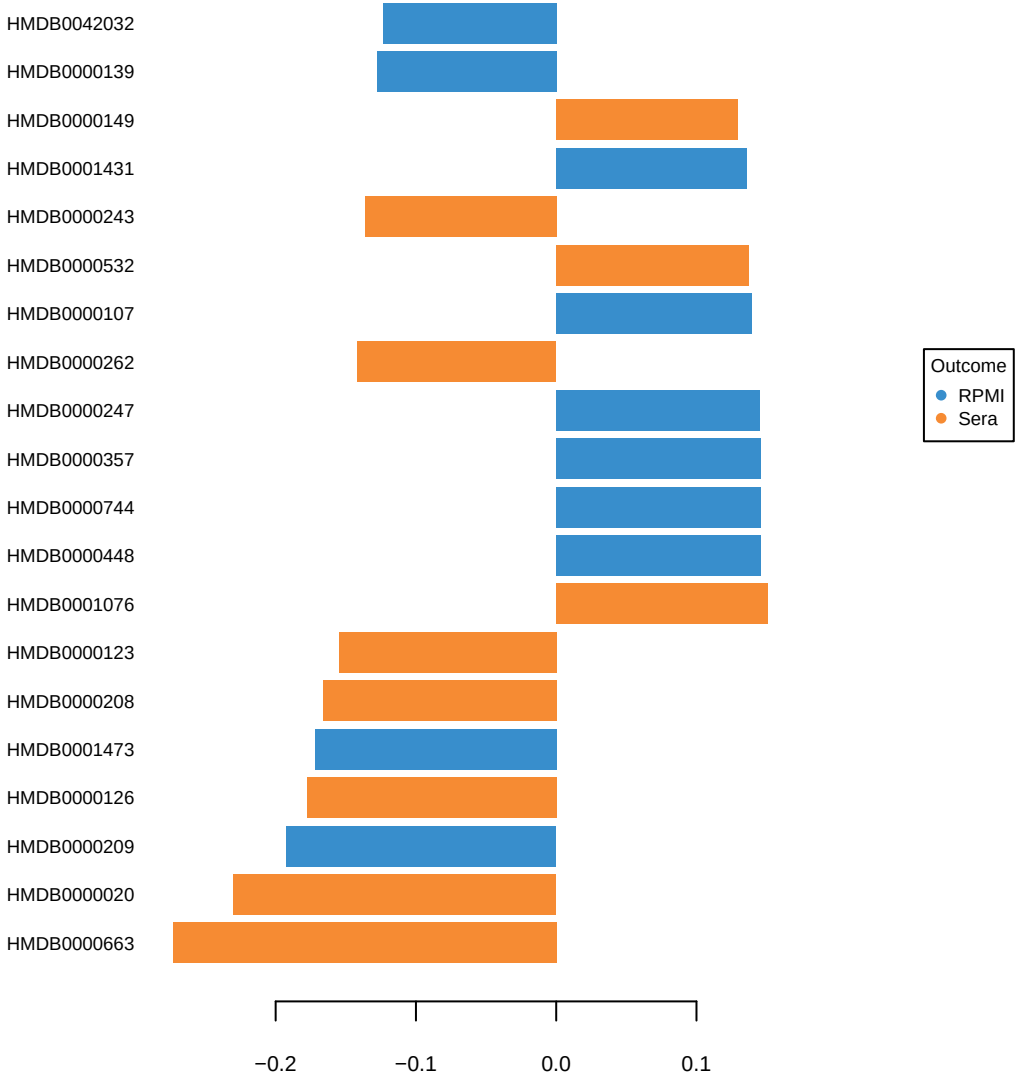



Contribution on comp 1
HMDB0000020
HMDB0000123
HMDB0000132
HMDB0000214
HMDB0001076
HMDB0000426
HMDB0000157
HMDB0000251
HMDB0000254
HMDB0000568
HMDB0000508
X3.Aminoglutaric.acid
HMDB0000005
HMDB0000243
HMDB0002917
HMDB0001514
HMDB0000306
HMDB0000812
HMDB0001844
HMDB0000294
HMDB0000744
HMDB0000482
HMDB0000192
HMDB0000618
HMDB0000168
HMDB0000749
HMDB0000273
HMDB0000640
HMDB0000191
HMDB0000149
HMDB0000452
L..13C5.15N..Valine
HMDB0003338
HMDB0000428
HMDB0000161
HMDB0002931
HMDB0000207
HMDB0000099
HMDB0001043
−0.10
−0.05
0.00
0.05
0.10
Outcome
RPMI
Sera

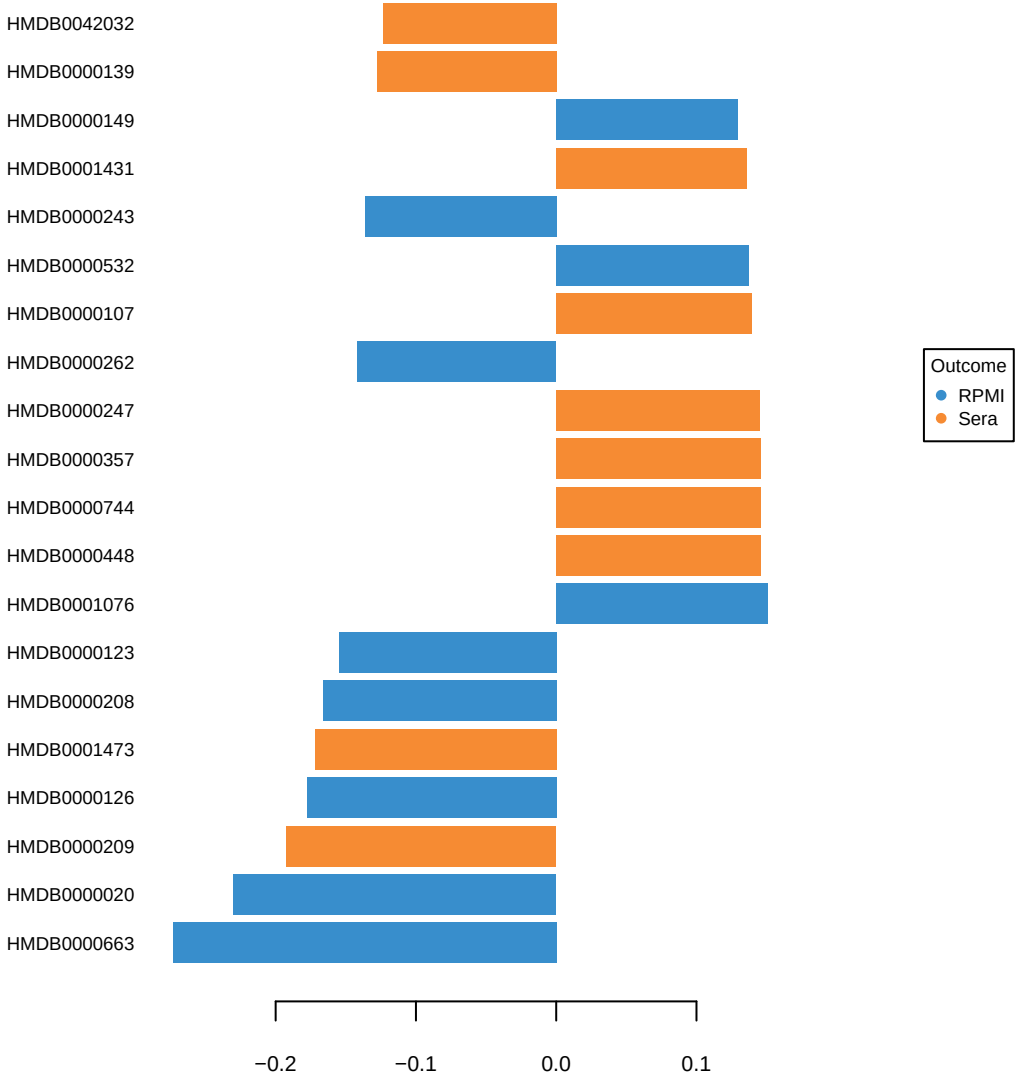

Contribution on comp 1
HMDB0000020
HMDB0000123
HMDB0000132
HMDB0000214
HMDB0001076
HMDB0000426
HMDB0000157
HMDB0000251
HMDB0000254
HMDB0000568
HMDB0000508
X3.Aminoglutaric.acid
HMDB0000005
HMDB0000243
HMDB0002917
HMDB0001514
HMDB0000306
HMDB0000812
HMDB0001844
HMDB0000294
HMDB0000744
HMDB0000482
HMDB0000192
HMDB0000618
HMDB0000168
HMDB0000749
HMDB0000273
HMDB0000640
HMDB0000191
HMDB0000149
HMDB0000452
L..13C5.15N..Valine
HMDB0003338
HMDB0000428
HMDB0000161
HMDB0002931
HMDB0000207
HMDB0000099
HMDB0001043
−0.10
−0.05
0.00
0.05
0.10
Outcome
RPMI
Sera

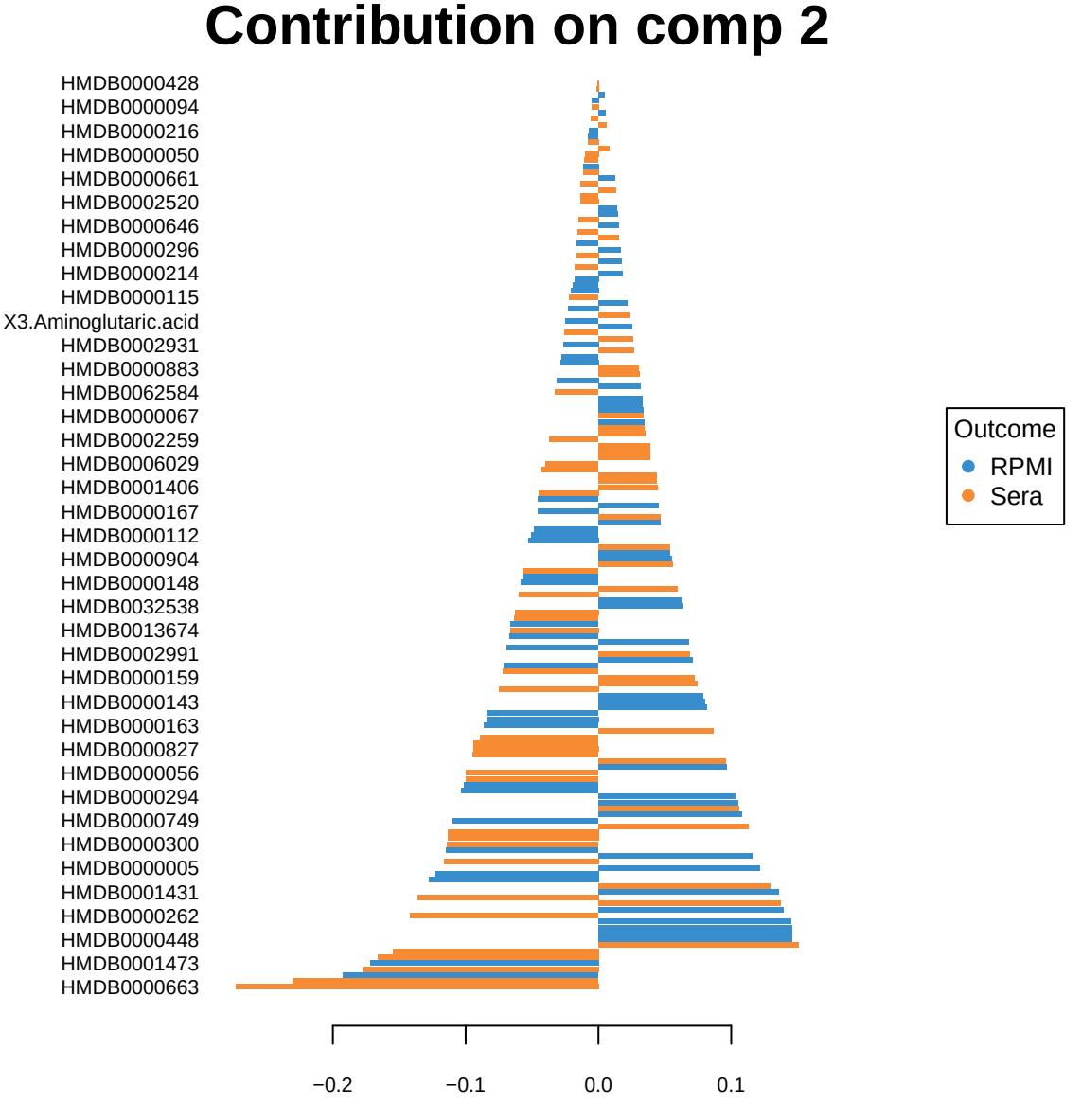

Color key
−3.16
0
3.16
PLSDA Component 2
Status
RPMI
Sera
Sera_7
Sera_6
RPMI_1
RPMI_0
RPMI_5
RPMI_4
Sera_10
Sera_11
Sera_8
Sera_9
RPMI_3
RPMI_2

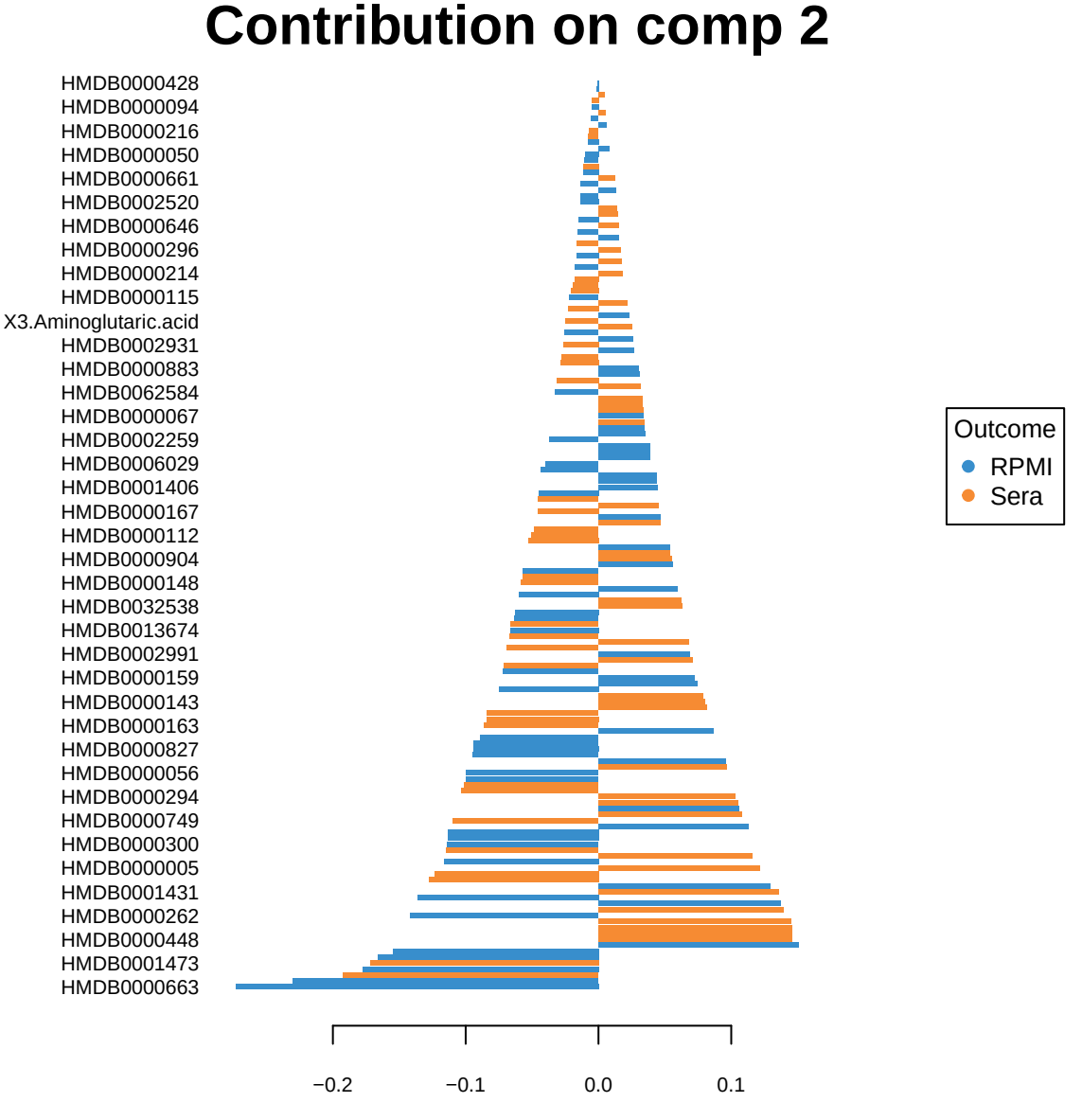
Metabolomics 2 PLSDA max loa

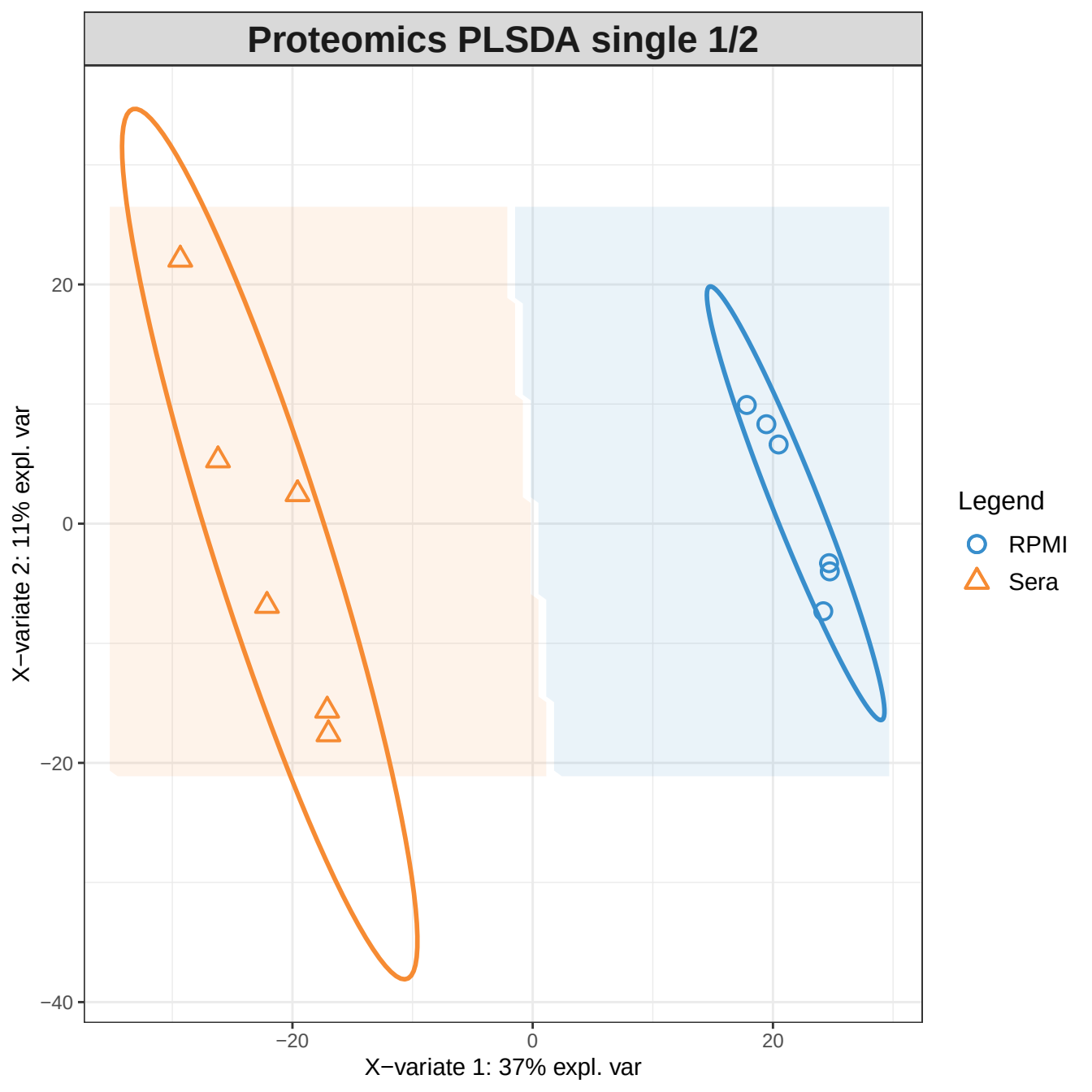


Metabolomics 2 PLSDA min loac

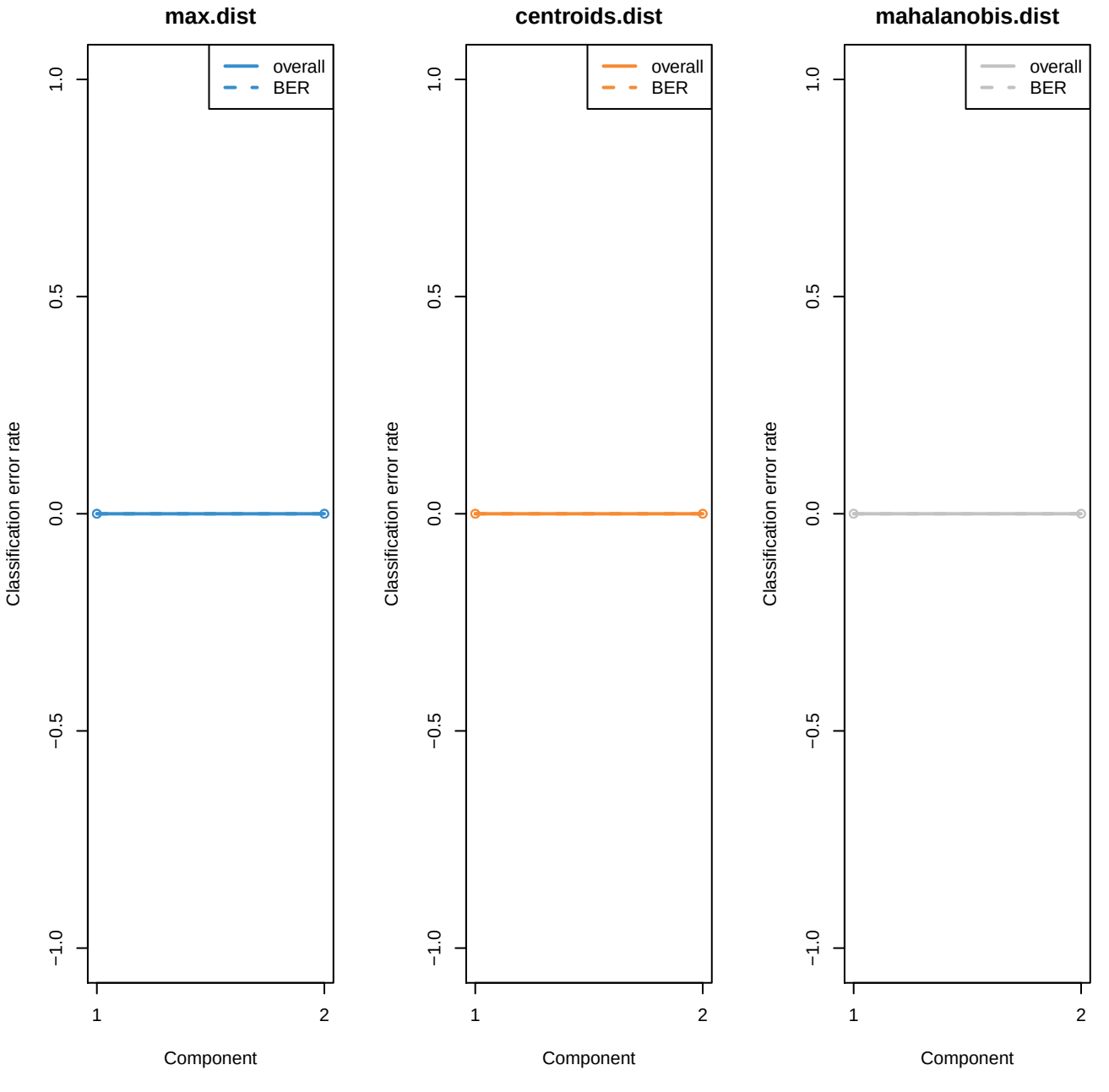


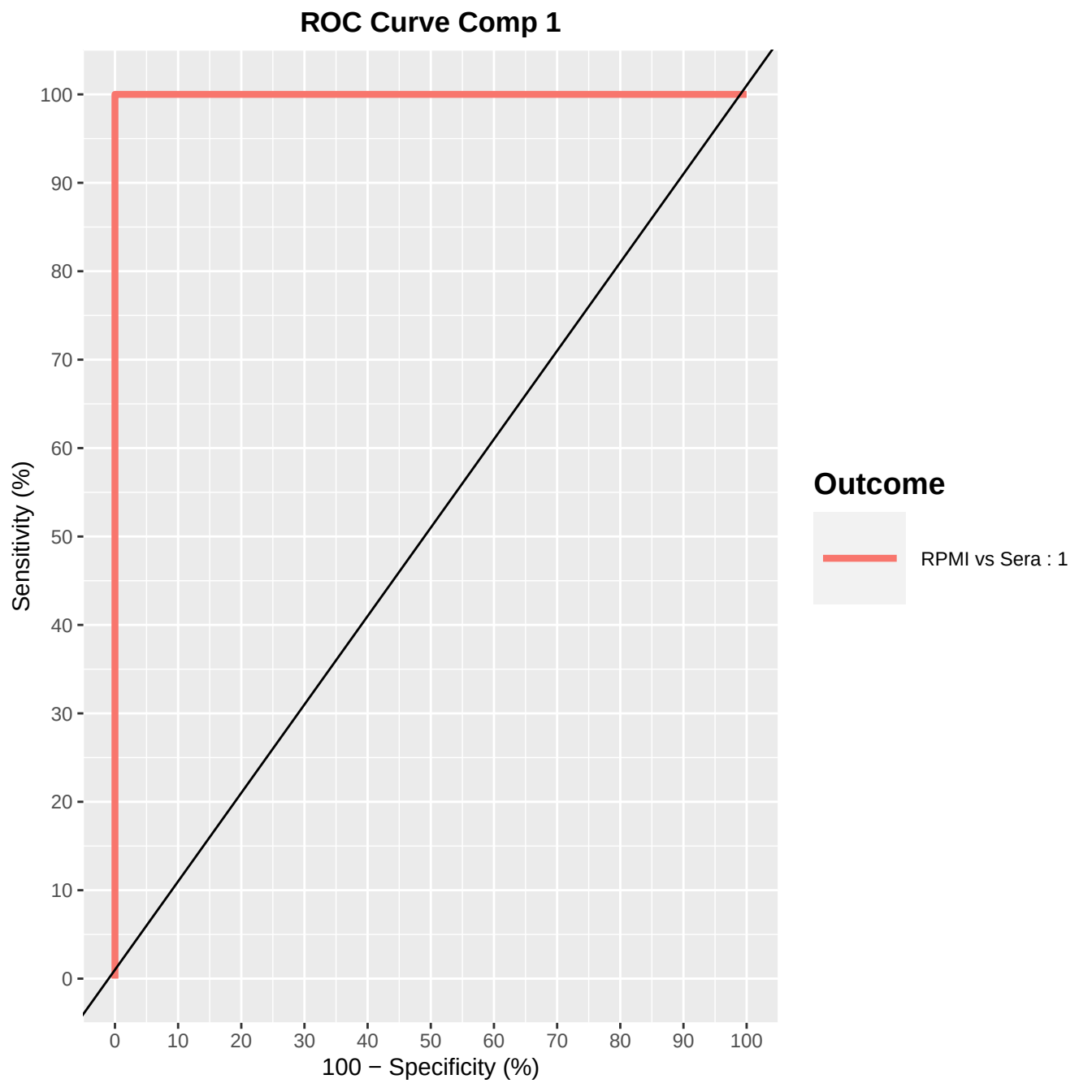

Contribution on comp 2
HMDB0000428
HMDB0000094
HMDB0000216
HMDB0000050
HMDB0000661
HMDB0002520
HMDB0000646
HMDB0000296
HMDB0000214
HMDB0000115
X3.Aminoglutaric.acid
HMDB0002931
HMDB0000883
HMDB0062584
HMDB0000067
HMDB0002259
HMDB0006029
HMDB0001406
HMDB0000167
HMDB0000112
HMDB0000904
HMDB0000148
HMDB0032538
HMDB0013674
HMDB0002991
HMDB0000159
HMDB0000143
HMDB0000163
HMDB0000827
HMDB0000056
HMDB0000294
HMDB0000749
HMDB0000300
HMDB0000005
HMDB0001431
HMDB0000262
HMDB0000448
HMDB0001473
HMDB0000663
−0.2
−0.1
0.0
0.1
Outcome
RPMI
Sera

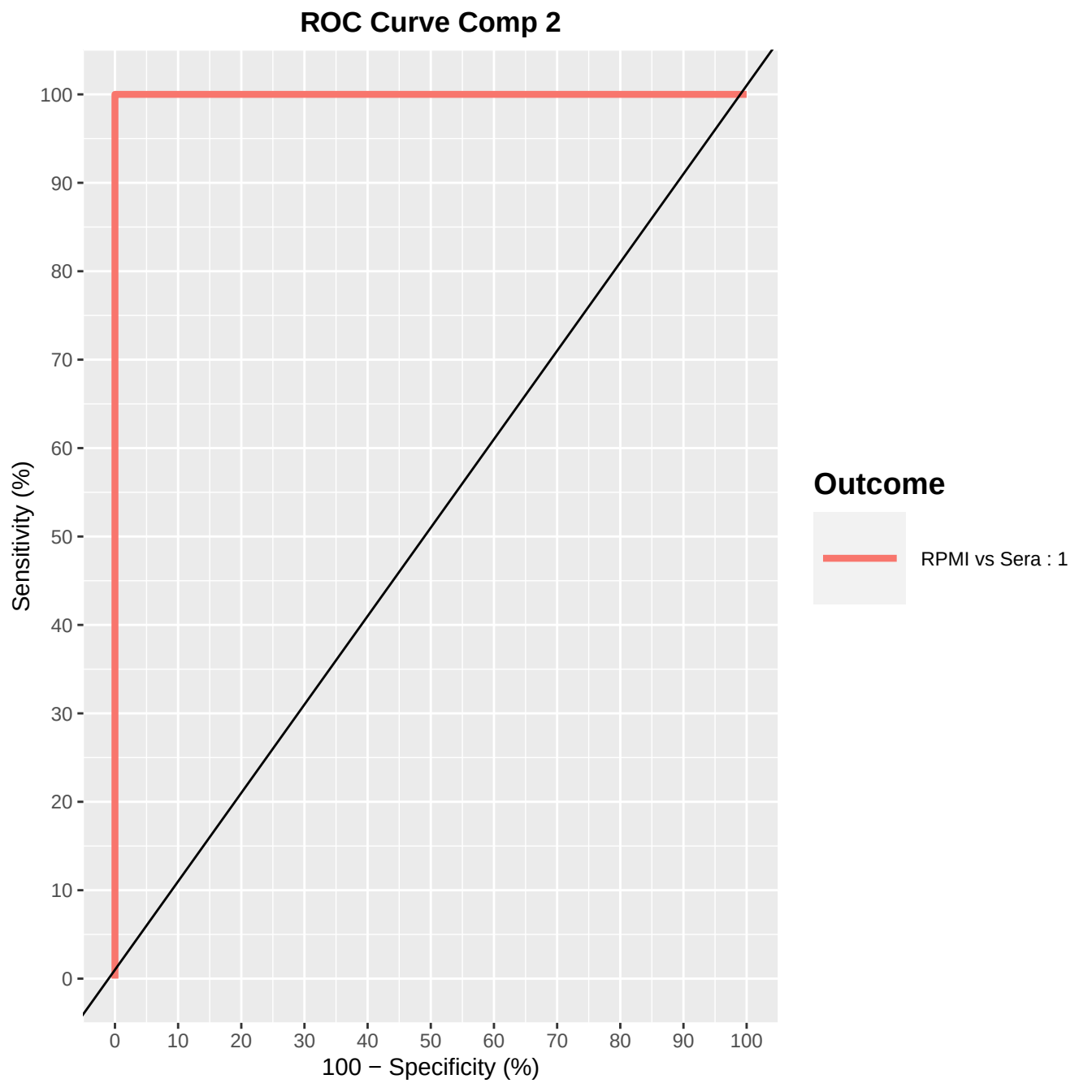

Contribution on comp 2
HMDB0000428
HMDB0000094
HMDB0000216
HMDB0000050
HMDB0000661
HMDB0002520
HMDB0000646
HMDB0000296
HMDB0000214
HMDB0000115
X3.Aminoglutaric.acid
HMDB0002931
HMDB0000883
HMDB0062584
HMDB0000067
HMDB0002259
HMDB0006029
HMDB0001406
HMDB0000167
HMDB0000112
HMDB0000904
HMDB0000148
HMDB0032538
HMDB0013674
HMDB0002991
HMDB0000159
HMDB0000143
HMDB0000163
HMDB0000827
HMDB0000056
HMDB0000294
HMDB0000749
HMDB0000300
HMDB0000005
HMDB0001431
HMDB0000262
HMDB0000448
HMDB0001473
HMDB0000663
−0.2
−0.1
0.0
0.1
Outcome
RPMI
Sera

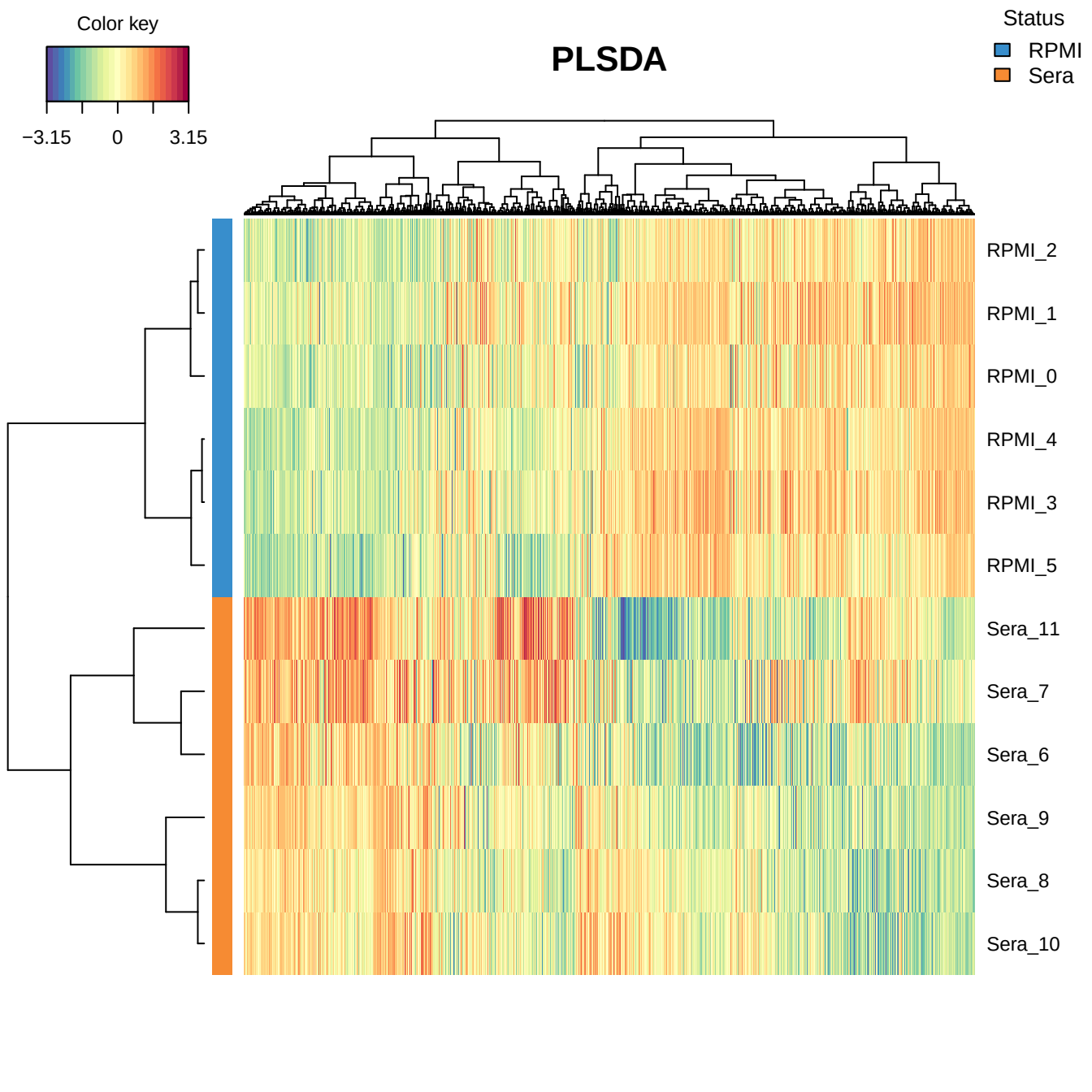

Proteomics PLSDA single 1/2
20
0
−20
−40
X−variate 2: 11% expl. var
−20
0
20
X−variate 1: 37% expl. var
Legend
RPMI
Sera

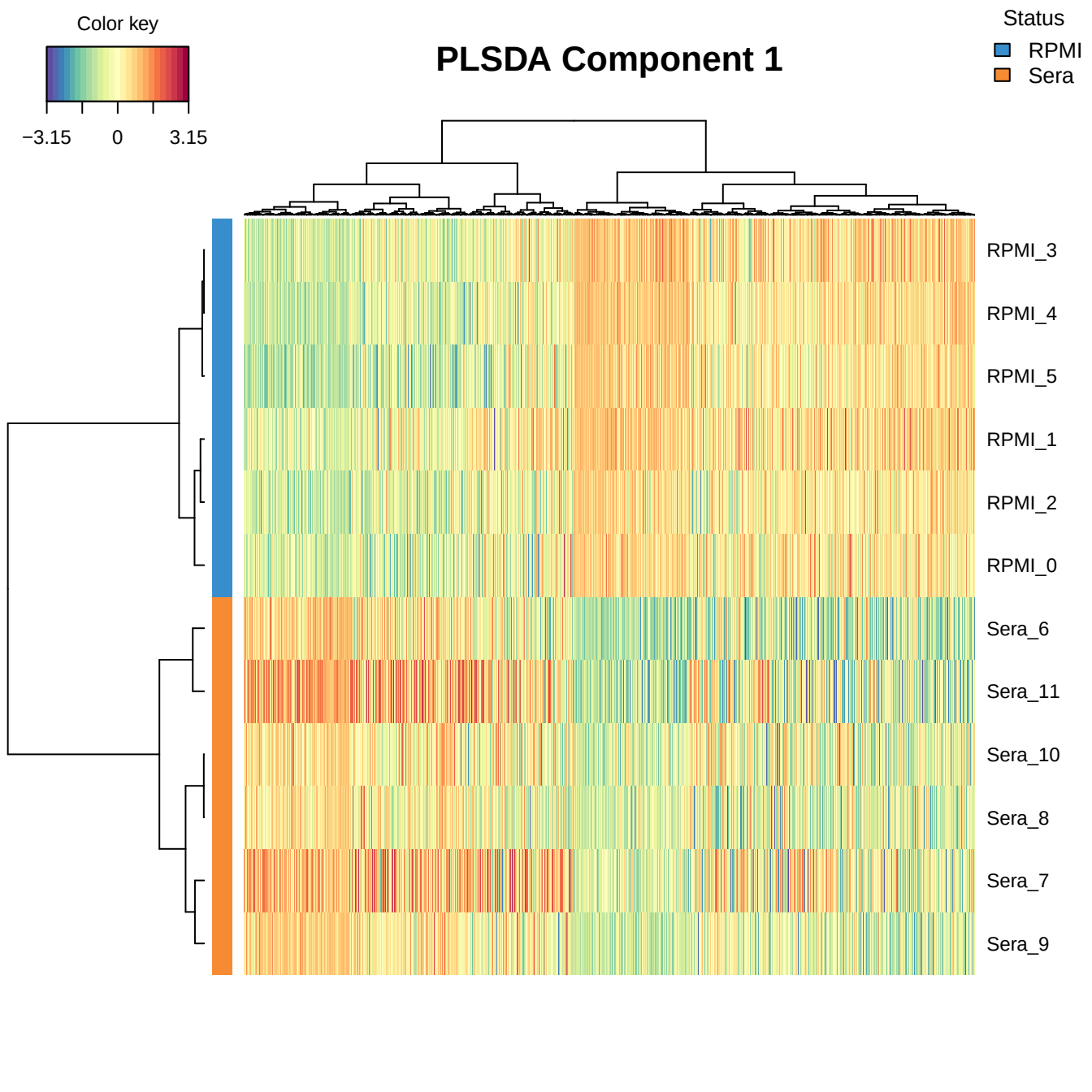
Proteomics PLSDA single 1/2
20
0
−20
−40
X−variate 2: 11% expl. var
−20
0
20
X−variate 1: 37% expl. var
Legend
RPMI
Sera


max.dist
centroids.dist
mahalanobis.dist
overall
BER
Classification error rate
1.0
0.5
0.0
−0.5
−1.0
1
2
Component

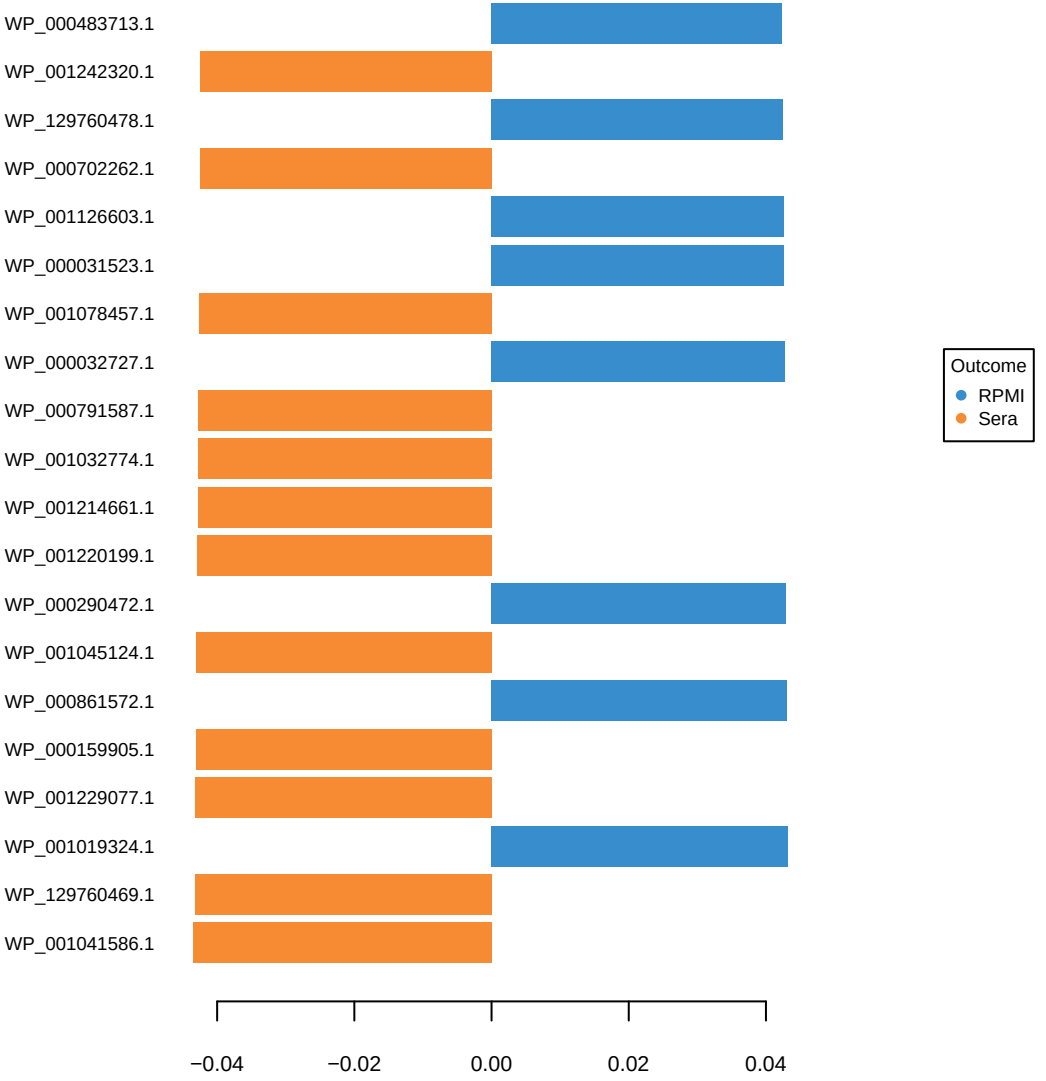

ROC Curve Comp 1
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1


ROC Curve Comp 2
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1

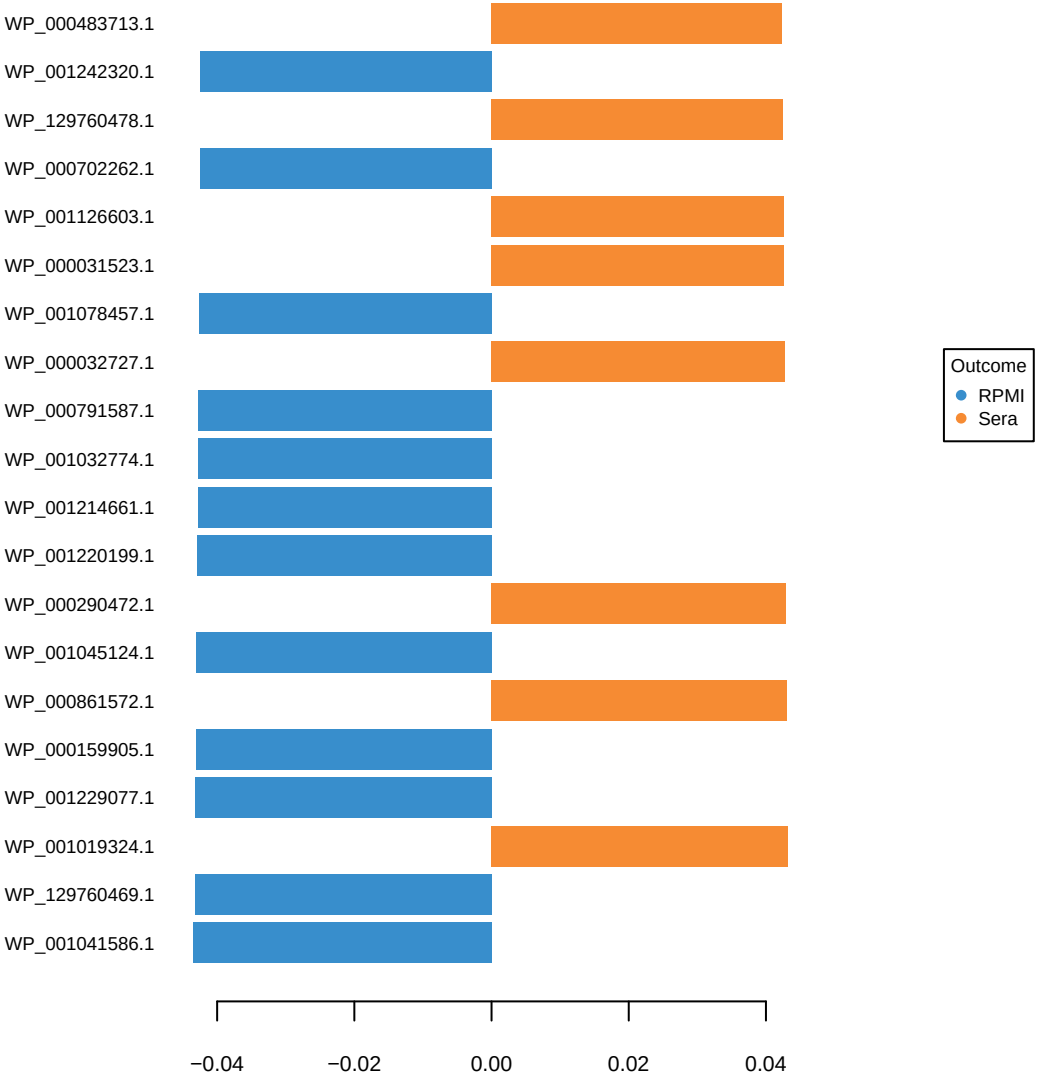

Color key
−3.15
0
3.15
PLSDA
Status
RPMI
Sera
RPMI_2
RPMI_1
RPMI_0
RPMI_4
RPMI_3
RPMI_5
Sera_11
Sera_7
Sera_6
Sera_9
Sera_8
Sera_10


Color key
−3.15
0
3.15
PLSDA Component 1
Status
RPMI
Sera
RPMI_3
RPMI_4
RPMI_5
RPMI_1
RPMI_2
RPMI_0
Sera_6
Sera_11
Sera_10
Sera_8
Sera_7
Sera_9

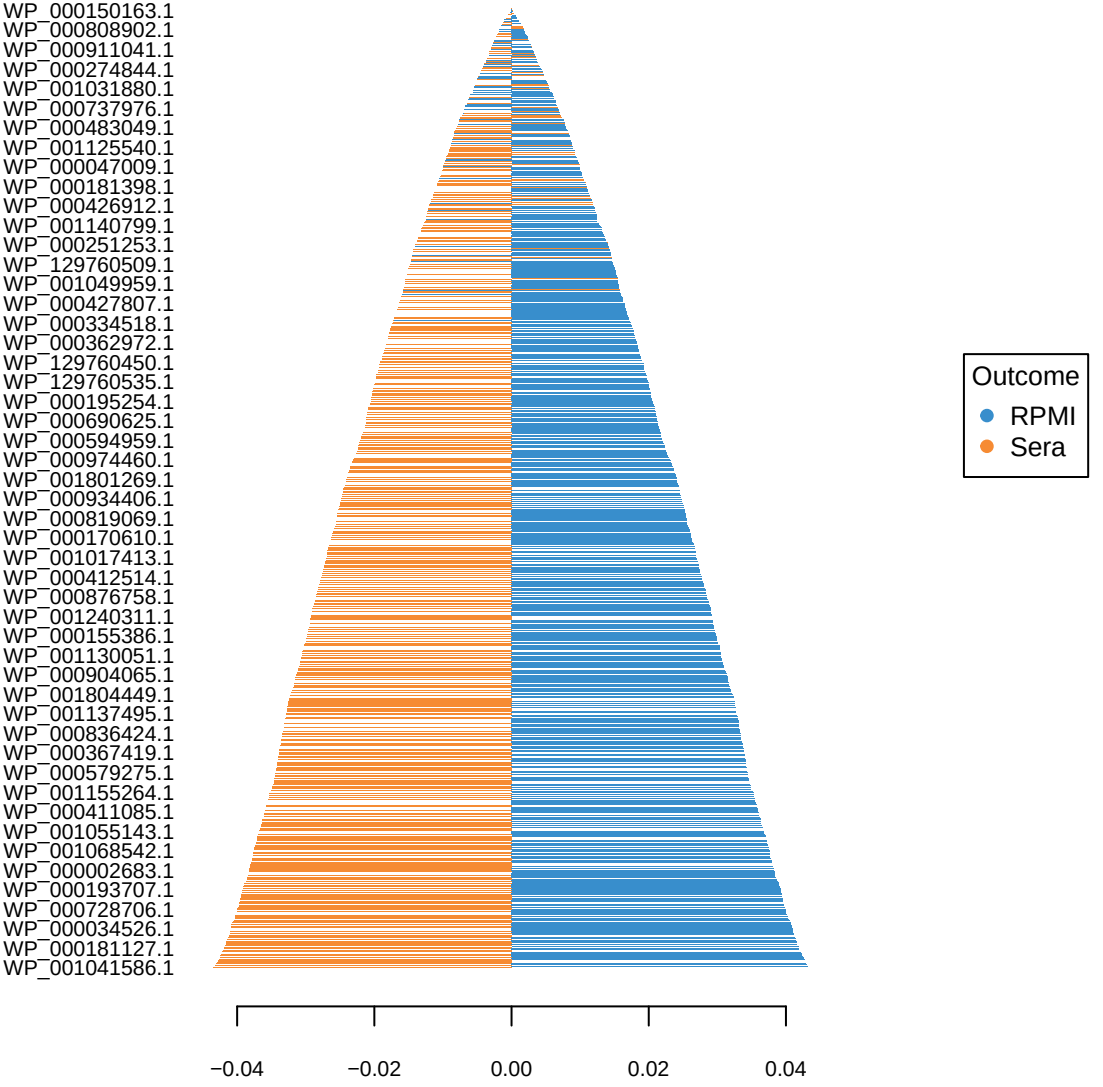
Proteomics 1 PLSDA max loadi



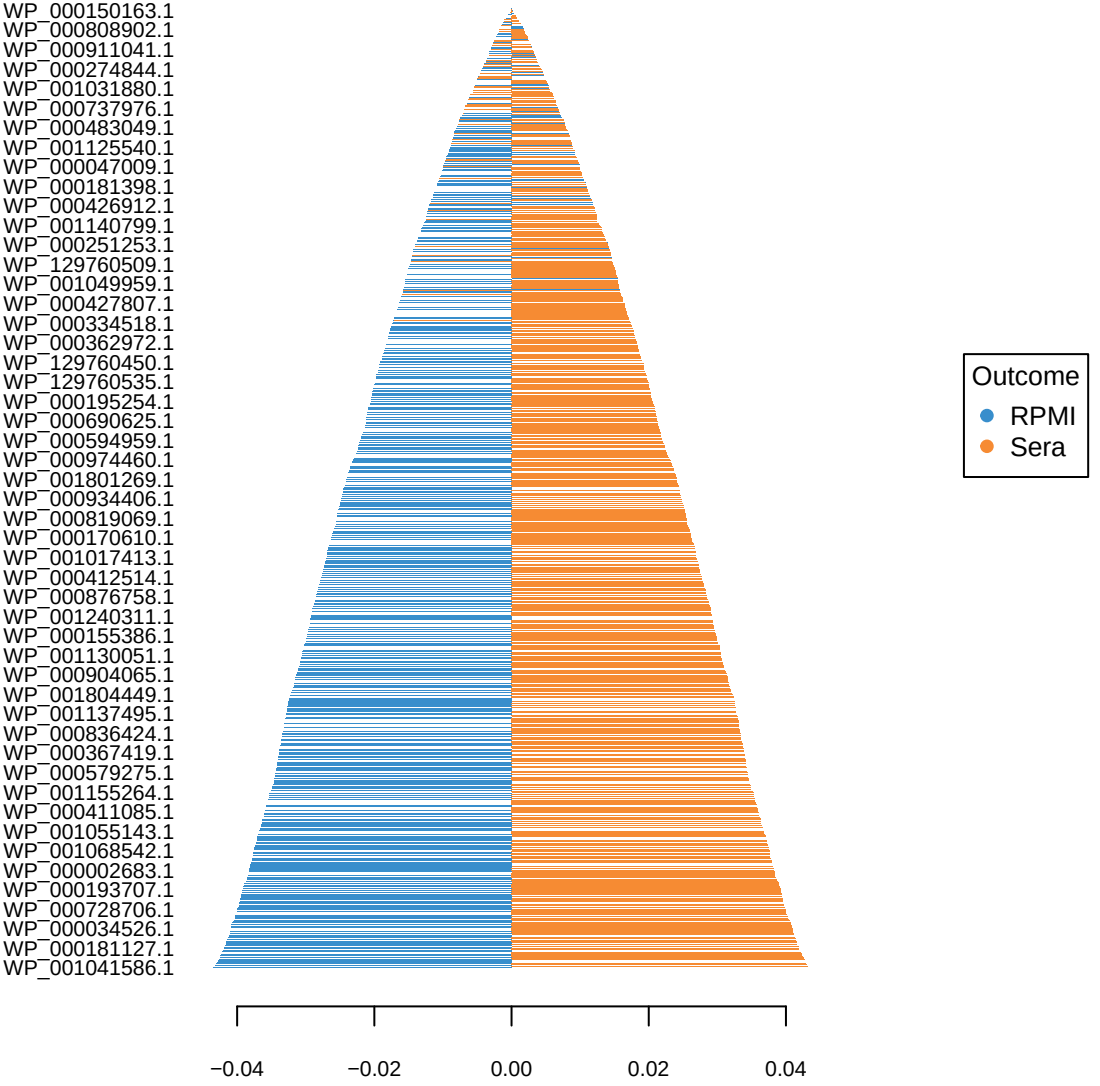
Proteomics 1 PLSDA min loadi

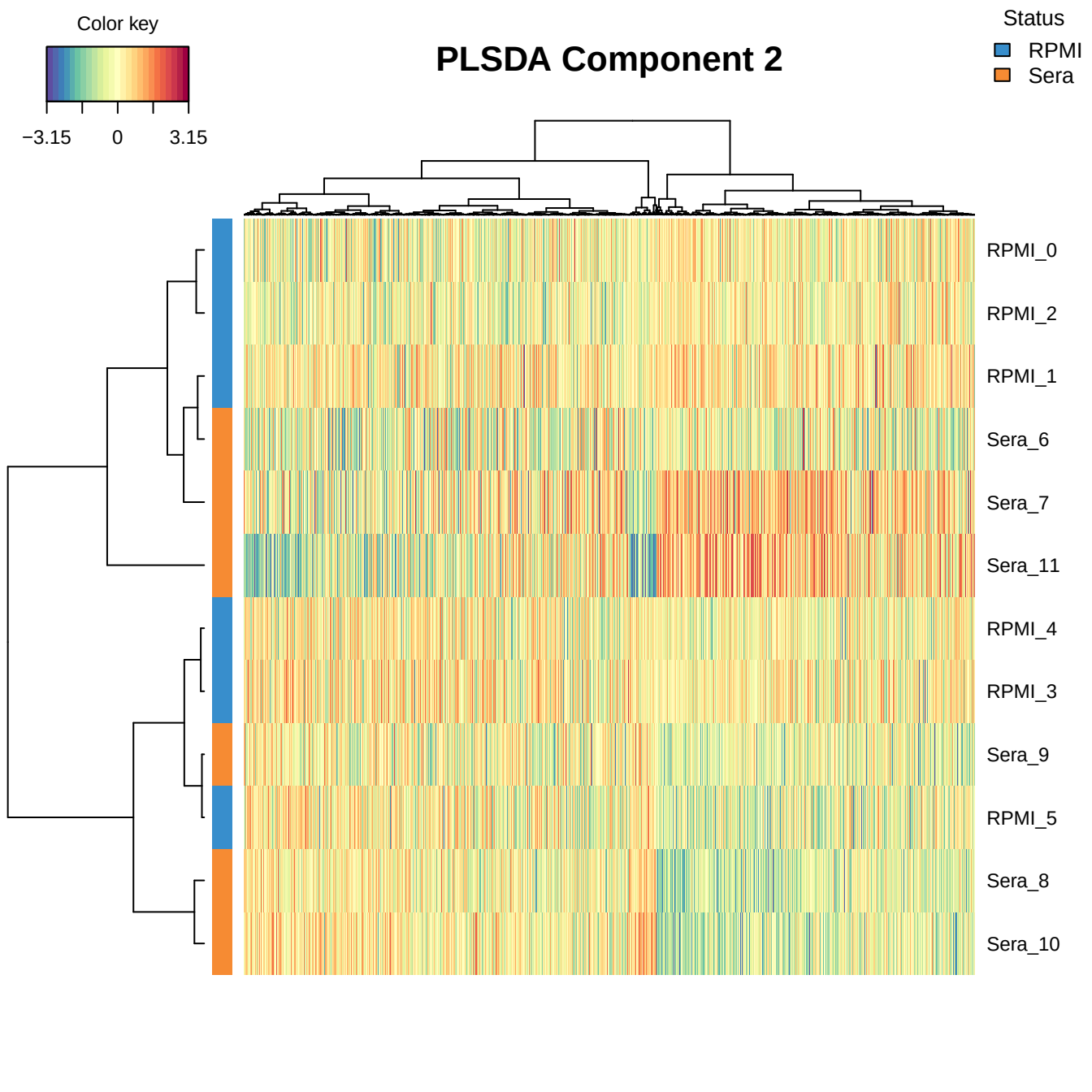


Contribution on comp 1

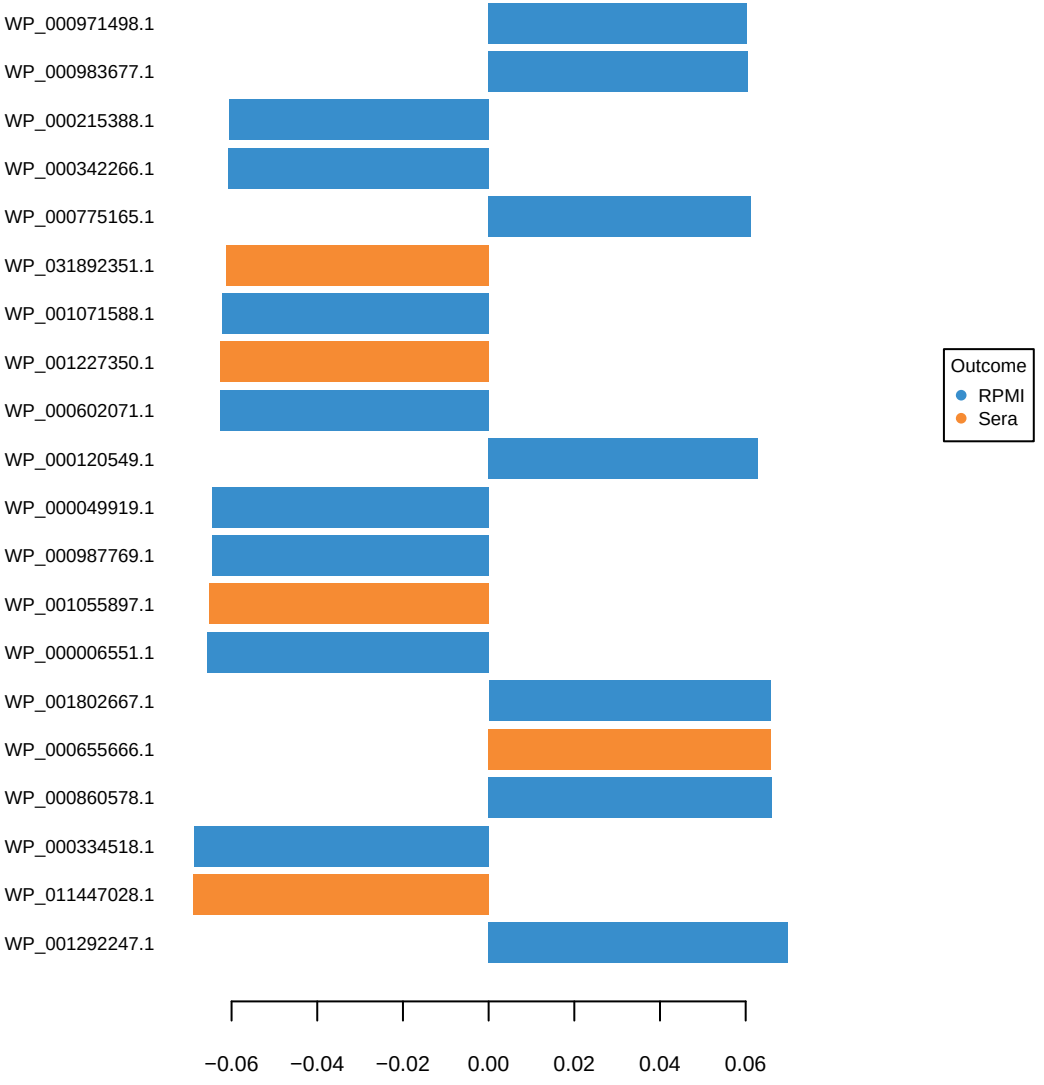


Contribution on comp 1

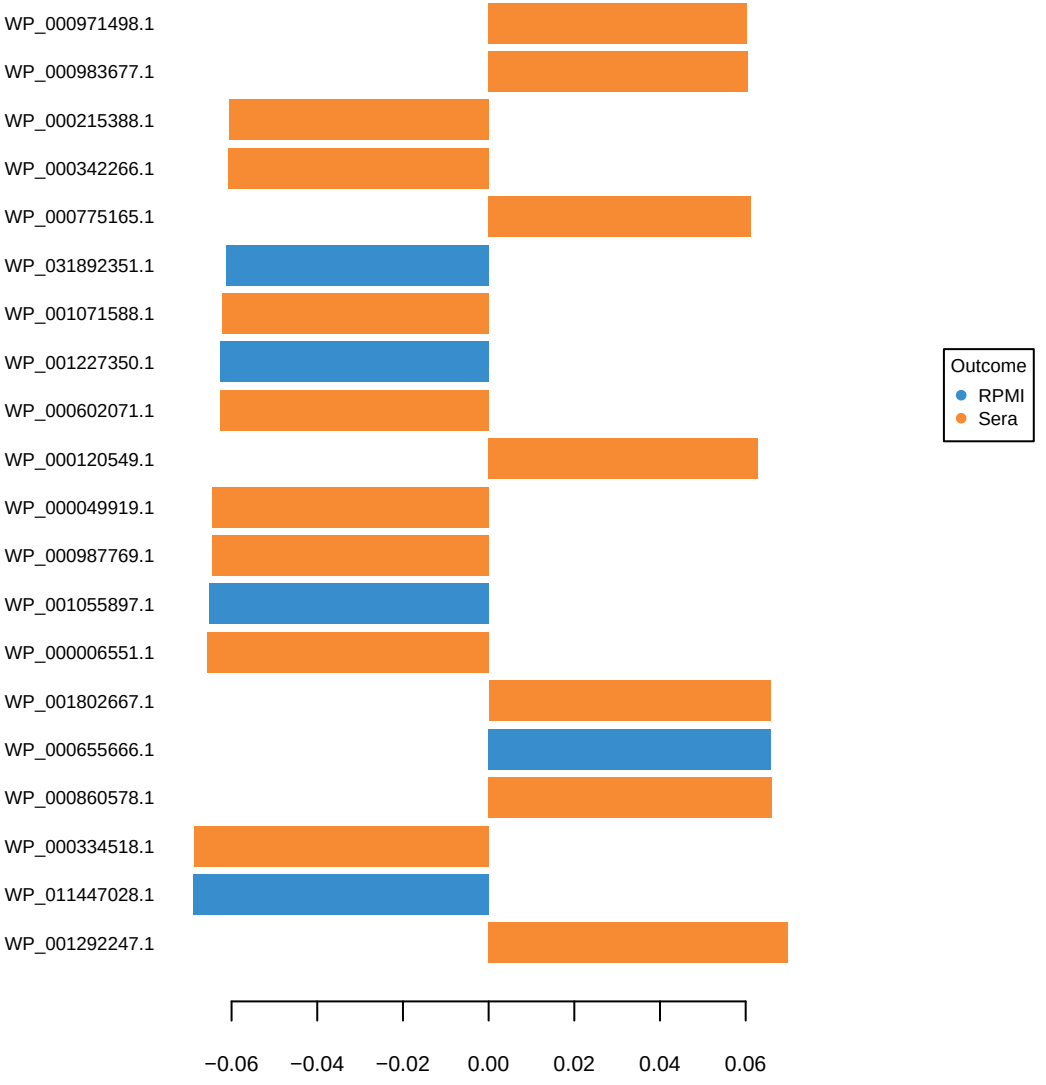



Color key
−3.15
0
3.15
PLSDA Component 2
Status
RPMI
Sera
RPMI_0
RPMI_2
RPMI_1
Sera_6
Sera_7
Sera_11
RPMI_4
RPMI_3
Sera_9
RPMI_5
Sera_8
Sera_10

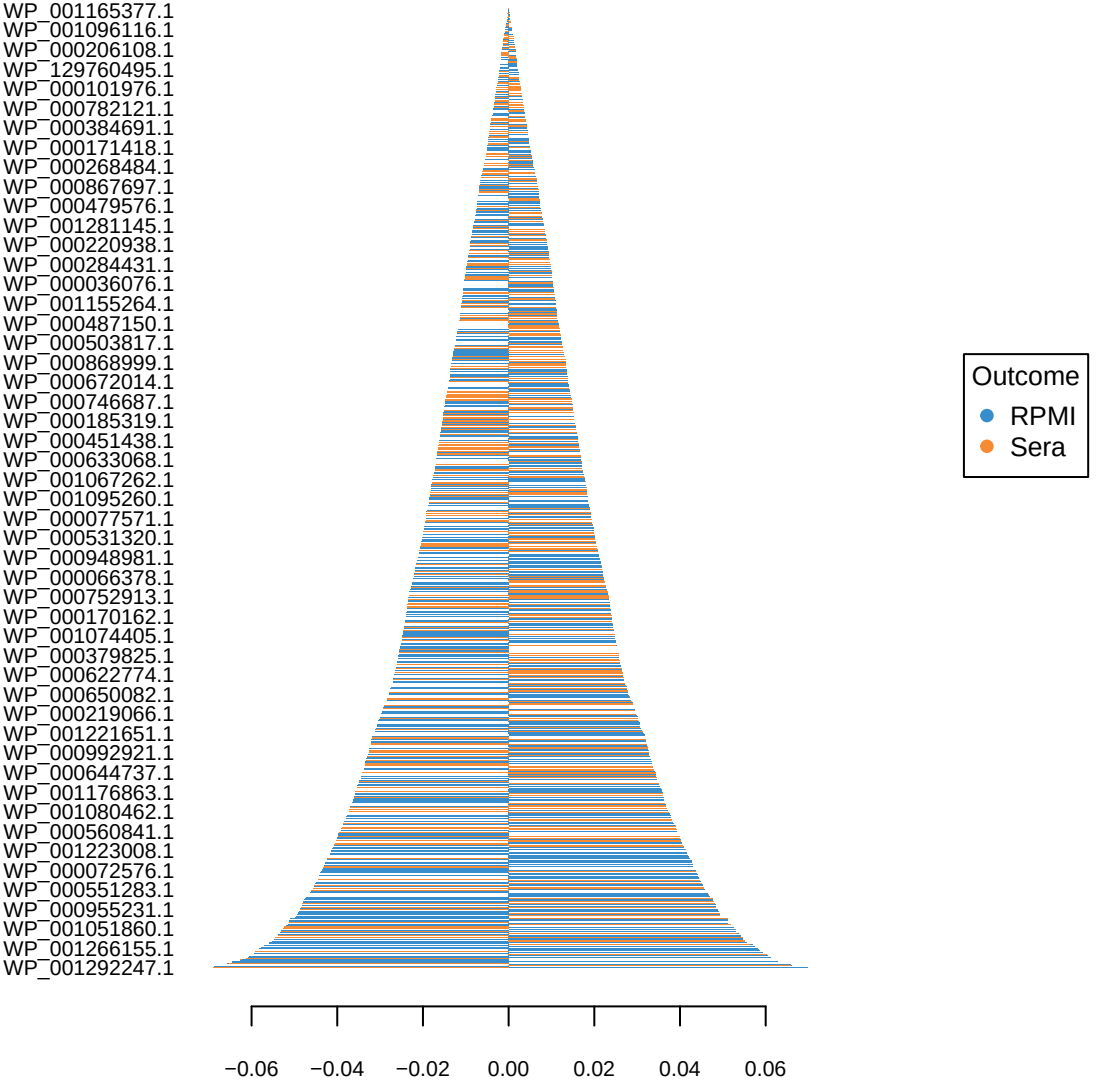
Proteomics 2 PLSDA max loadi



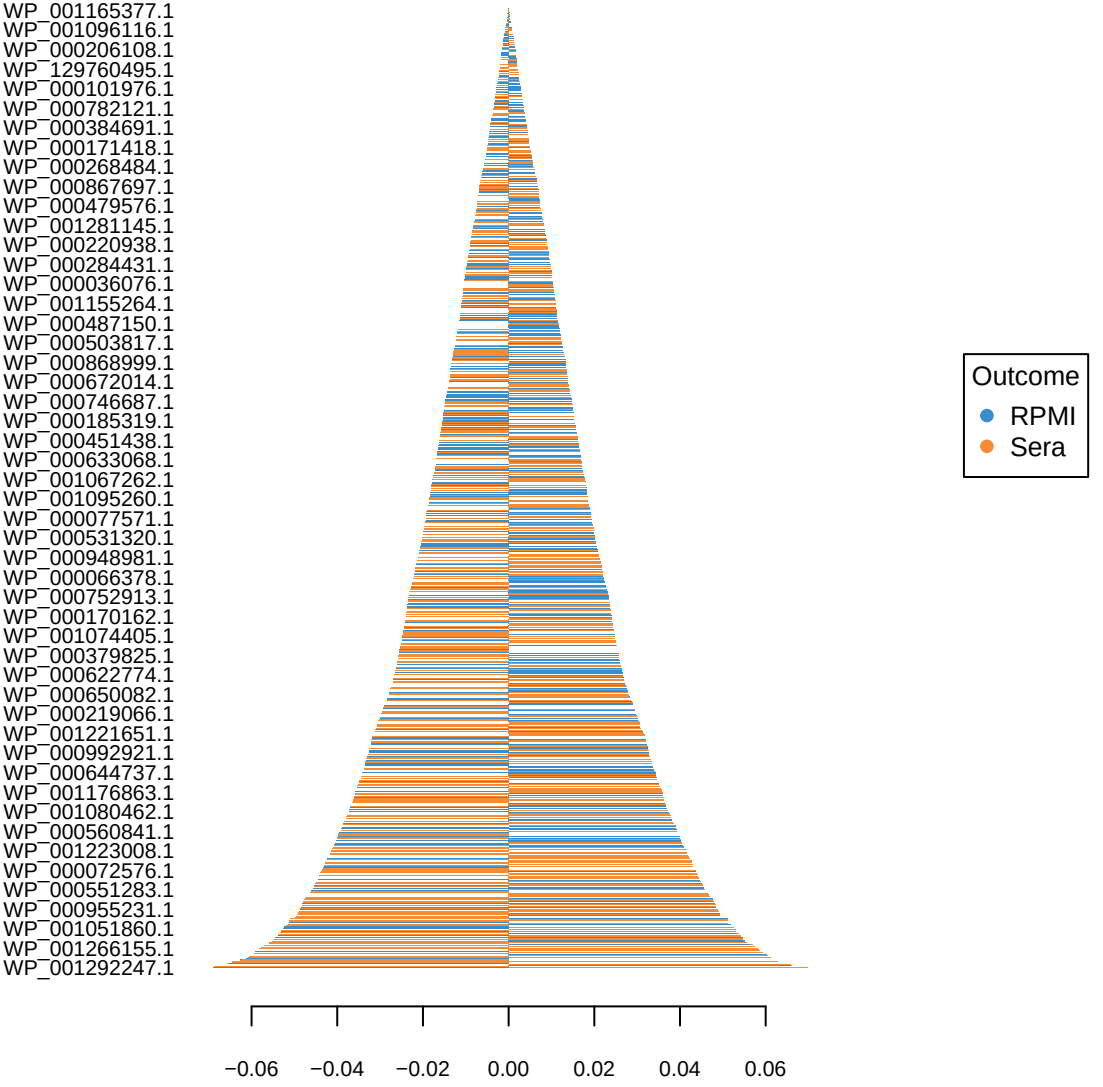
Proteomics 2 PLSDA min loadi

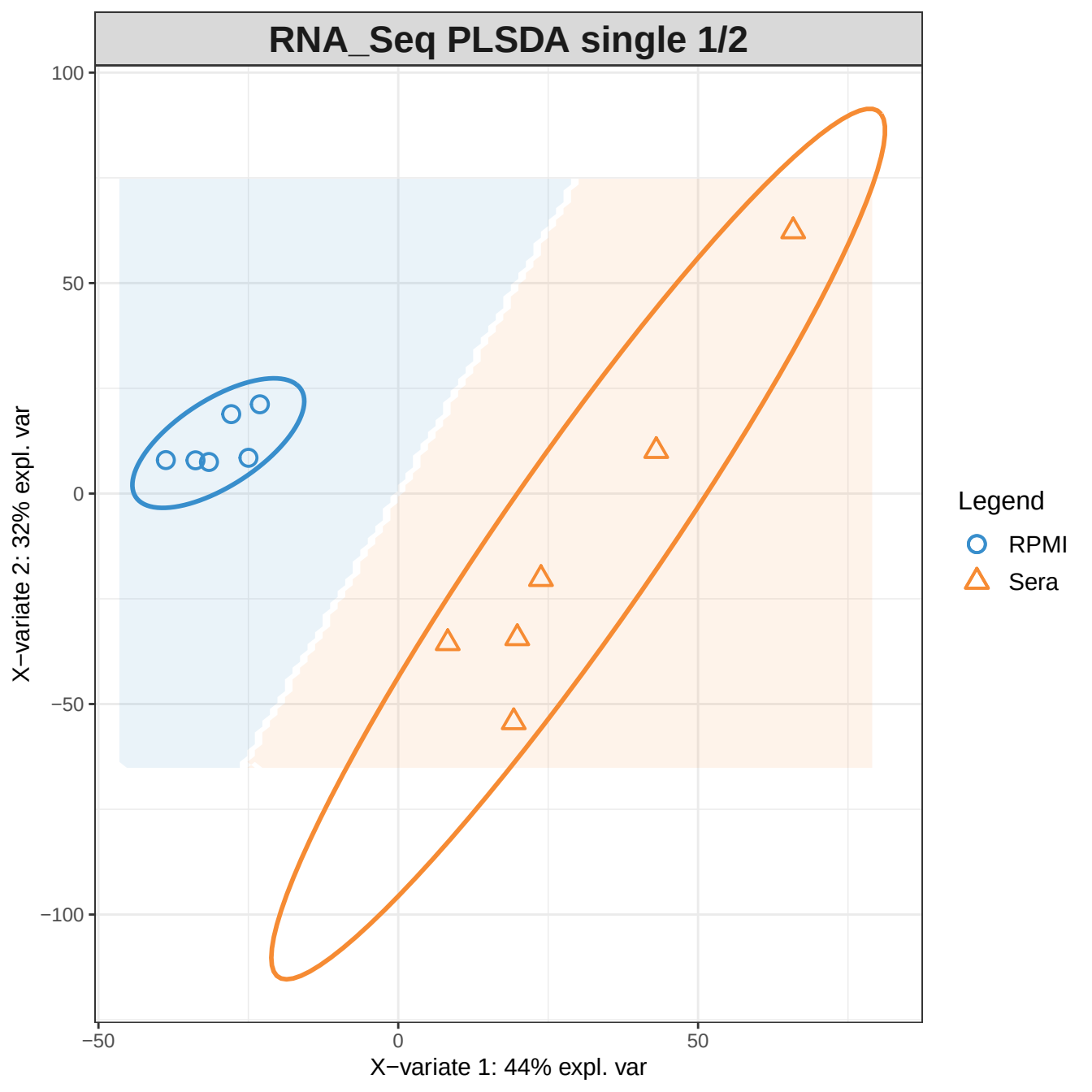


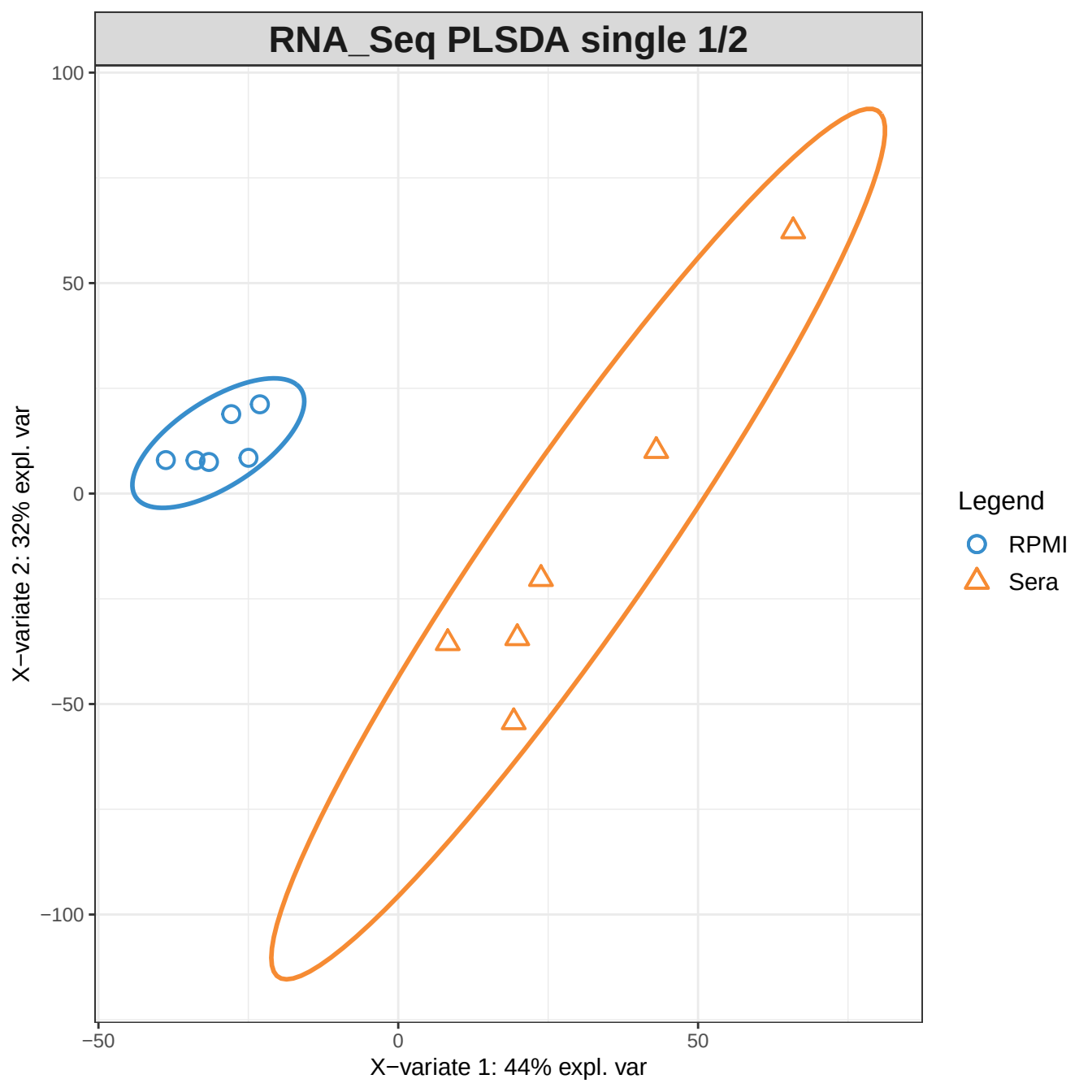
Contribution on comp 2

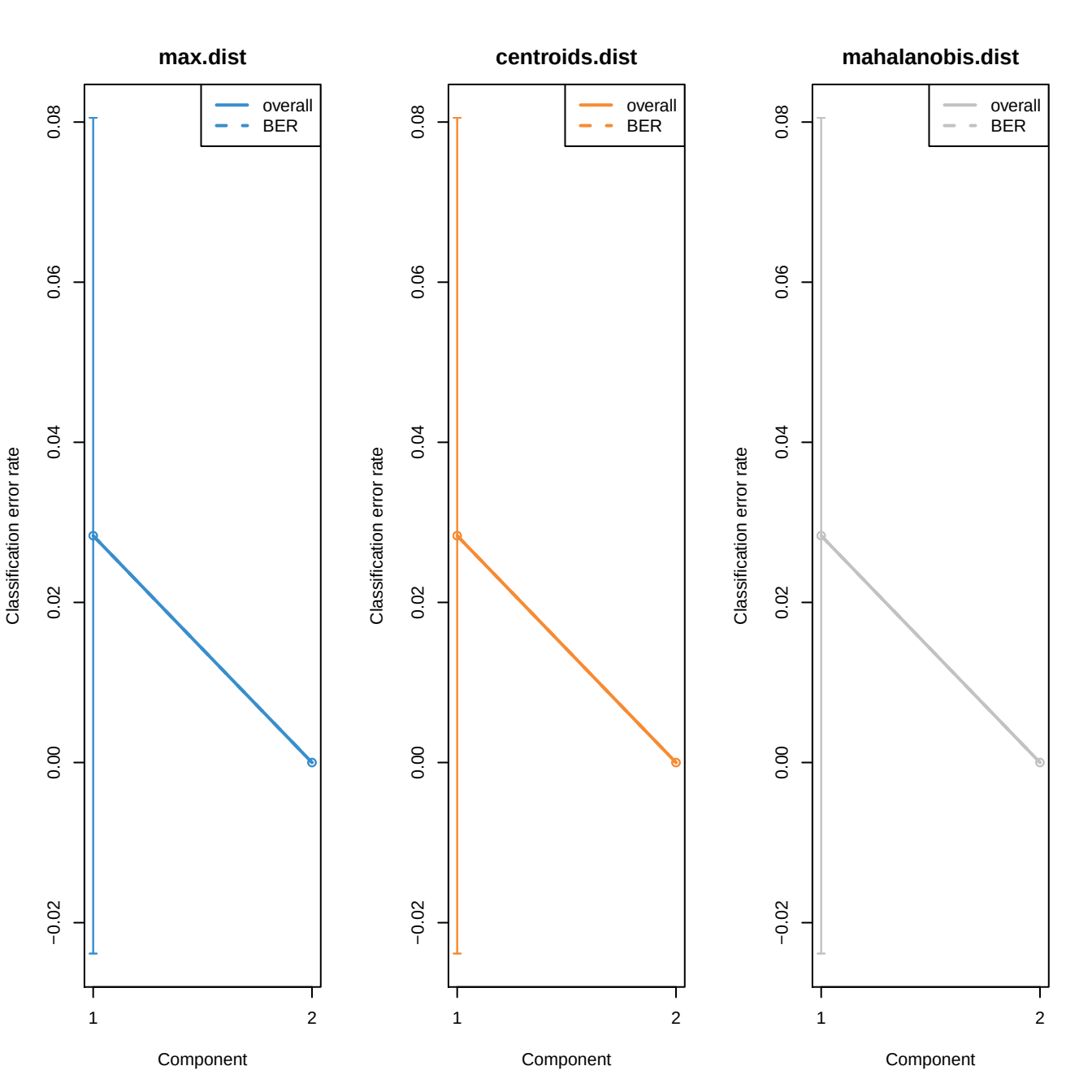


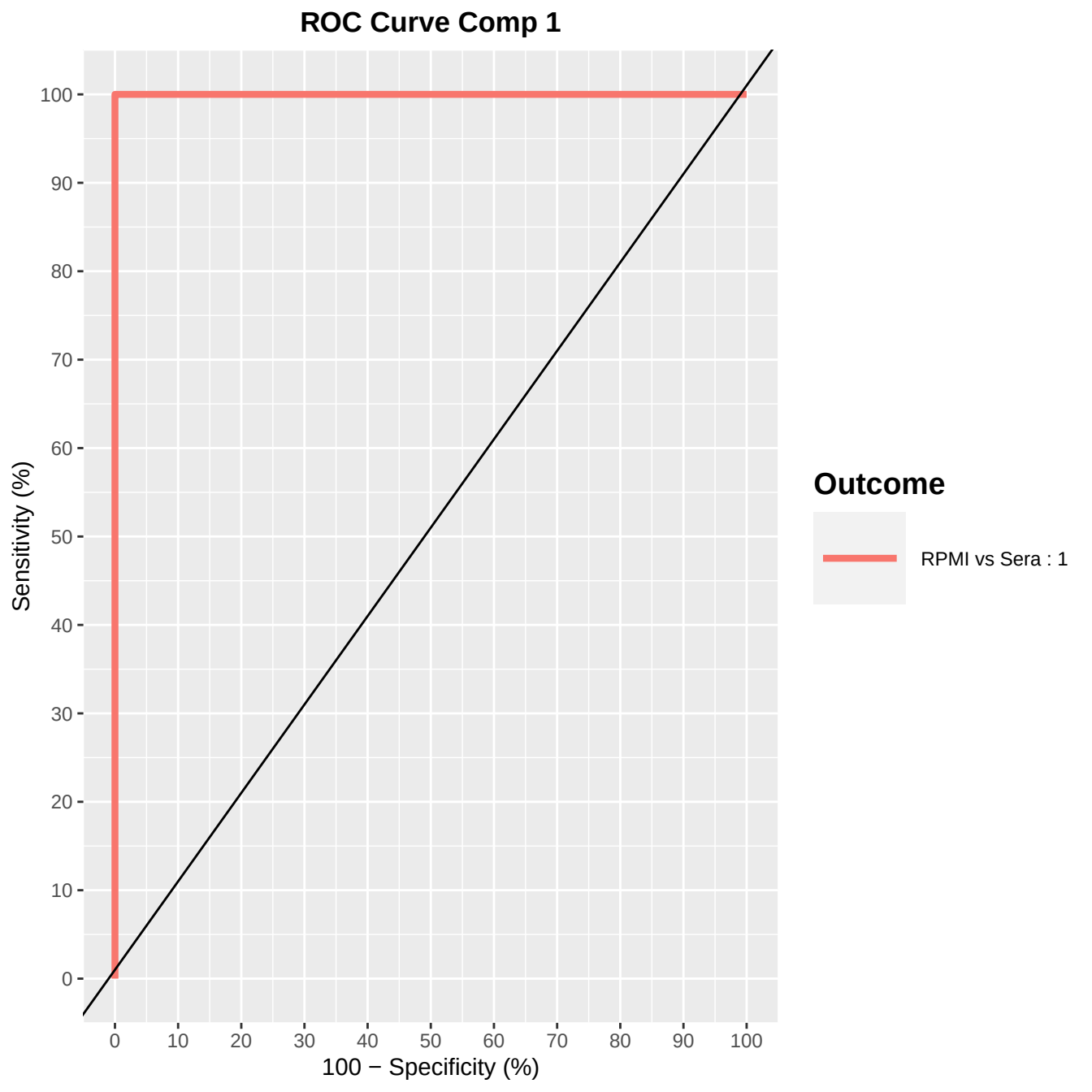
Contribution on comp 2

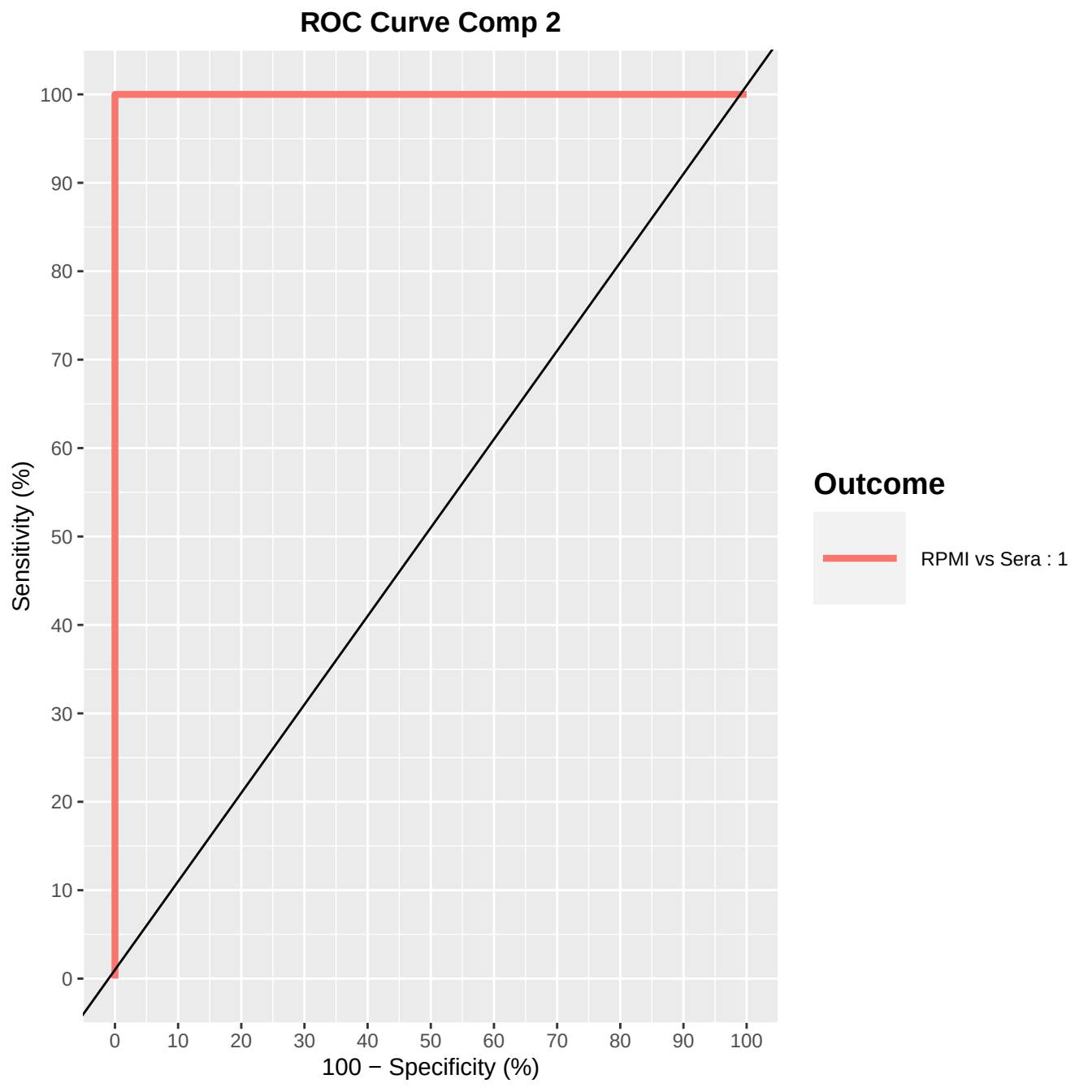


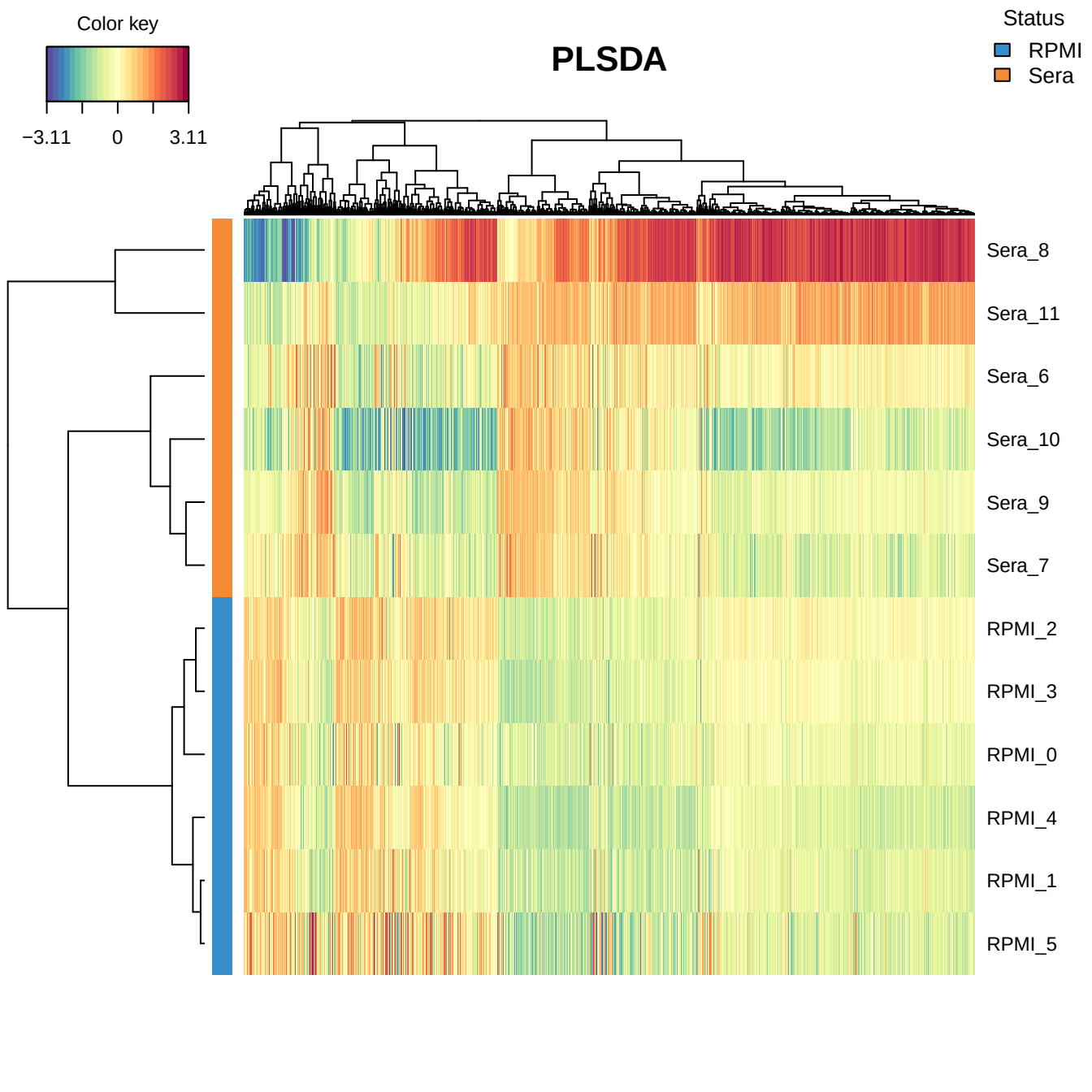

RNA_Seq PLSDA single 1/2
100
50
0
−50
−100
−50
0
50
X−variate 1: 44% expl. var
X−variate 2: 32% expl. var
Legend
RPMI
Sera

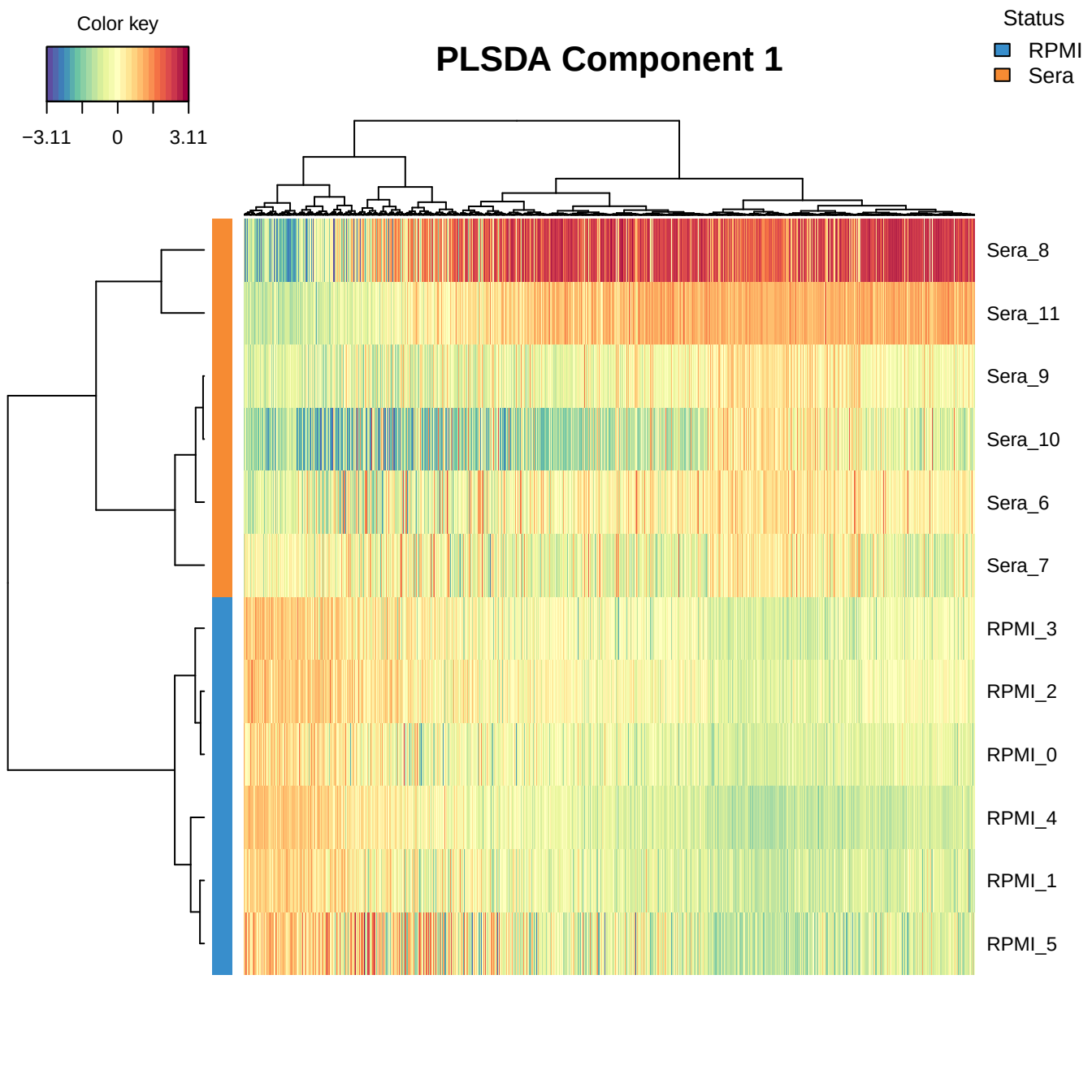

RNA_Seq PLSDA single 1/2
100
50
0
−50
−100
−50
0
50
X−variate 2: 32% expl. var
X−variate 1: 44% expl. var
Legend
RPMI
Sera


max.dist
centroids.dist
mahalanobis.dist
overall
BER
Classification error rate
Component
0.08
0.06
0.04
0.02
0.00
−0.02
1
2

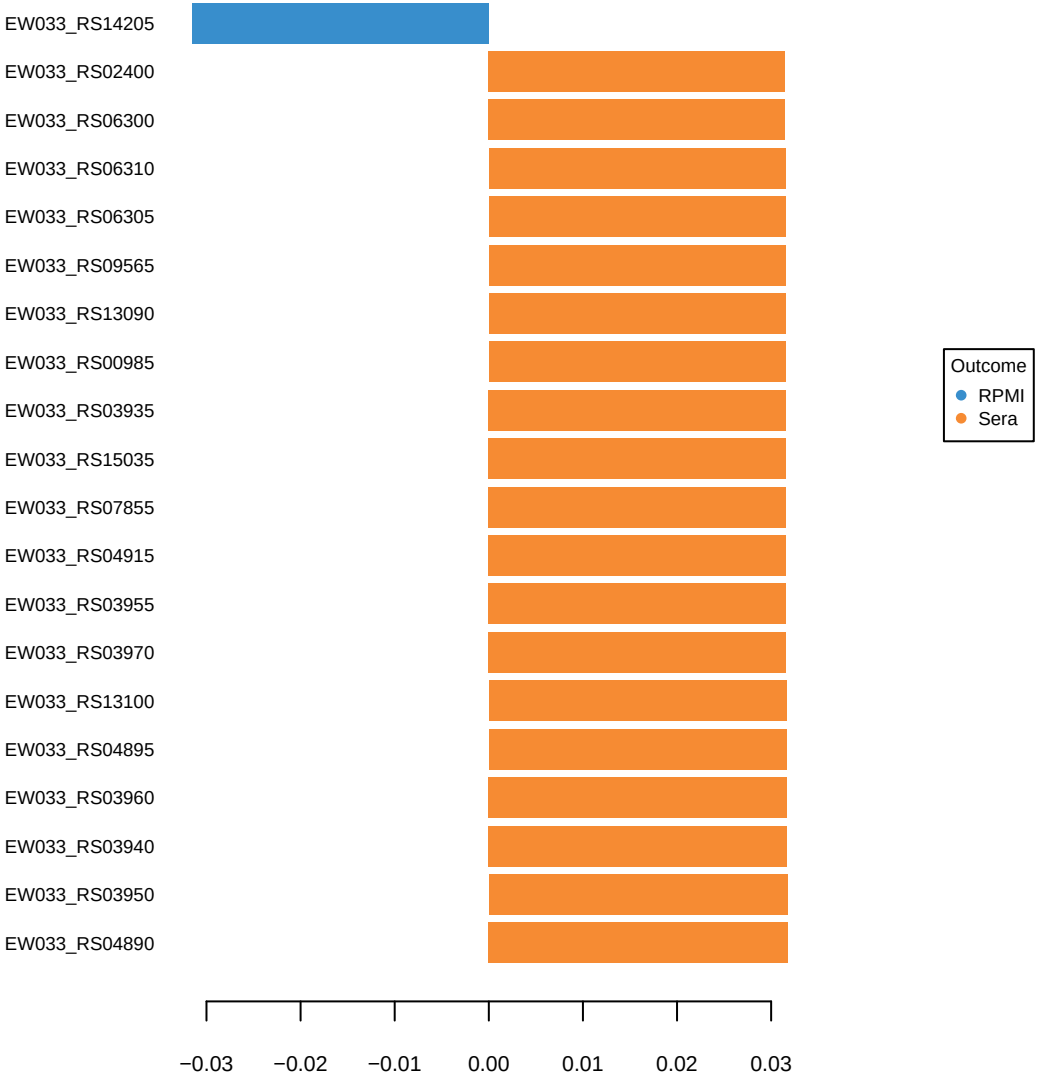

ROC Curve Comp 1
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1


ROC Curve Comp 2
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1

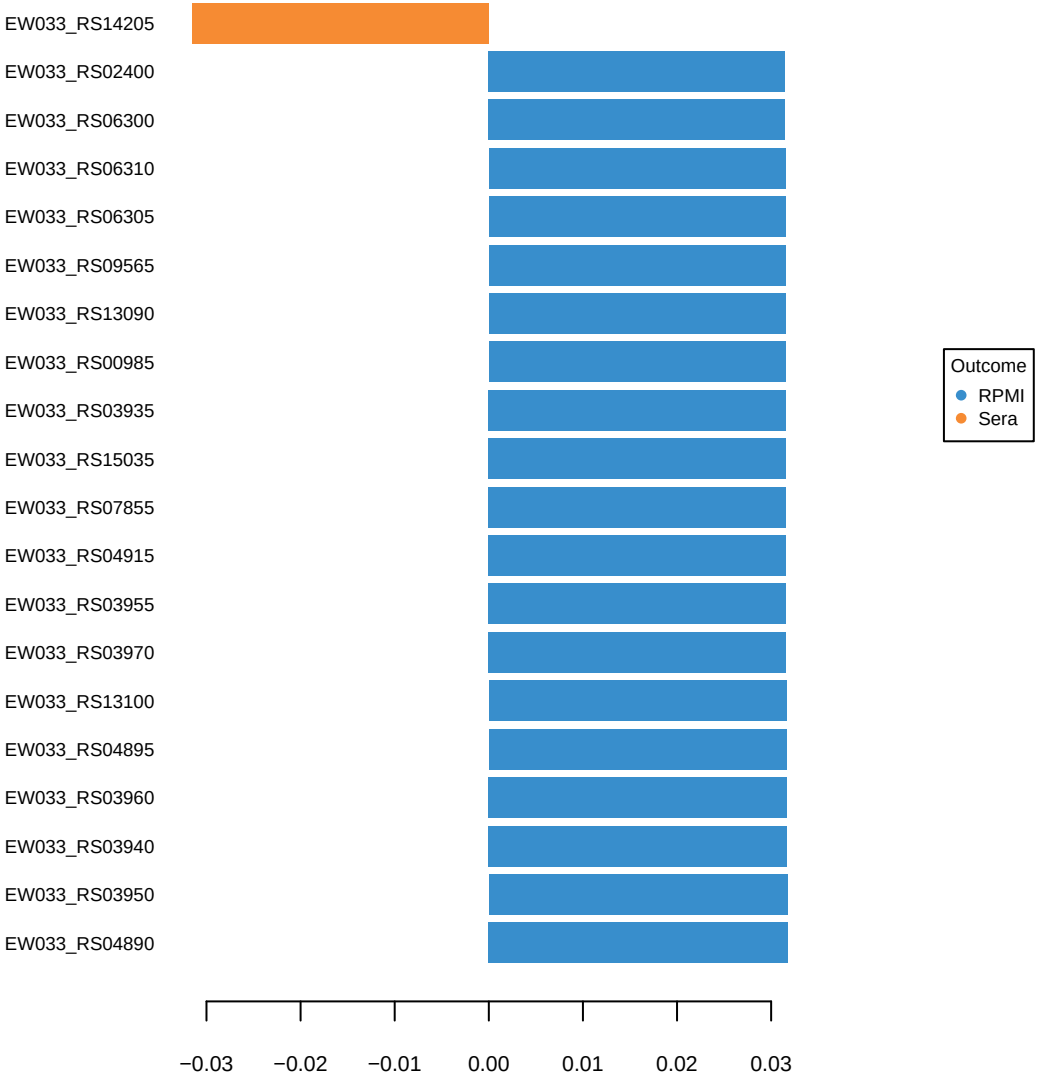

Color key
−3.11
0
3.11
PLSDA
Status
RPMI
Sera
Sera_8
Sera_11
Sera_6
Sera_10
Sera_9
Sera_7
RPMI_2
RPMI_3
RPMI_0
RPMI_4
RPMI_1
RPMI_5


Color key
−3.11
0
3.11
PLSDA Component 1
Status
RPMI
Sera
Sera_8
Sera_11
Sera_9
Sera_10
Sera_6
Sera_7
RPMI_3
RPMI_2
RPMI_0
RPMI_4
RPMI_1
RPMI_5

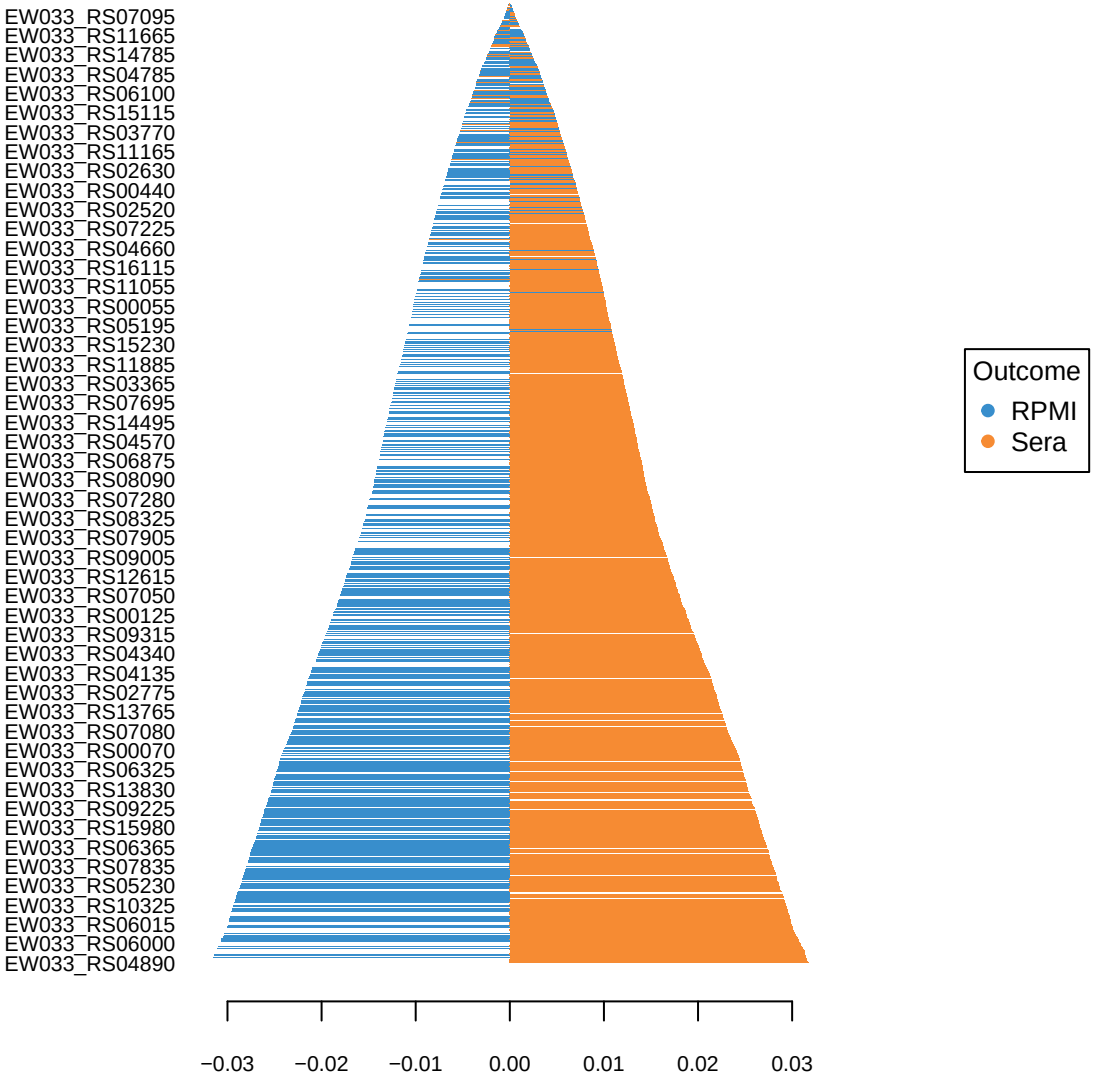
RNA_Seq 1 PLSDA max loadir



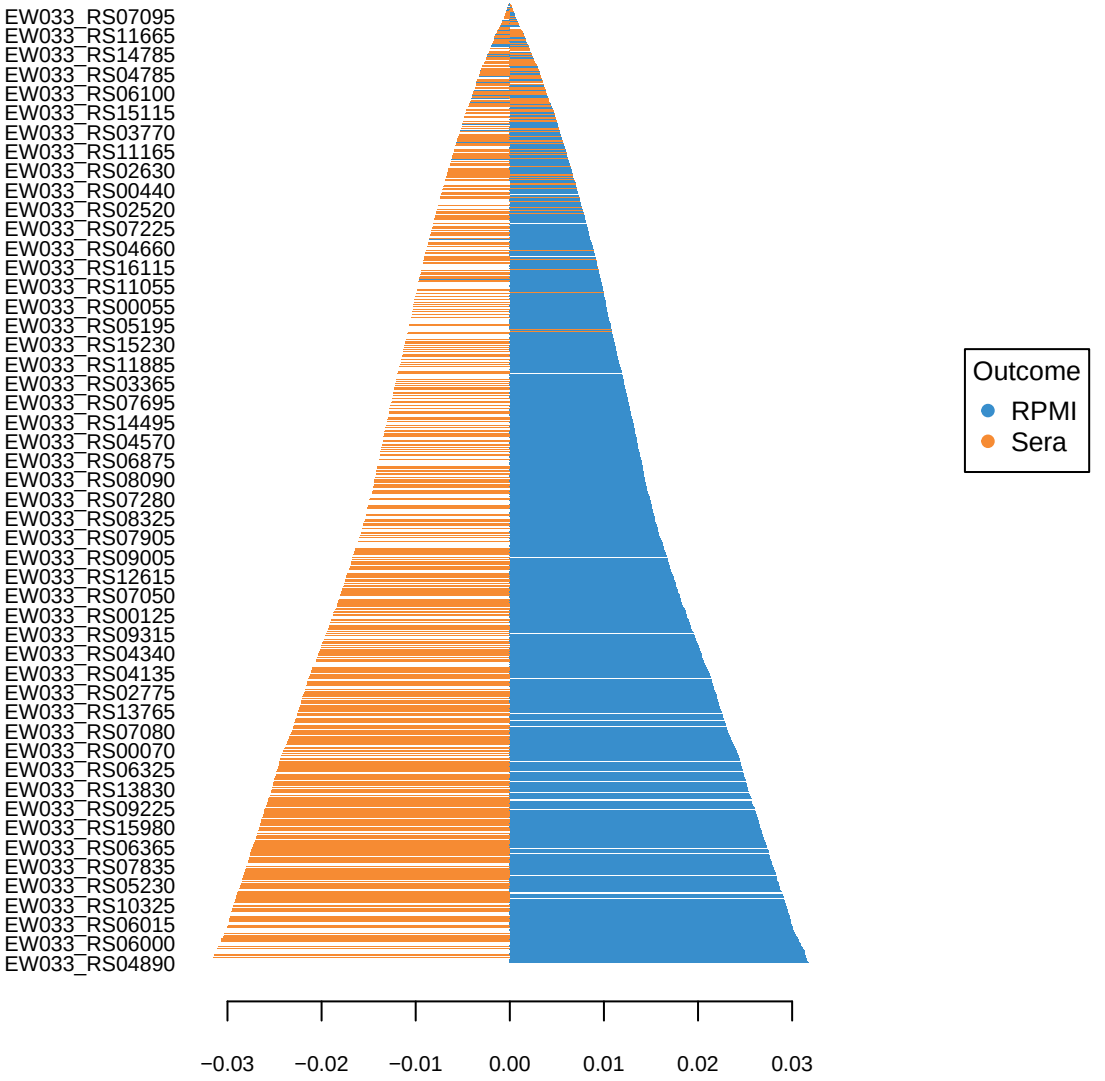
RNA_Seq 1 PLSDA min loadin

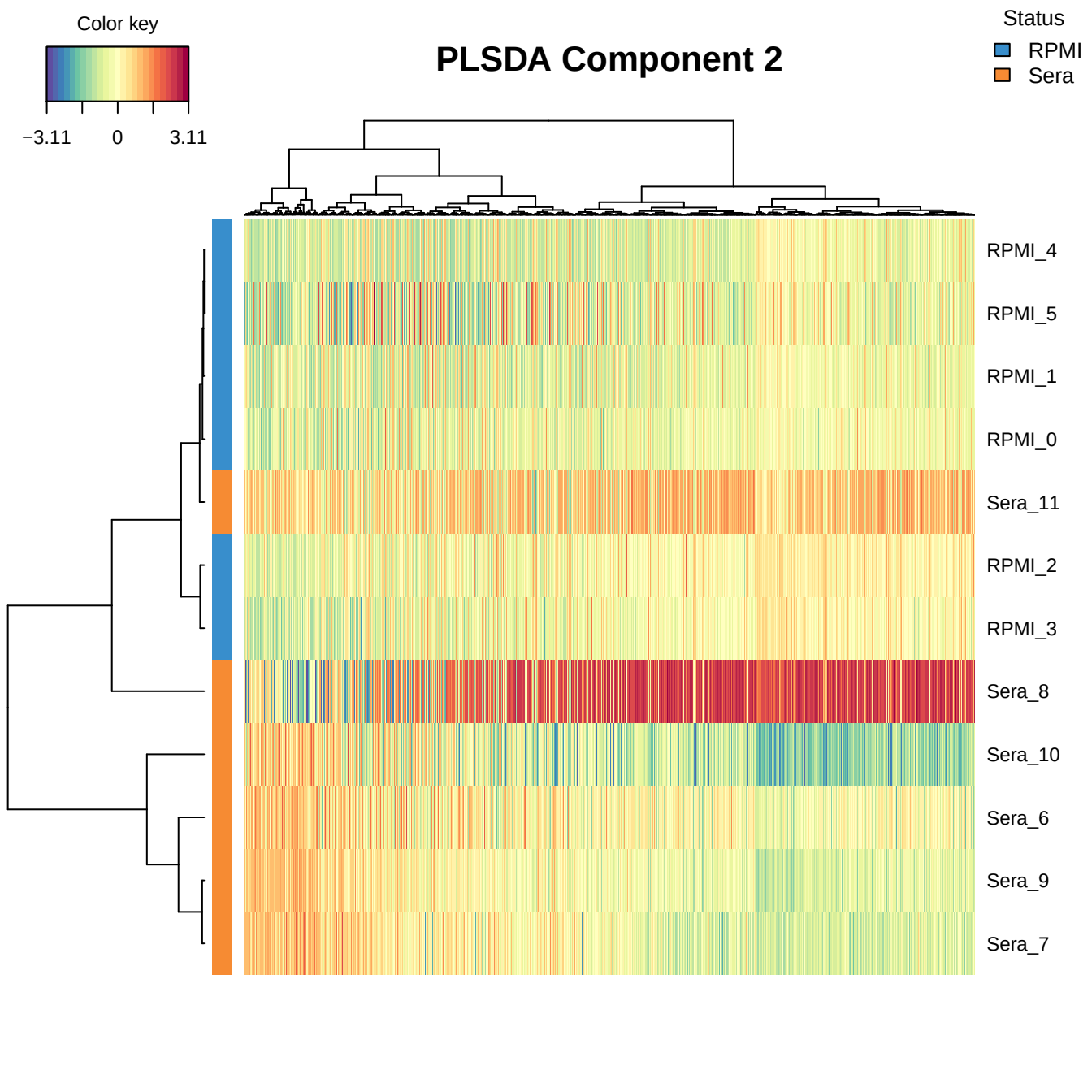


Contribution on comp 1

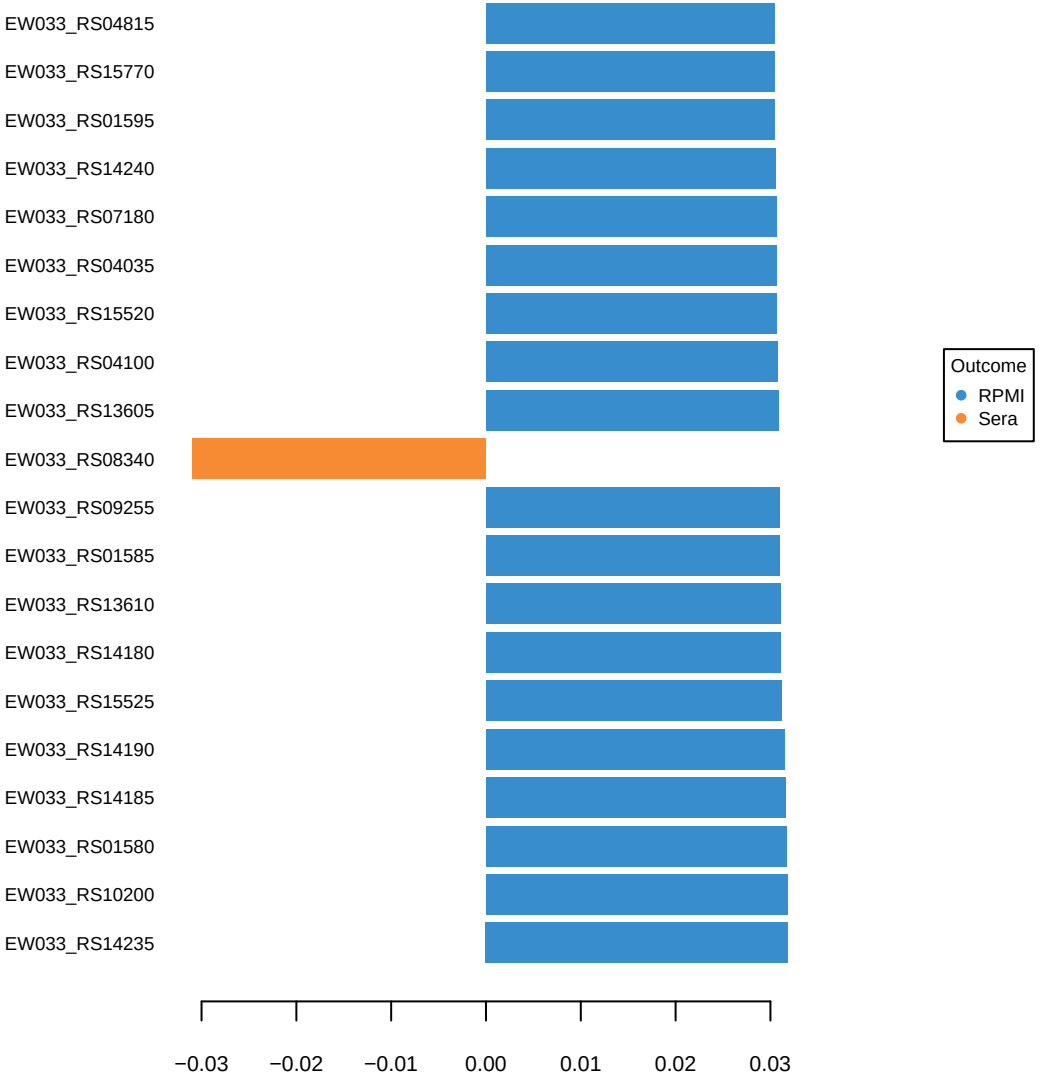


Contribution on comp 1

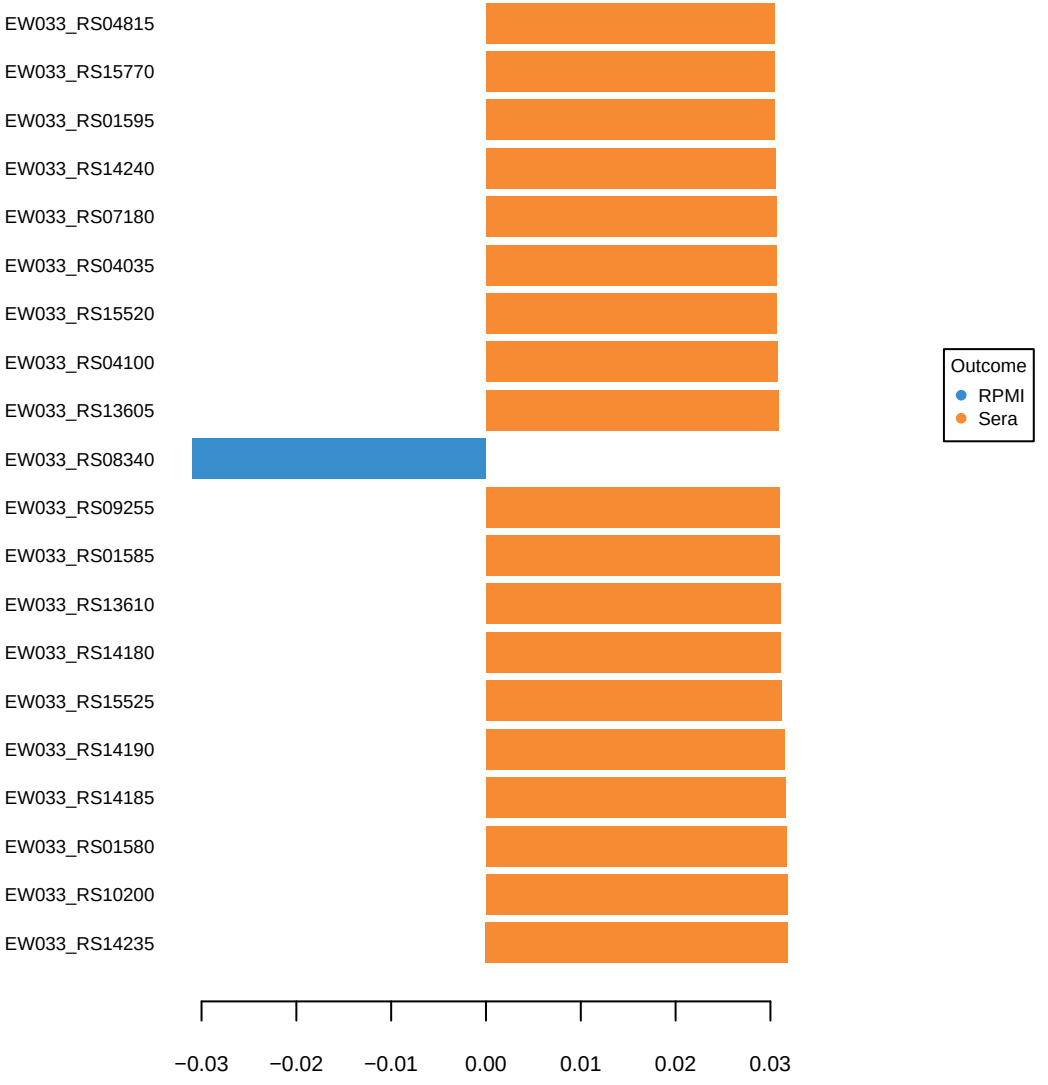



Color key
−3.11
0
3.11
PLSDA Component 2
Status
RPMI
Sera
RPMI_4
RPMI_5
RPMI_1
RPMI_0
Sera_11
RPMI_2
RPMI_3
Sera_8
Sera_10
Sera_6
Sera_9
Sera_7

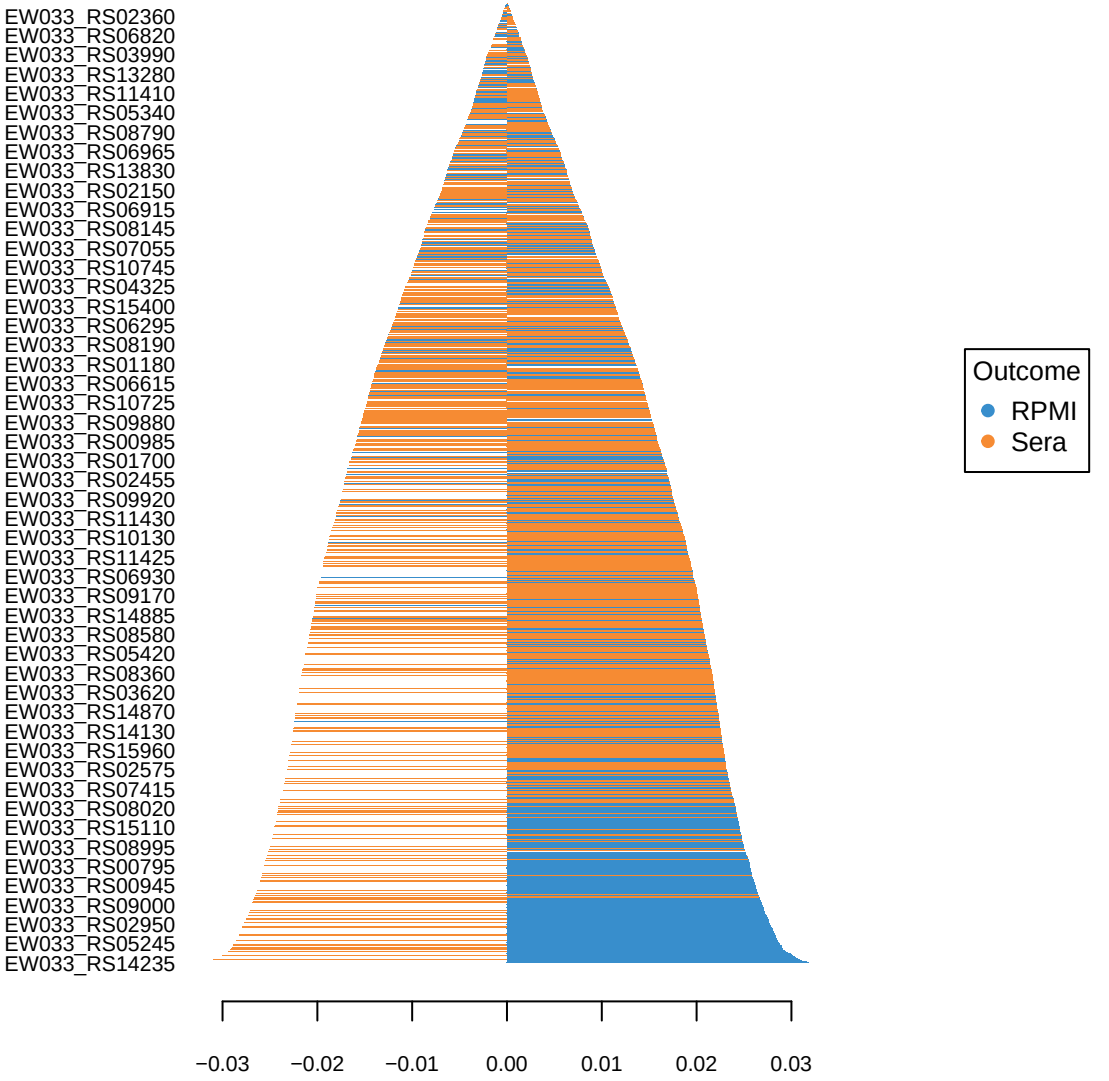
RNA_Seq 2 PLSDA max loadir



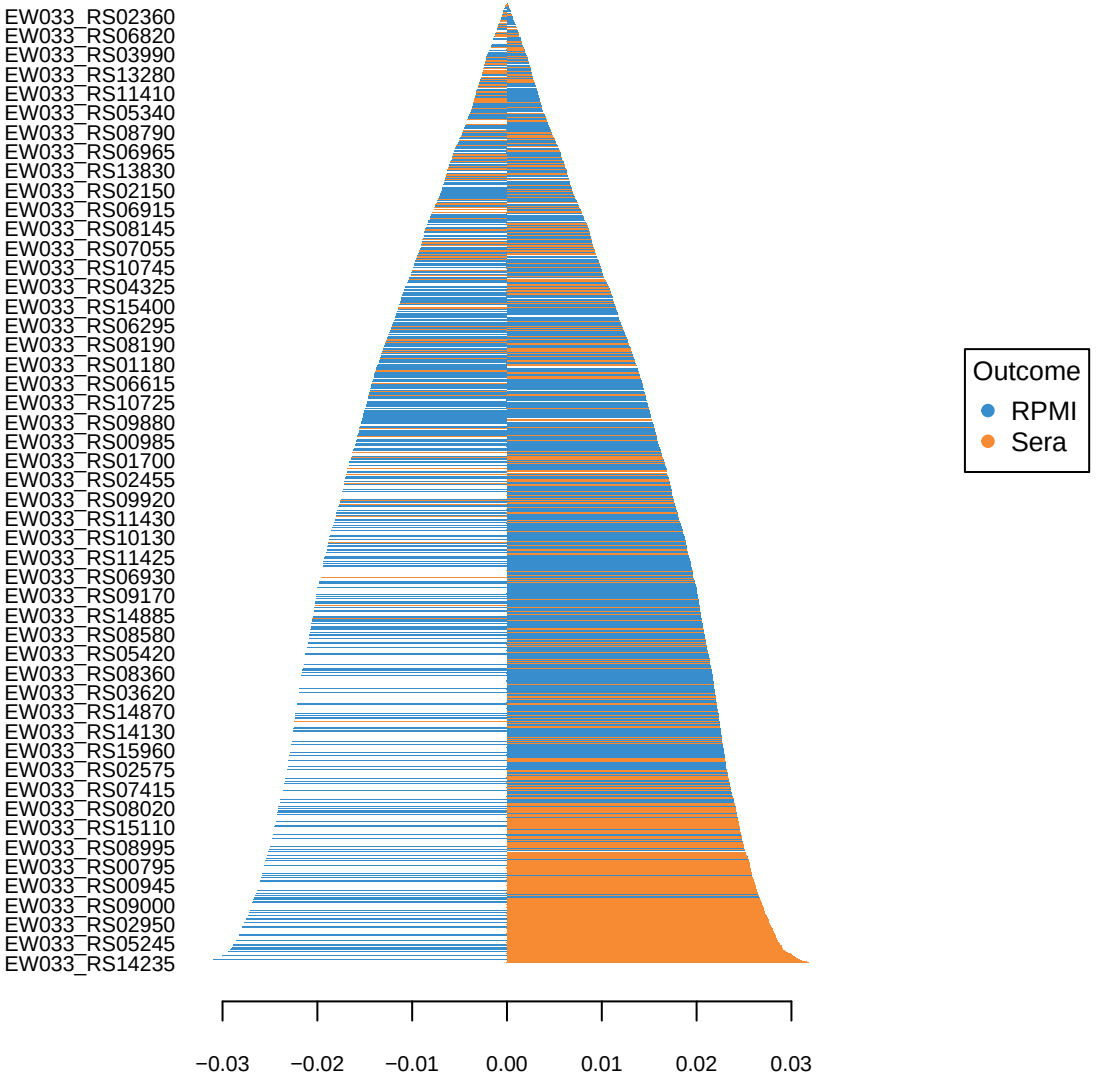
RNA_Seq 2 PLSDA min loadin

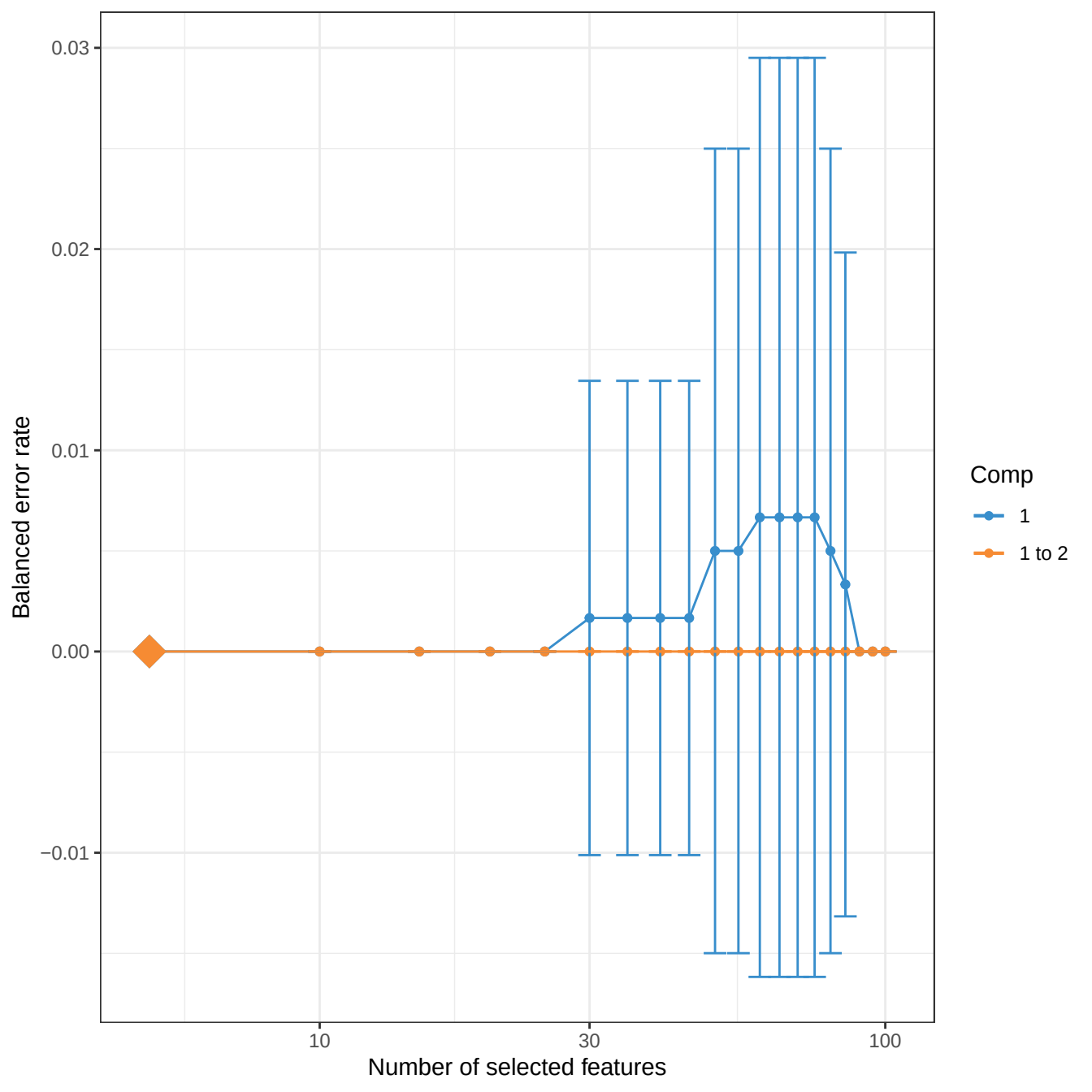


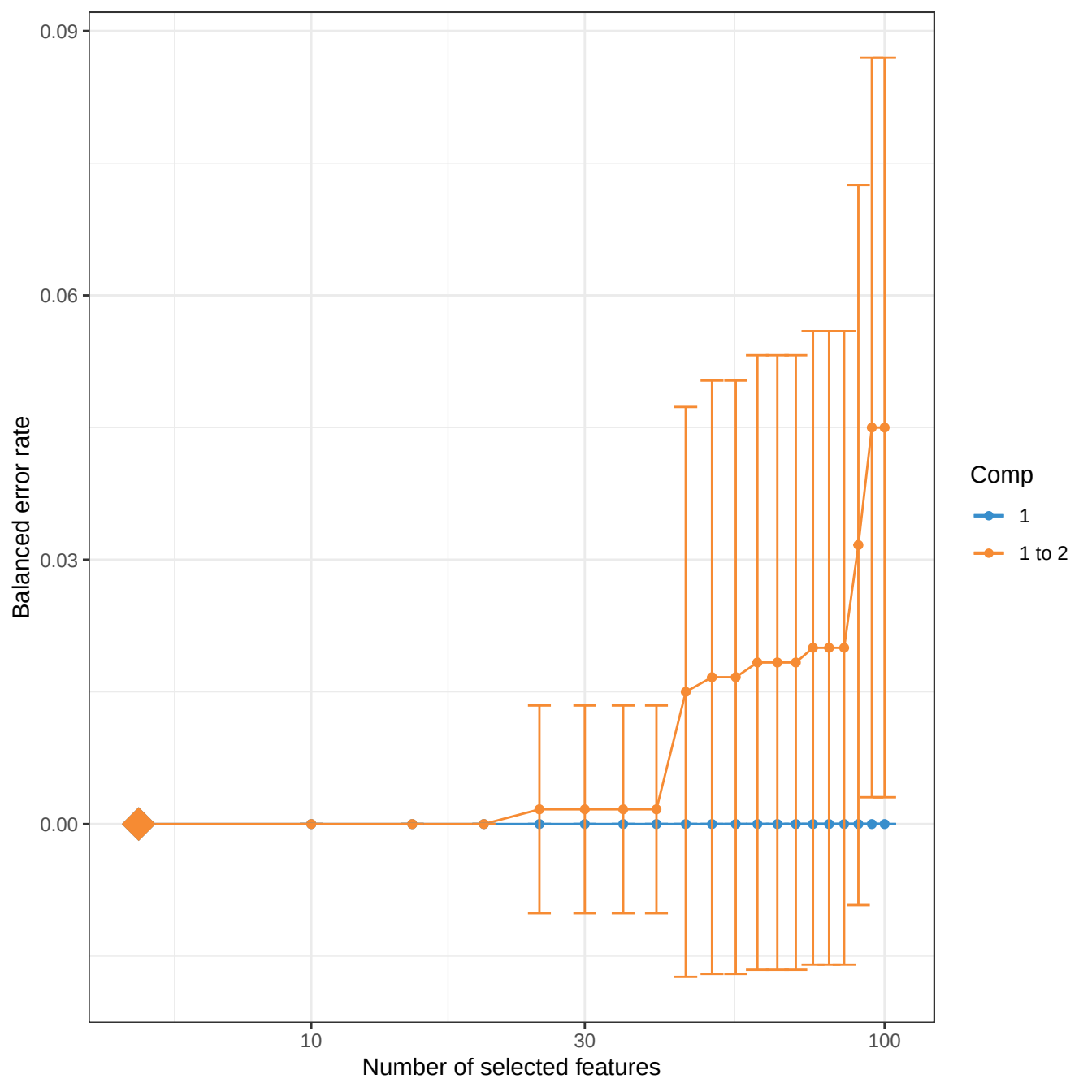
Contribution on comp 2

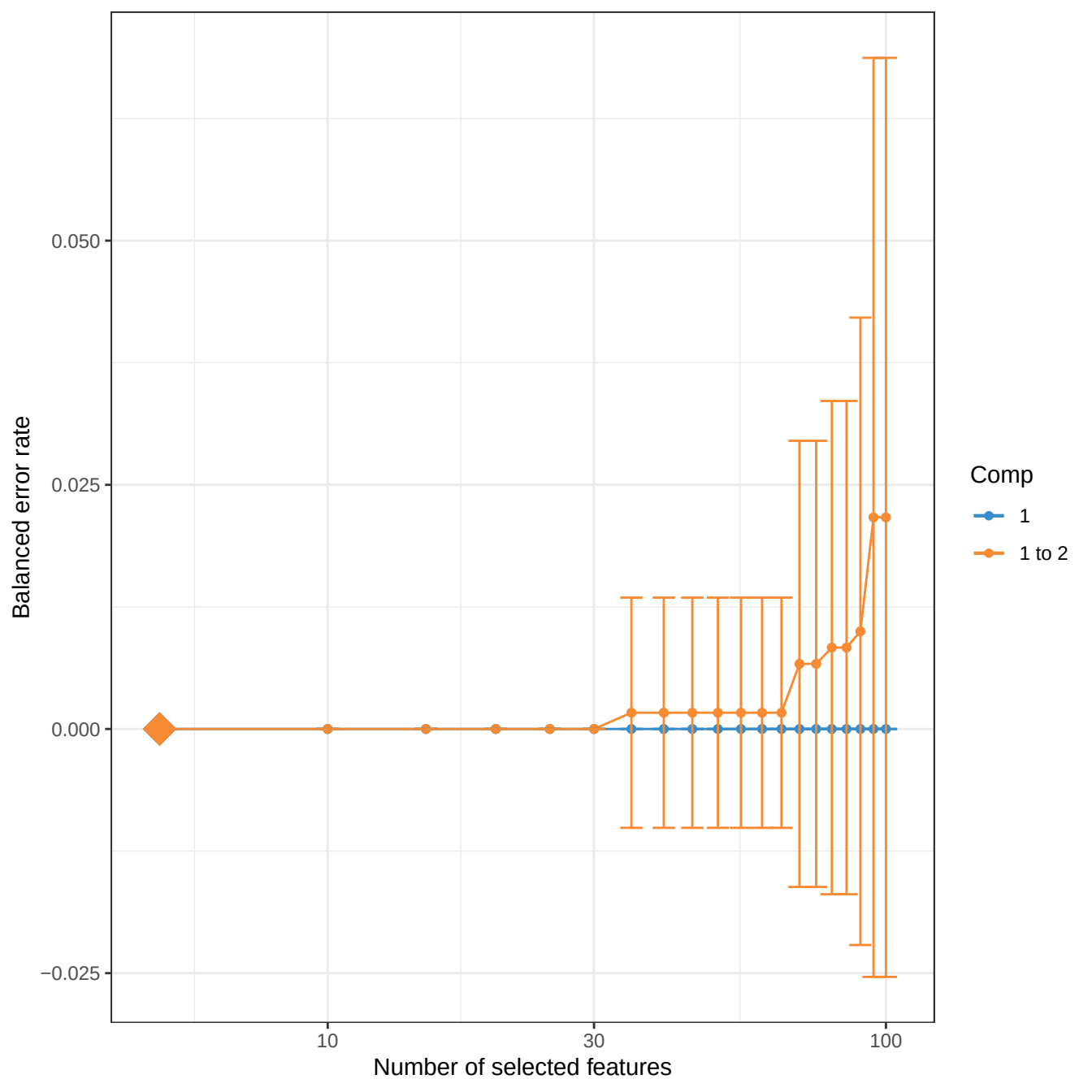


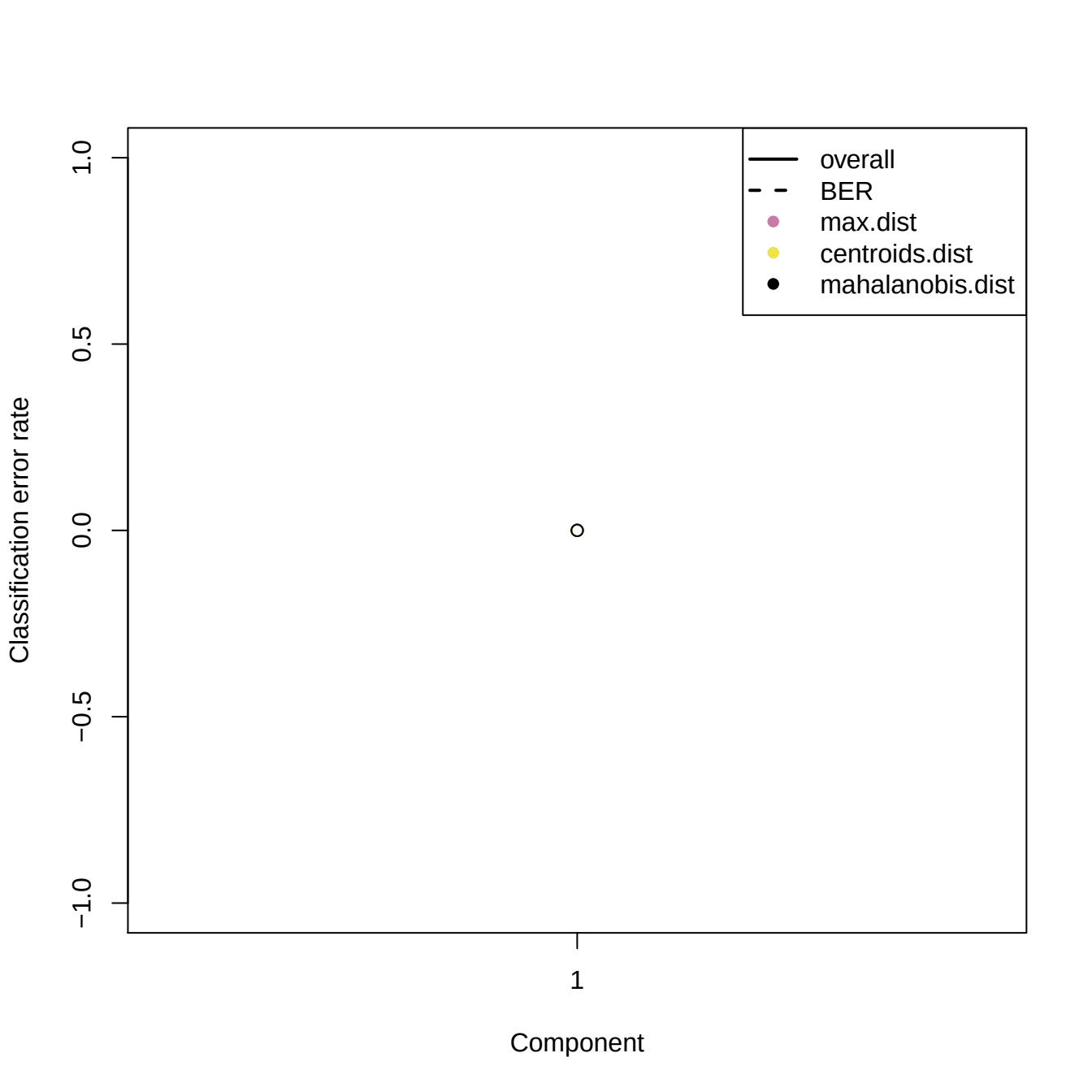
Contribution on comp 2

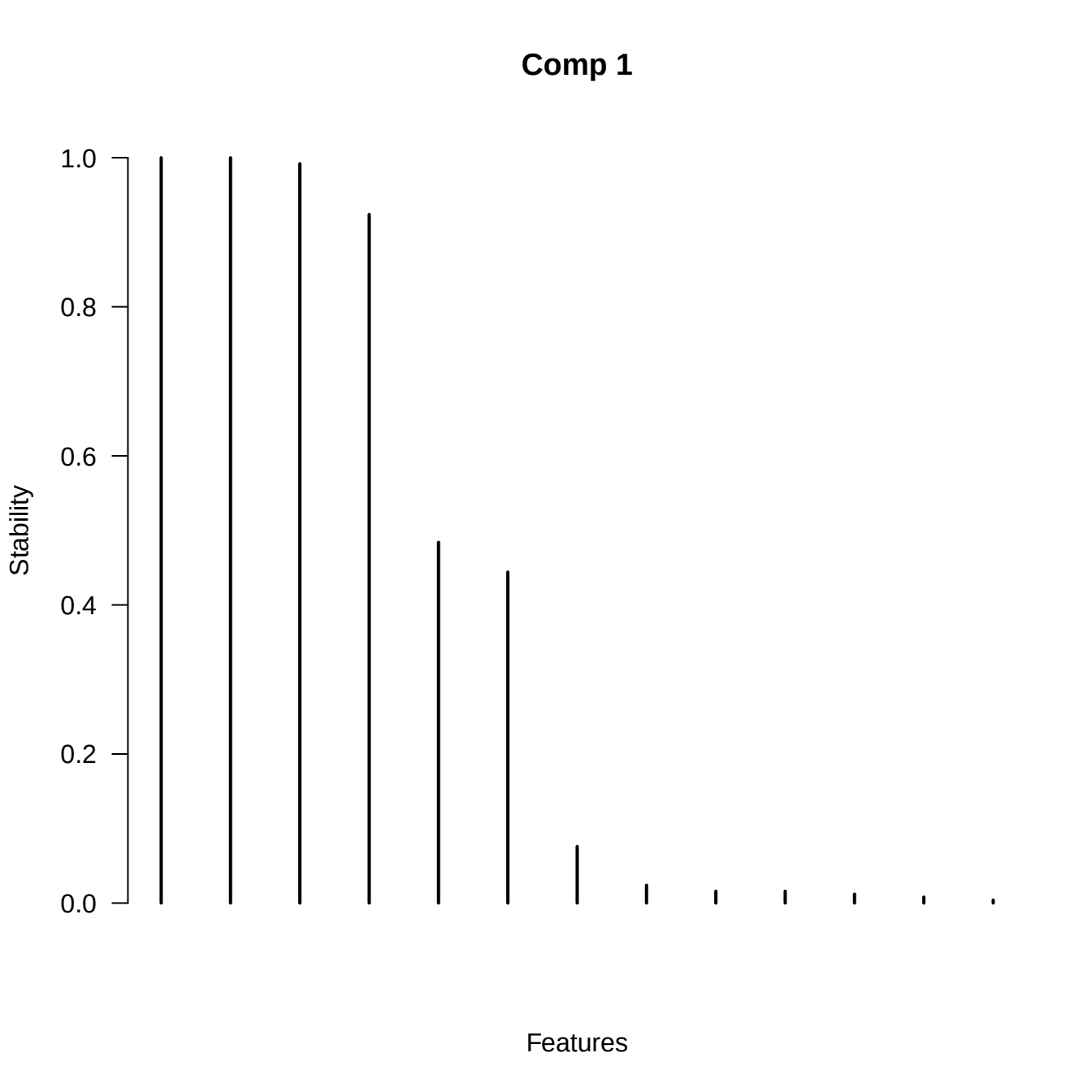


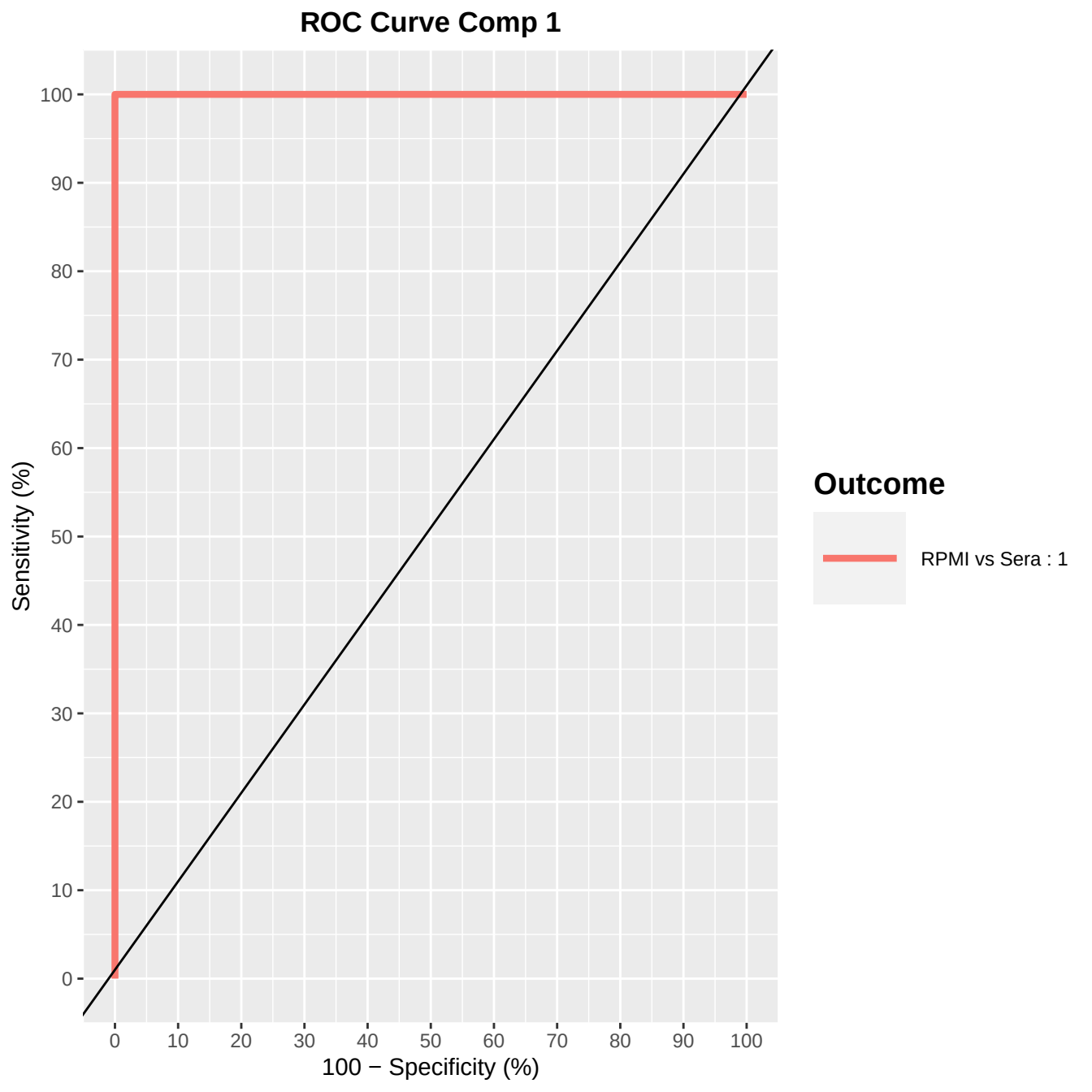

0.03
0.02
0.01
0.00
−0.01
Balanced error rate
10
30
100
Number of selected features
Comp
1
1 to 2

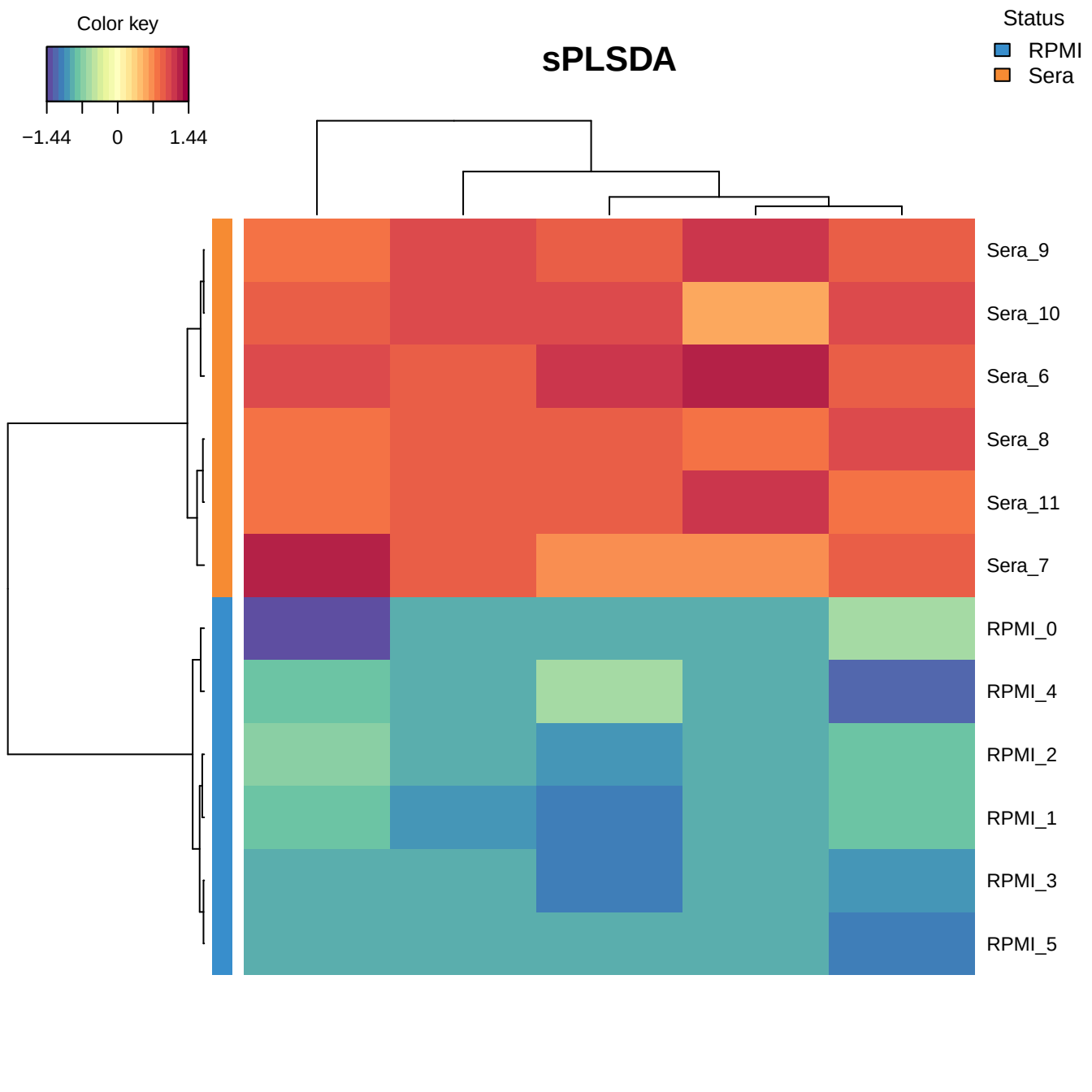

0.09
0.06
0.03
0.00
Balanced error rate
10
30
100
Number of selected features
Comp
1
1 to 2

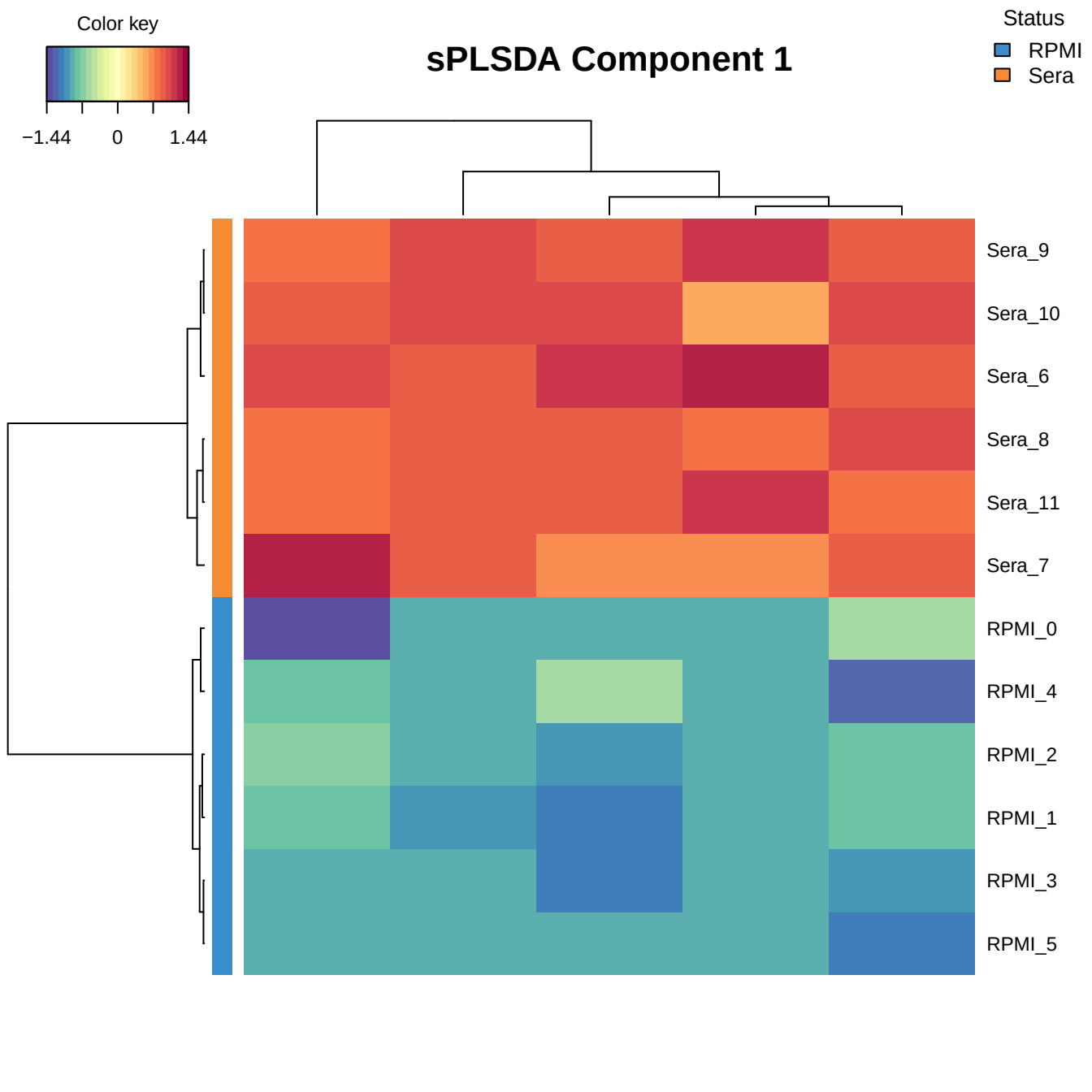

Balanced error rate
0.050
0.025
0.000
−0.025
10
30
100
Number of selected features
Comp
1
1 to 2


overall
BER
max.dist
centroids.dist
mahalanobis.dist
Classification error rate
1.0
0.5
0.0
−0.5
−1.0
1
Component

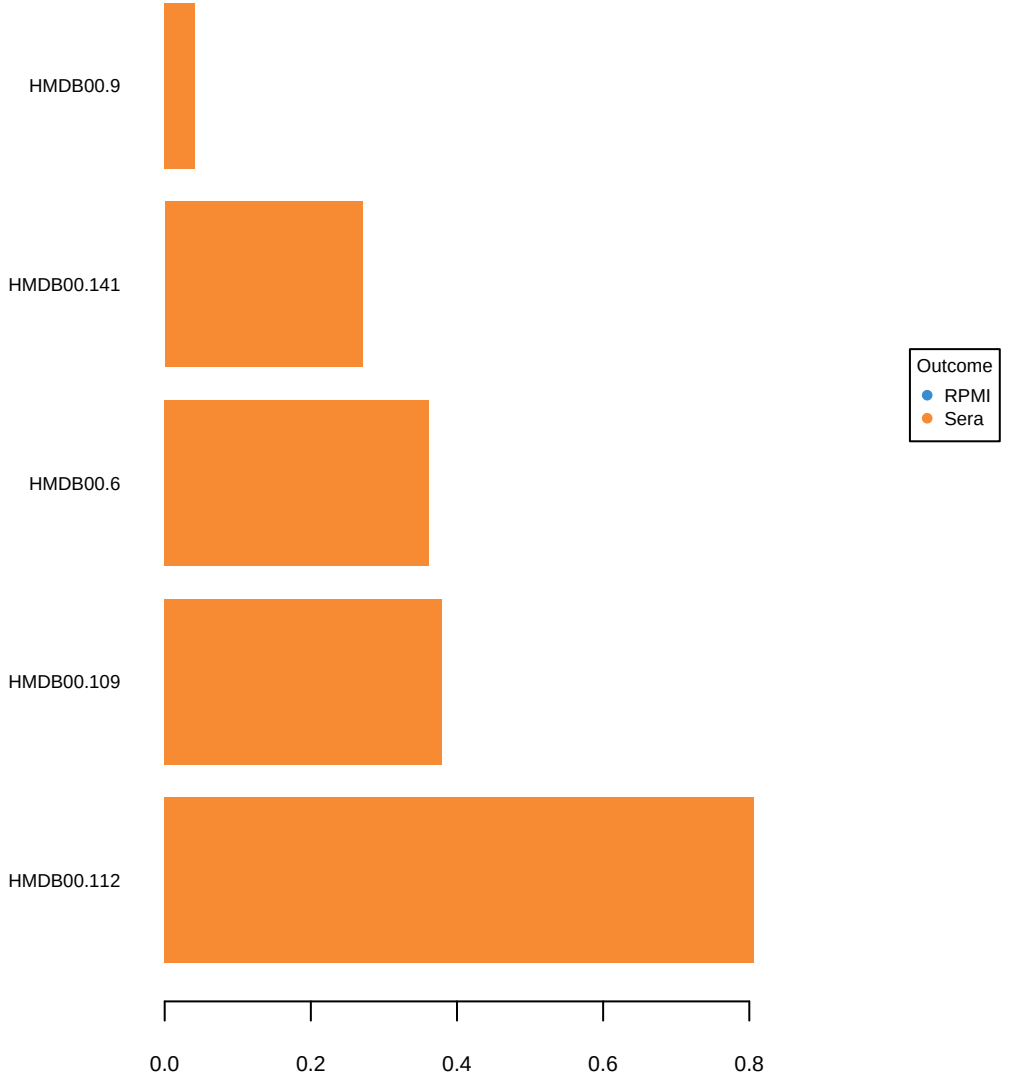

Comp 1
1.0
0.8
0.6
0.4
0.2
0.0
Stability
Features


ROC Curve Comp 1
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1

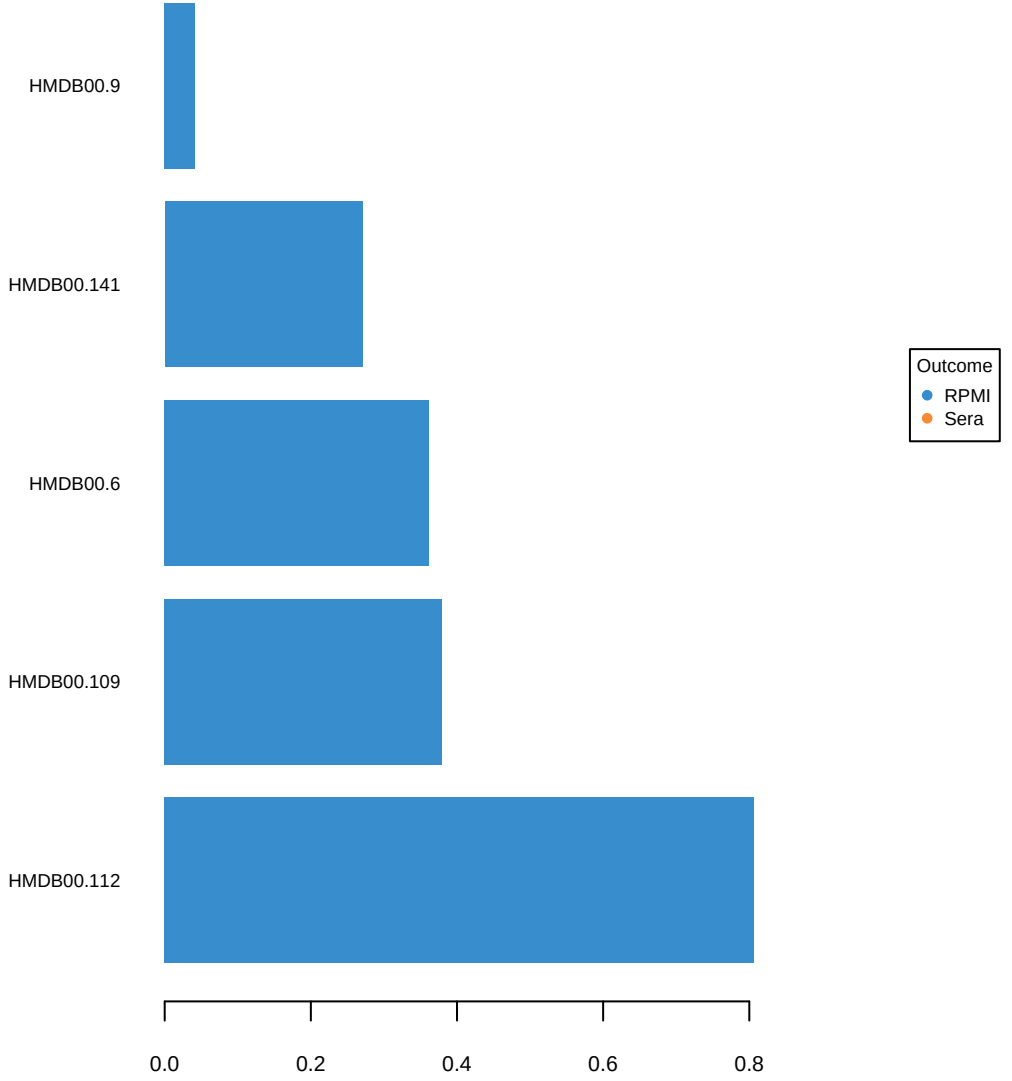

Color key
−1.44
0
1.44
sPLSDA
Status
RPMI
Sera
Sera_9
Sera_10
Sera_6
Sera_8
Sera_11
Sera_7
RPMI_0
RPMI_4
RPMI_2
RPMI_1
RPMI_3
RPMI_5

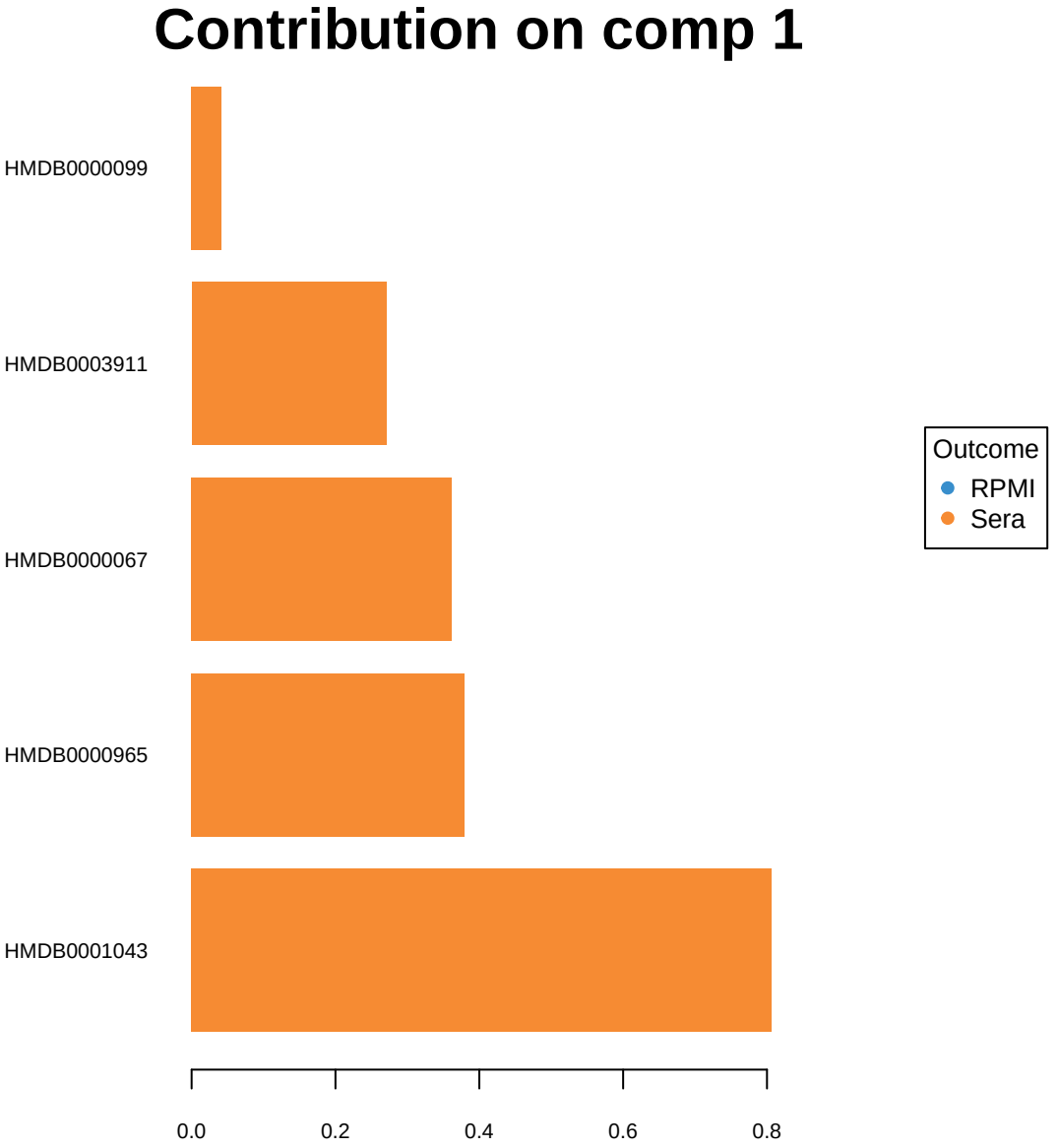

Color key
−1.44
0
1.44
sPLSDA Component 1
Status
RPMI
Sera
Sera_9
Sera_10
Sera_6
Sera_8
Sera_11
Sera_7
RPMI_0
RPMI_4
RPMI_2
RPMI_1
RPMI_3
RPMI_5

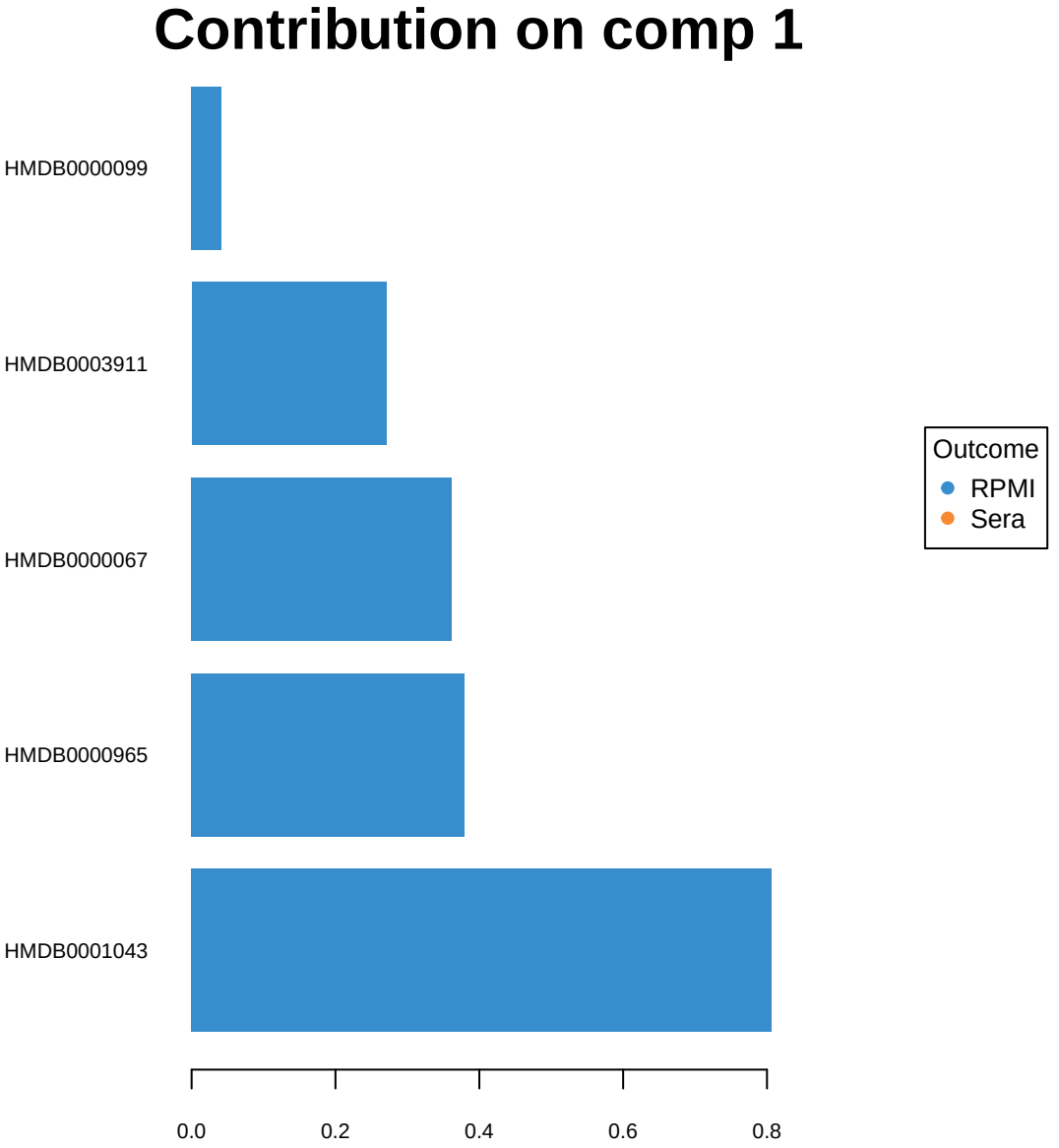
Metabolomics 1 sPLSDA max loa

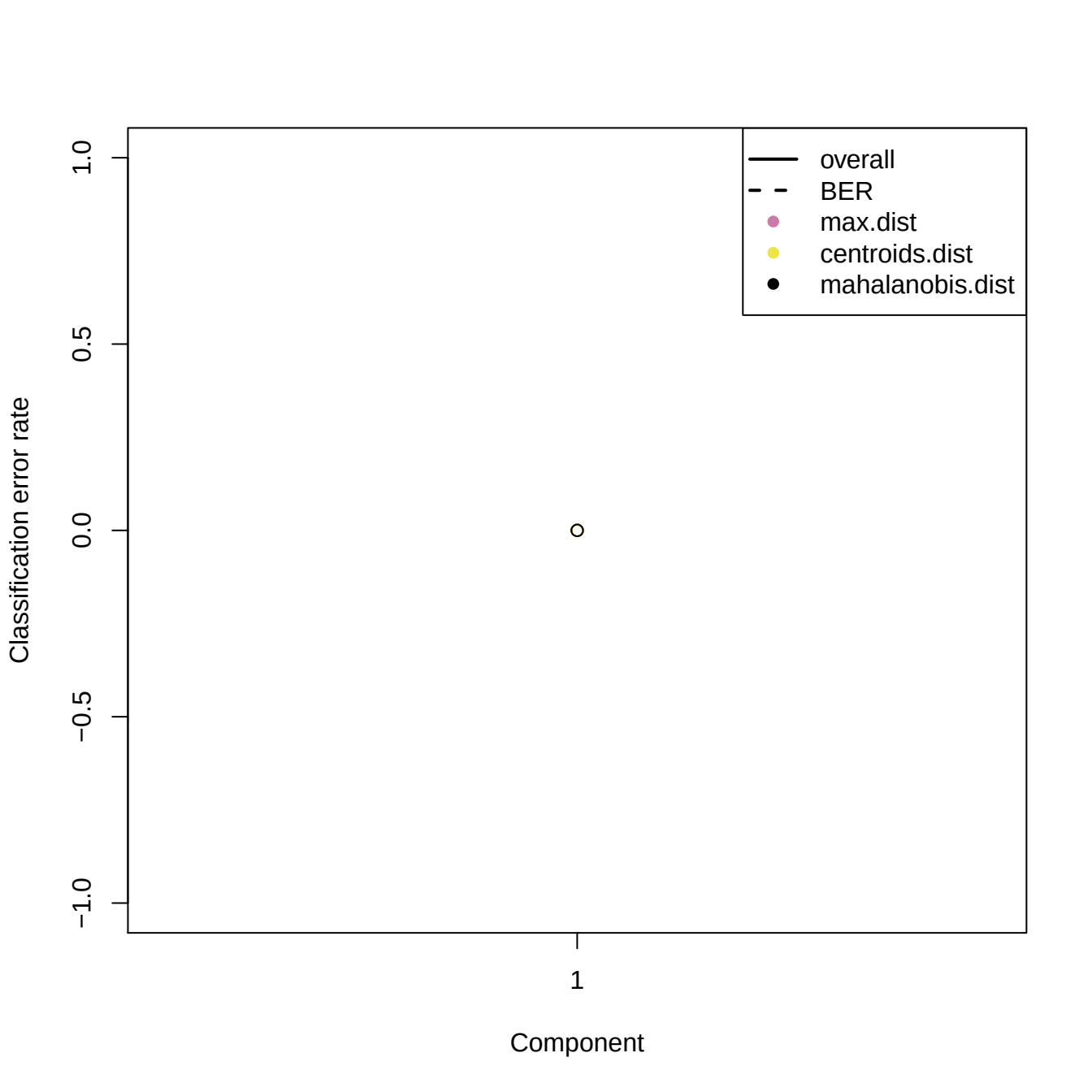


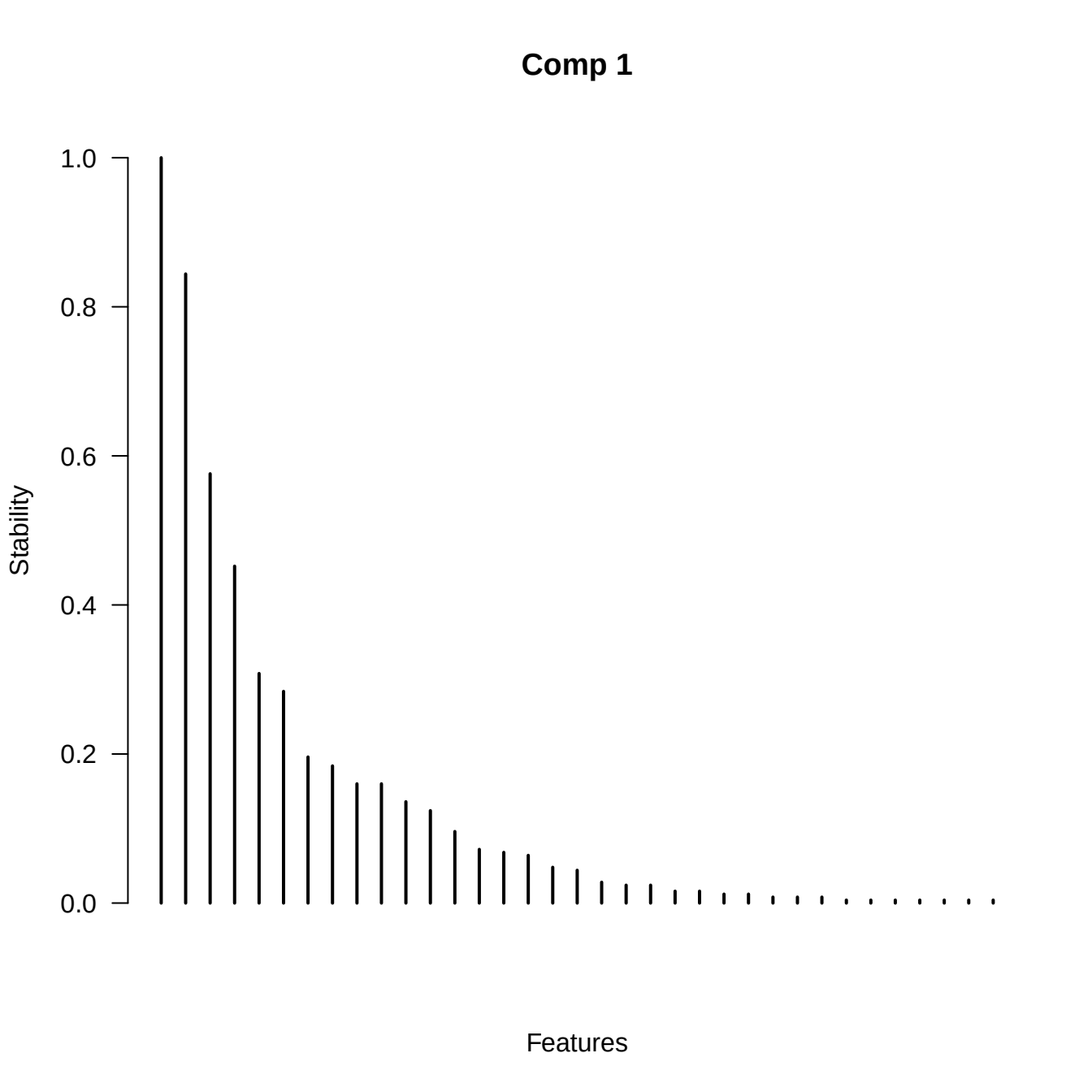
Metabolomics 1 sPLSDA min loa

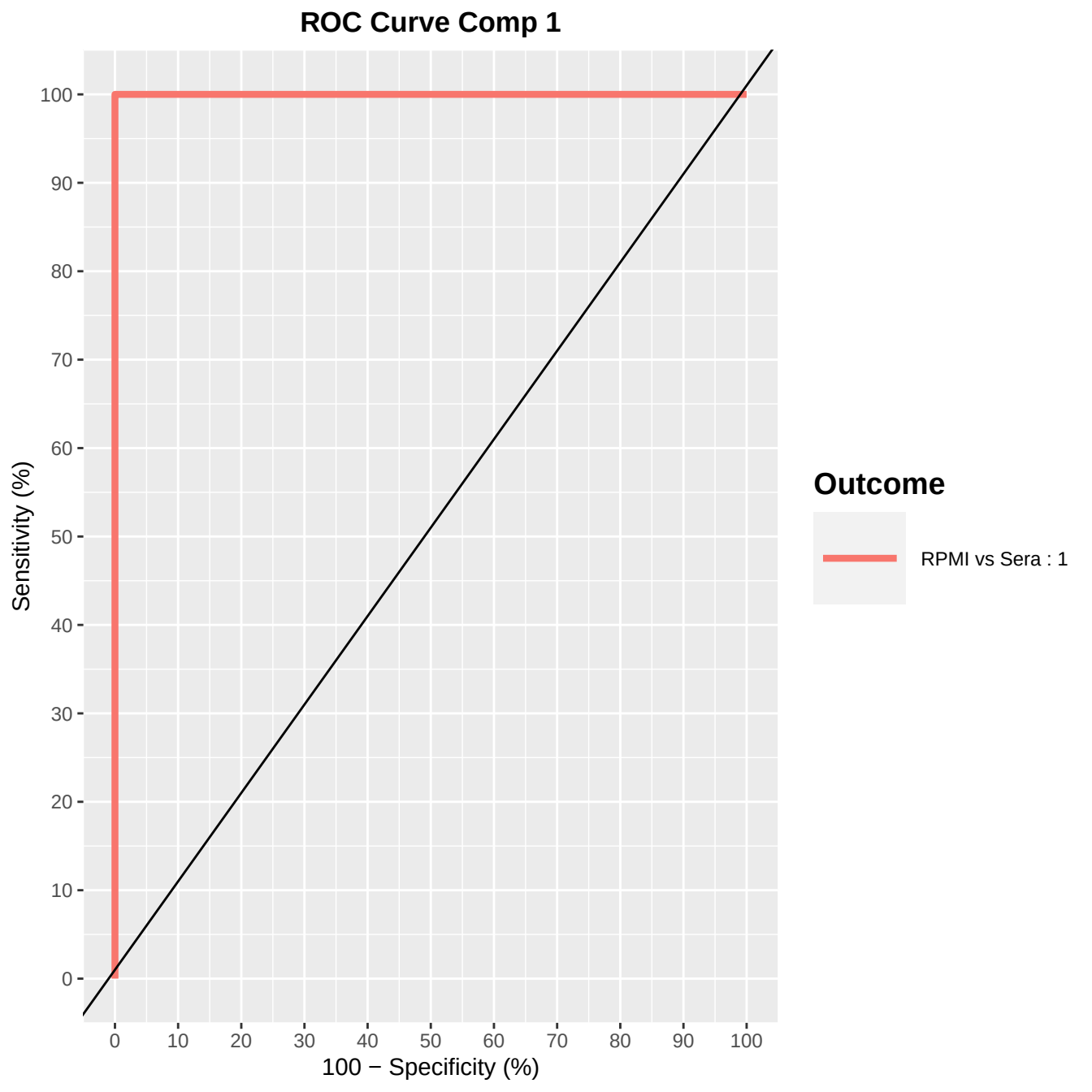


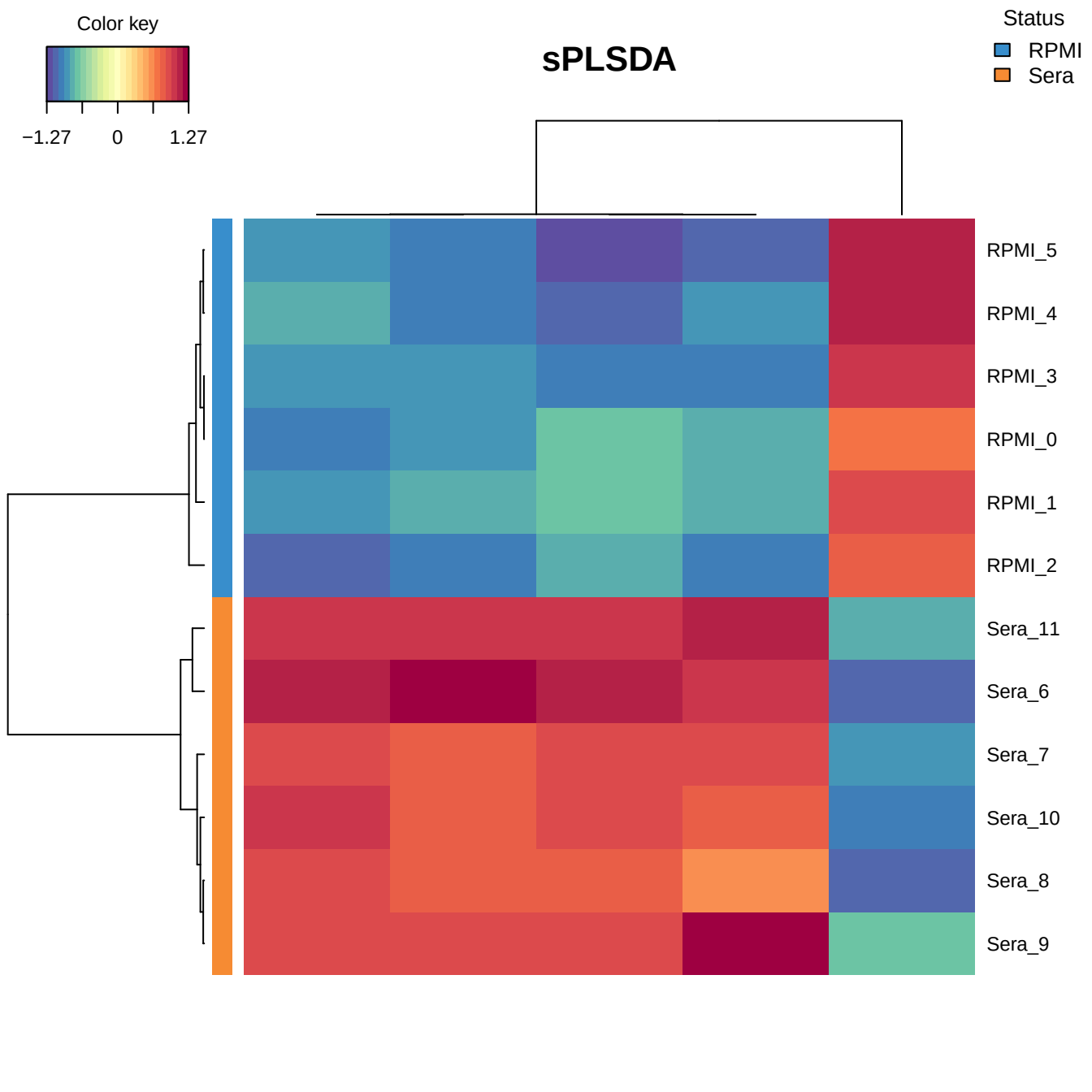

Contribution on comp 1
HMDB0000099
HMDB0003911
HMDB0000067
HMDB0000965
HMDB0001043
0.0
0.2
0.4
0.6
0.8
Outcome
RPMI
Sera

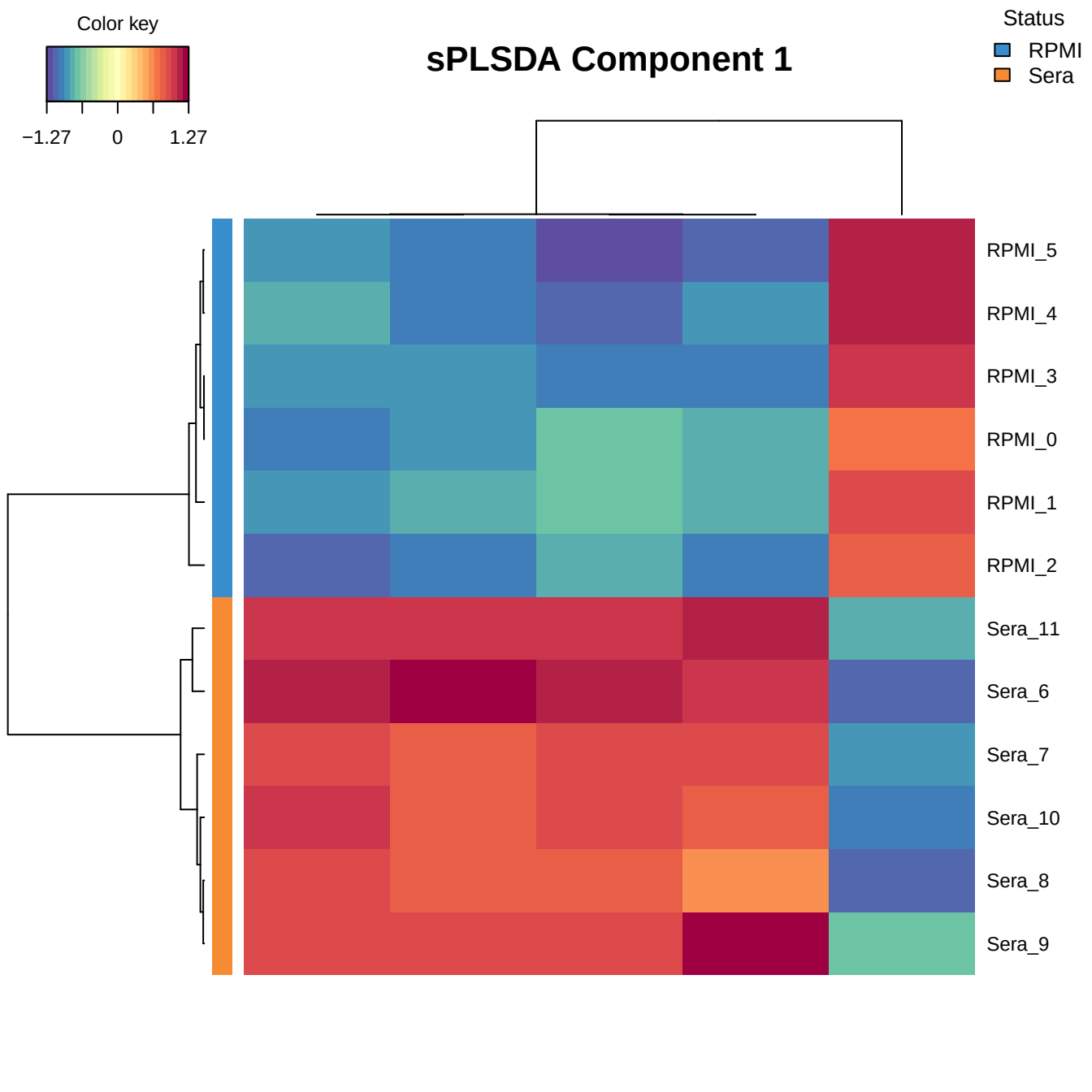

Contribution on comp 1
HMDB0000099
HMDB0003911
HMDB0000067
HMDB0000965
HMDB0001043
0.0
0.2
0.4
0.6
0.8
Outcome
RPMI
Sera


overall
BER
max.dist
centroids.dist
mahalanobis.dist
Classification error rate
1.0
0.5
0.0
−0.5
−1.0
1
Component

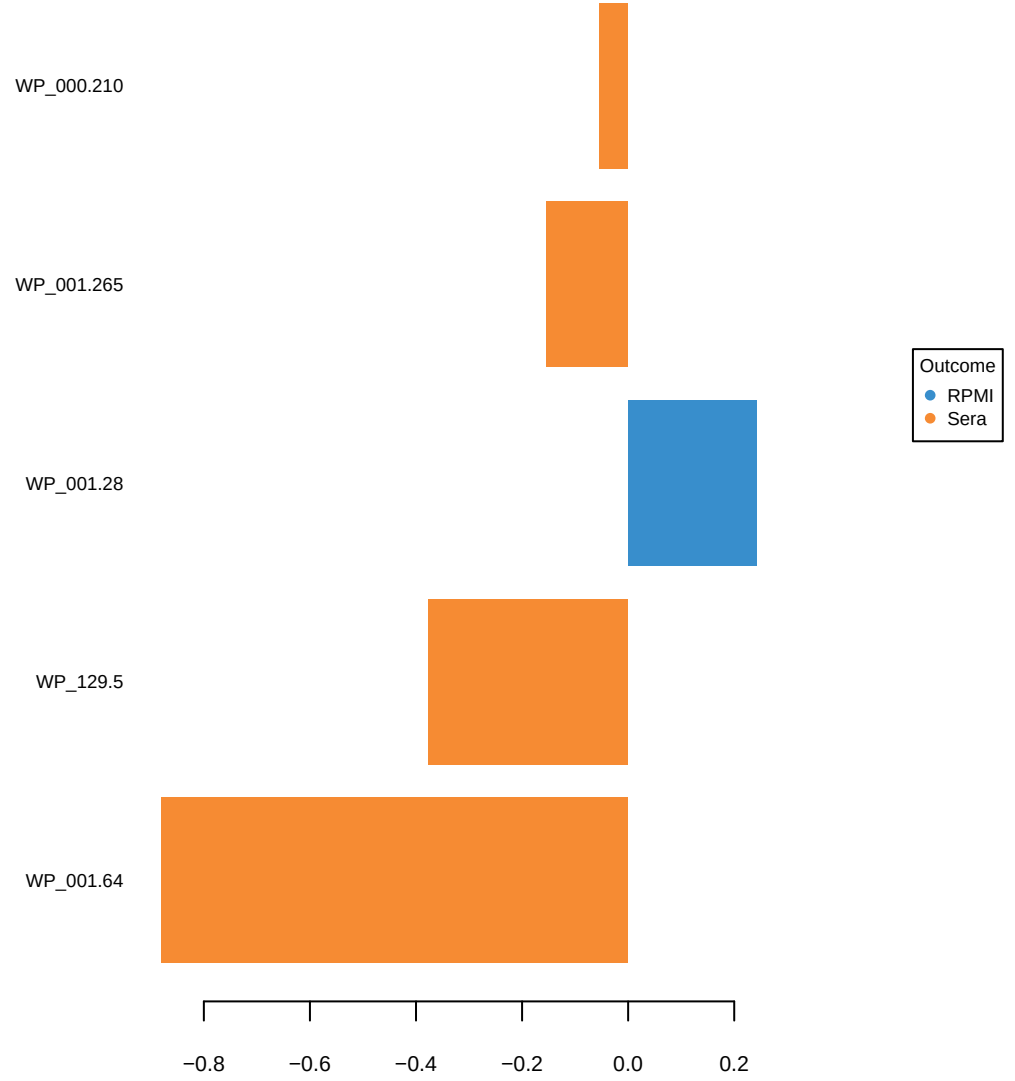

Comp 1
1.0
0.8
0.6
0.4
0.2
0.0
Stability
Features


ROC Curve Comp 1
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1

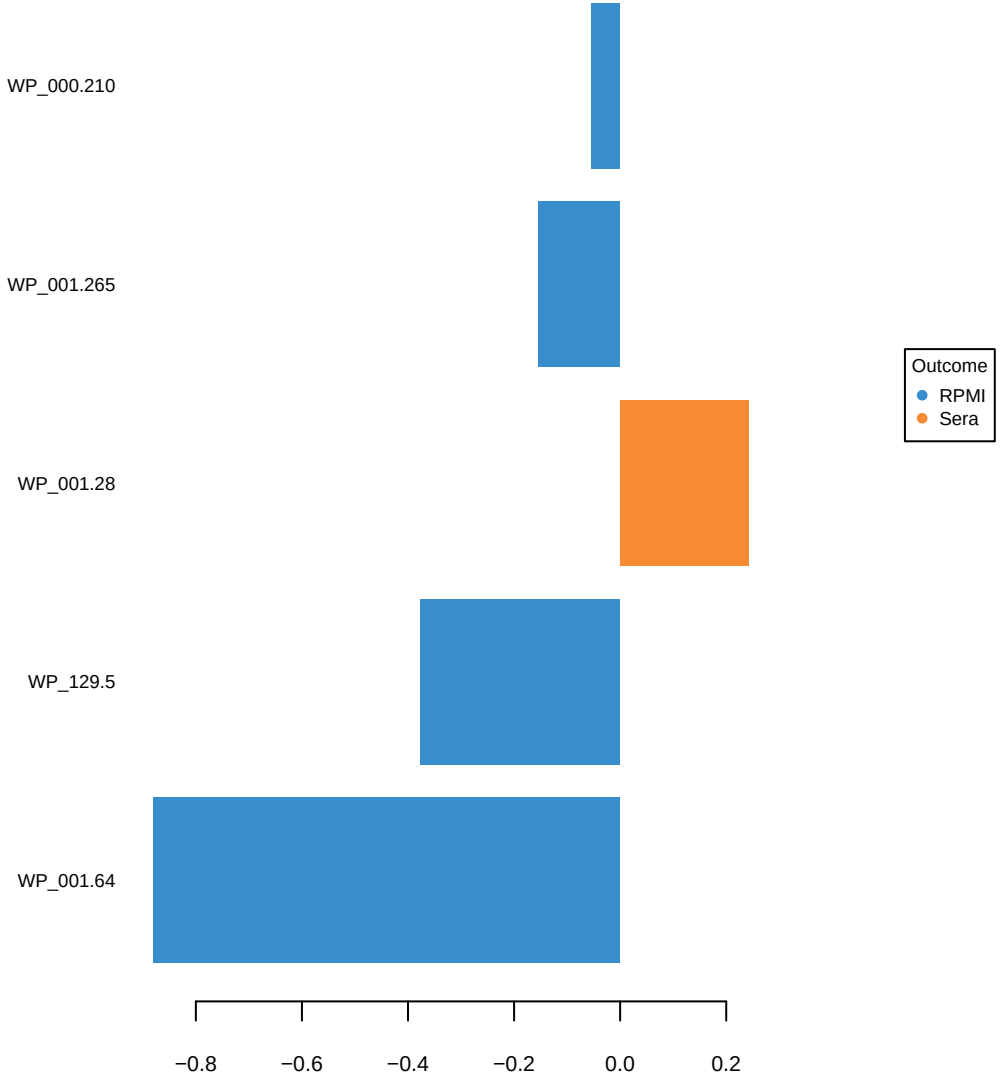

Color key
−1.27
0
1.27
sPLSDA
Status
RPMI
Sera
RPMI_5
RPMI_4
RPMI_3
RPMI_0
RPMI_1
RPMI_2
Sera_11
Sera_6
Sera_7
Sera_10
Sera_8
Sera_9

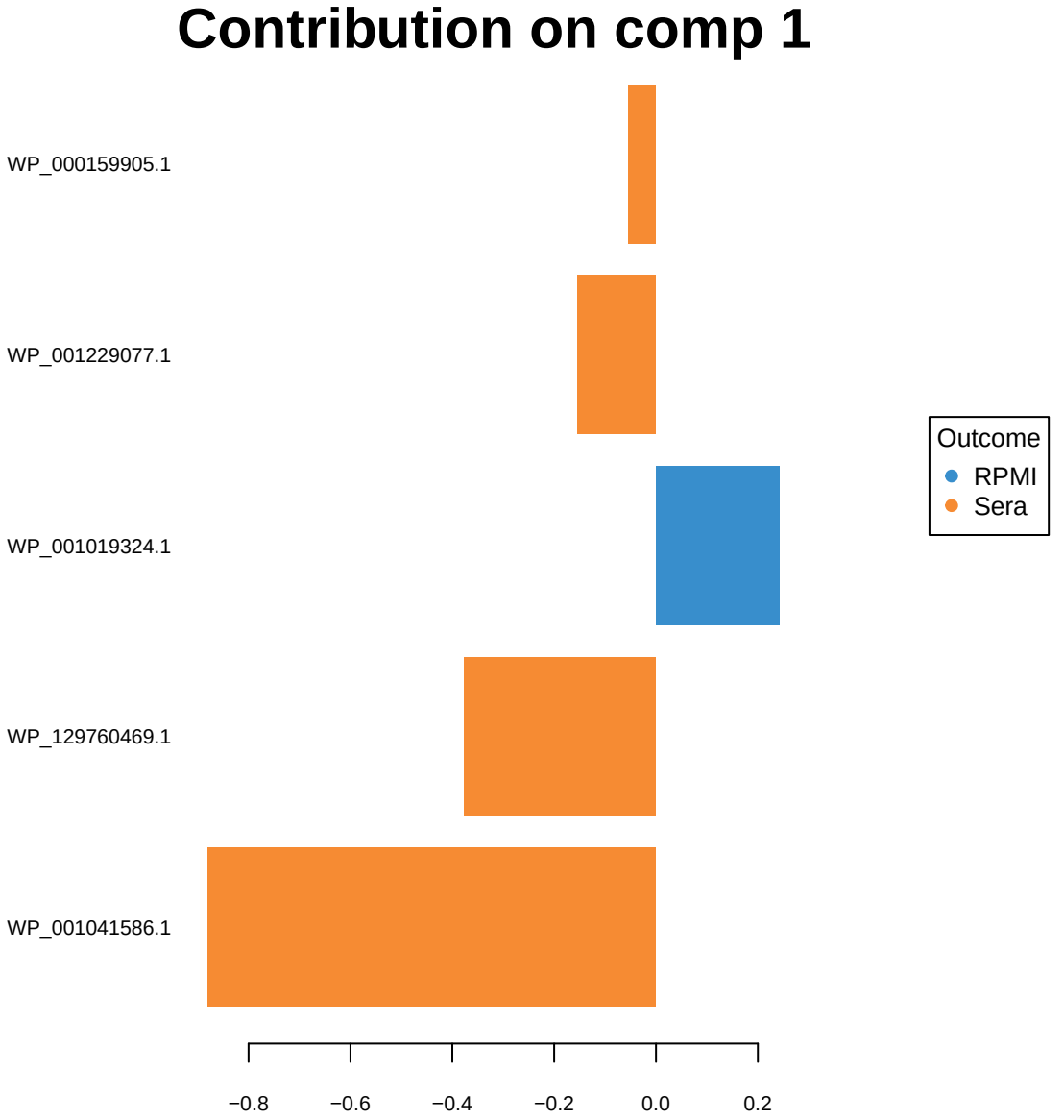

Color key
−1.27
0
1.27
sPLSDA Component 1
Status
RPMI
Sera
RPMI_5
RPMI_4
RPMI_3
RPMI_0
RPMI_1
RPMI_2
Sera_11
Sera_6
Sera_7
Sera_10
Sera_8
Sera_9

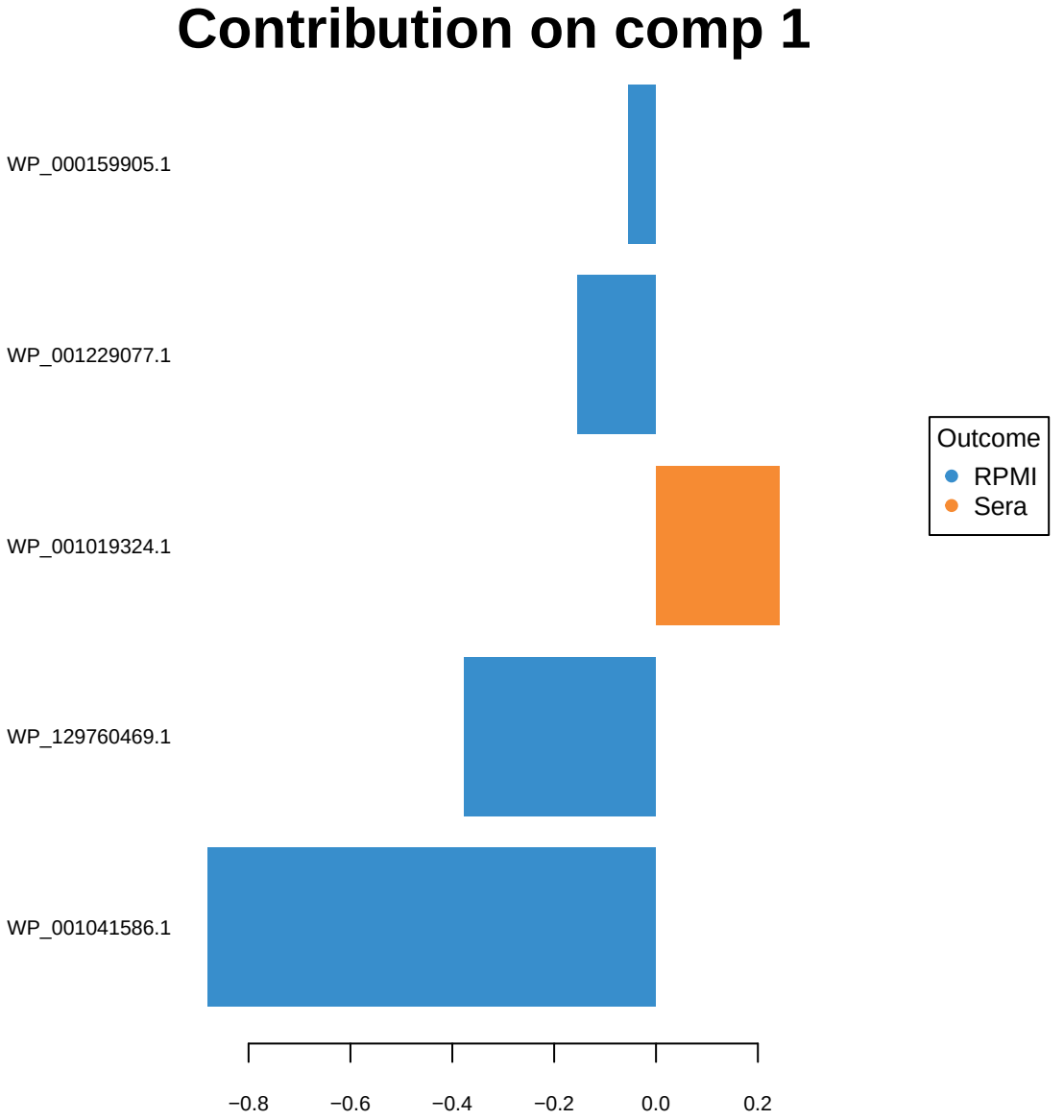
Proteomics 1 sPLSDA max load

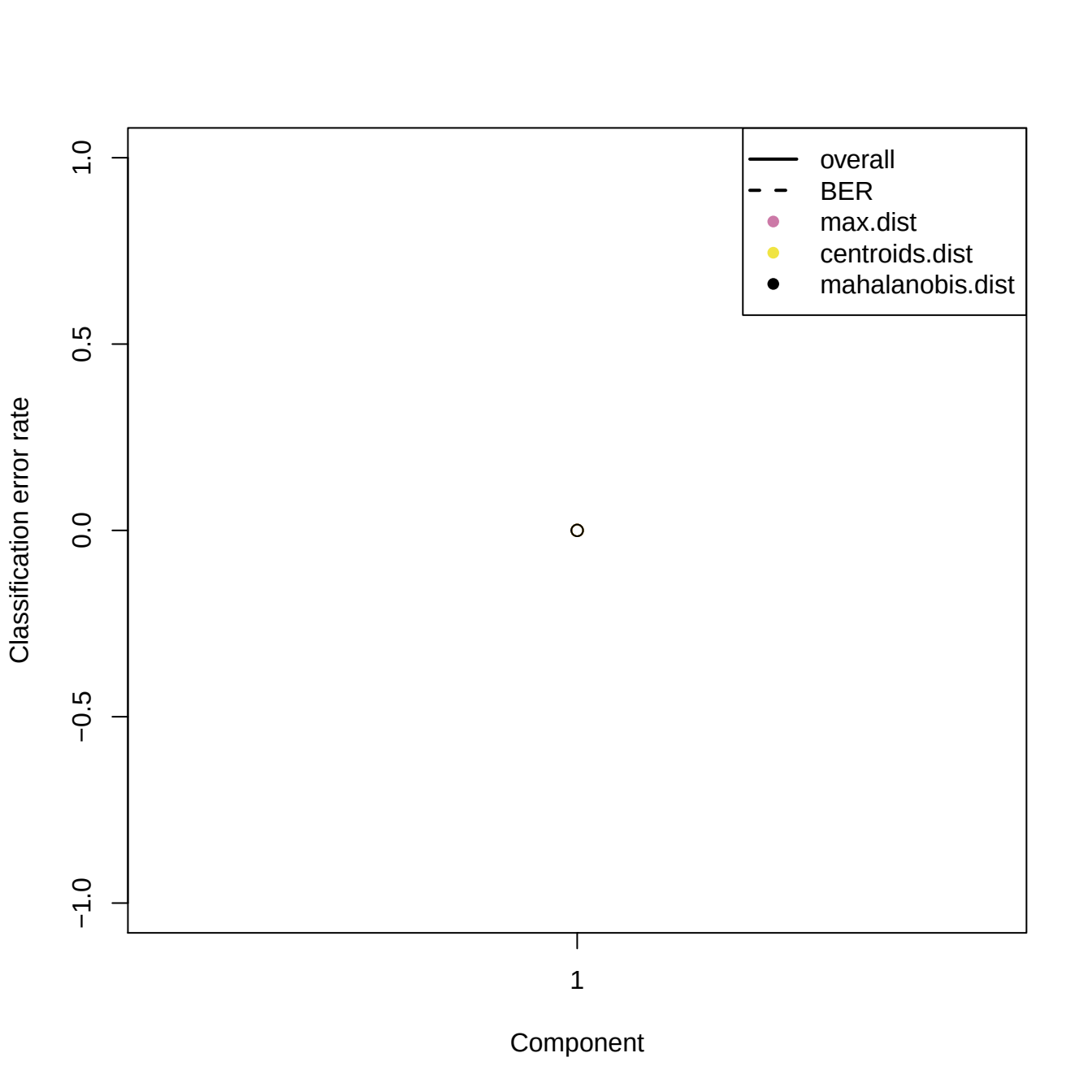


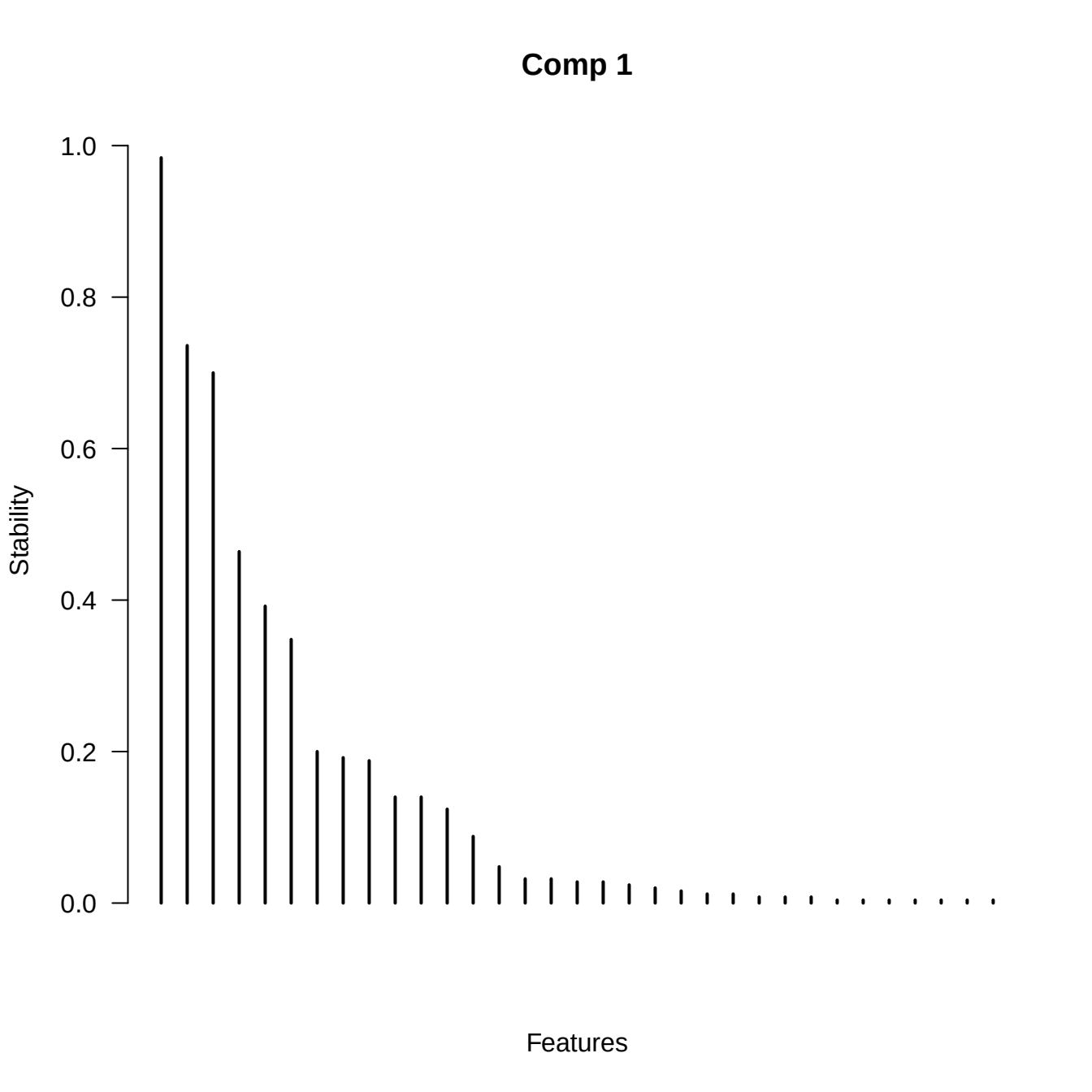
Proteomics 1 sPLSDA min load

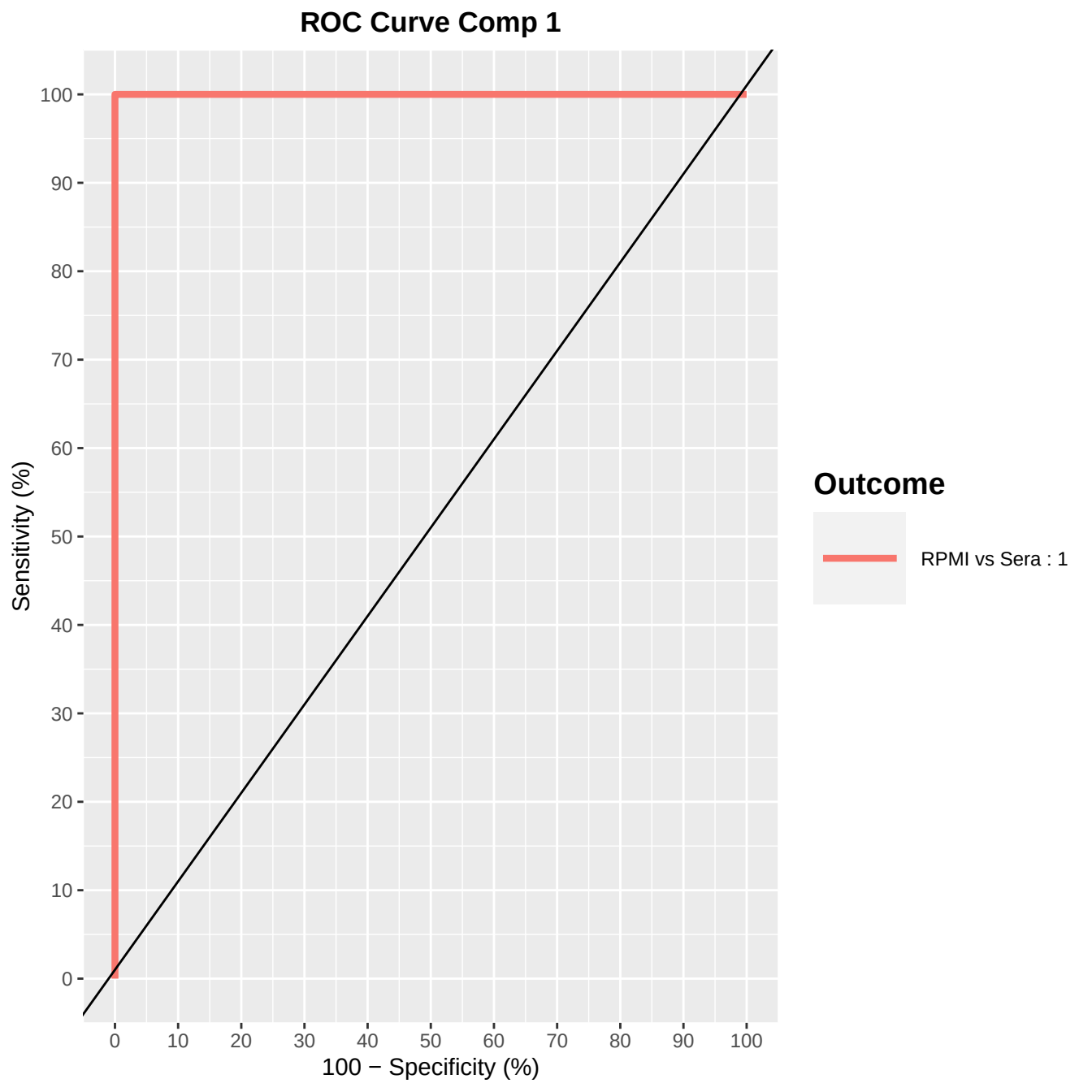


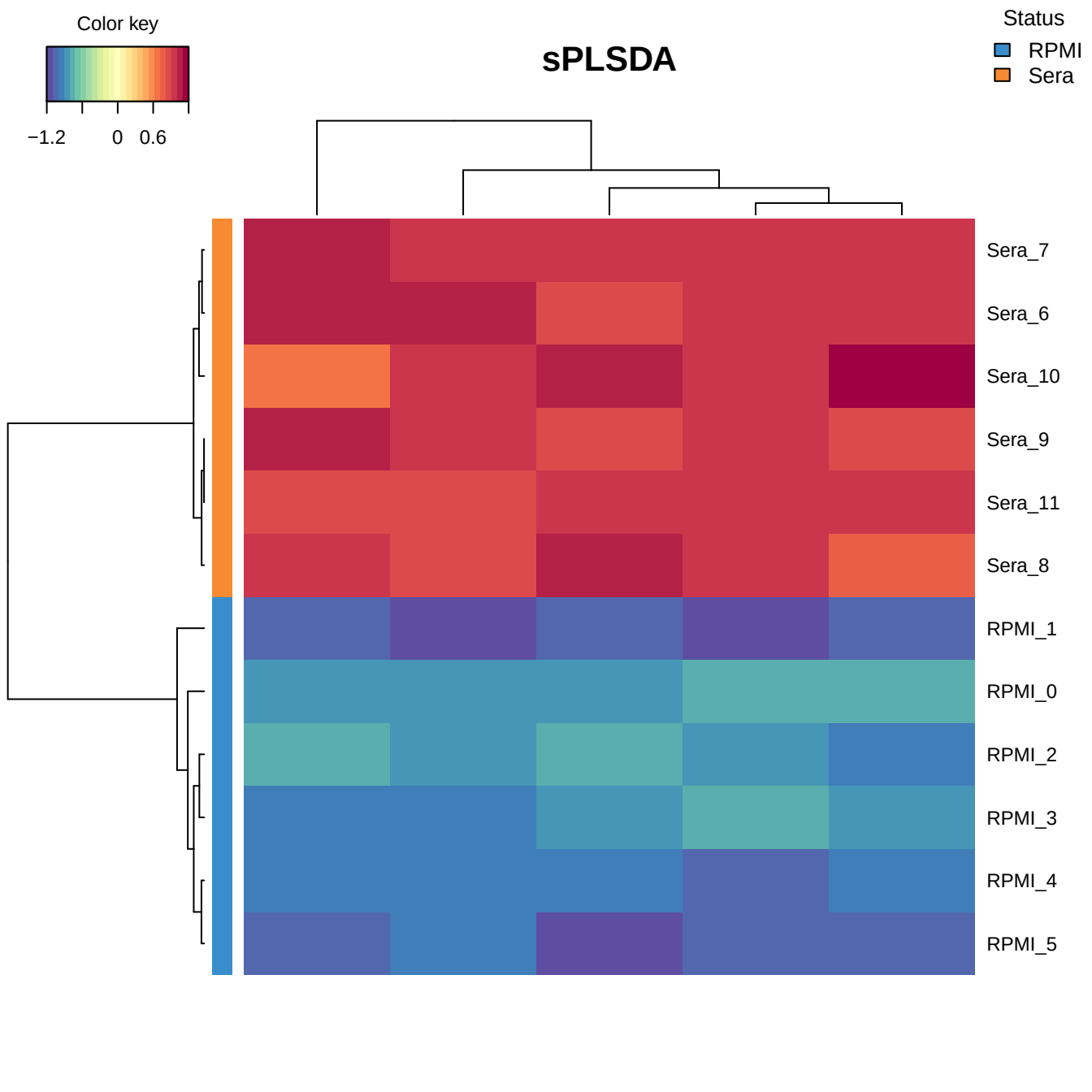

Contribution on comp 1
WP_000159905.1
WP_001229077.1
WP_001019324.1
WP_129760469.1
WP_001041586.1
−0.8
−0.6
−0.4
−0.2
0.0
0.2
Outcome
RPMI
Sera

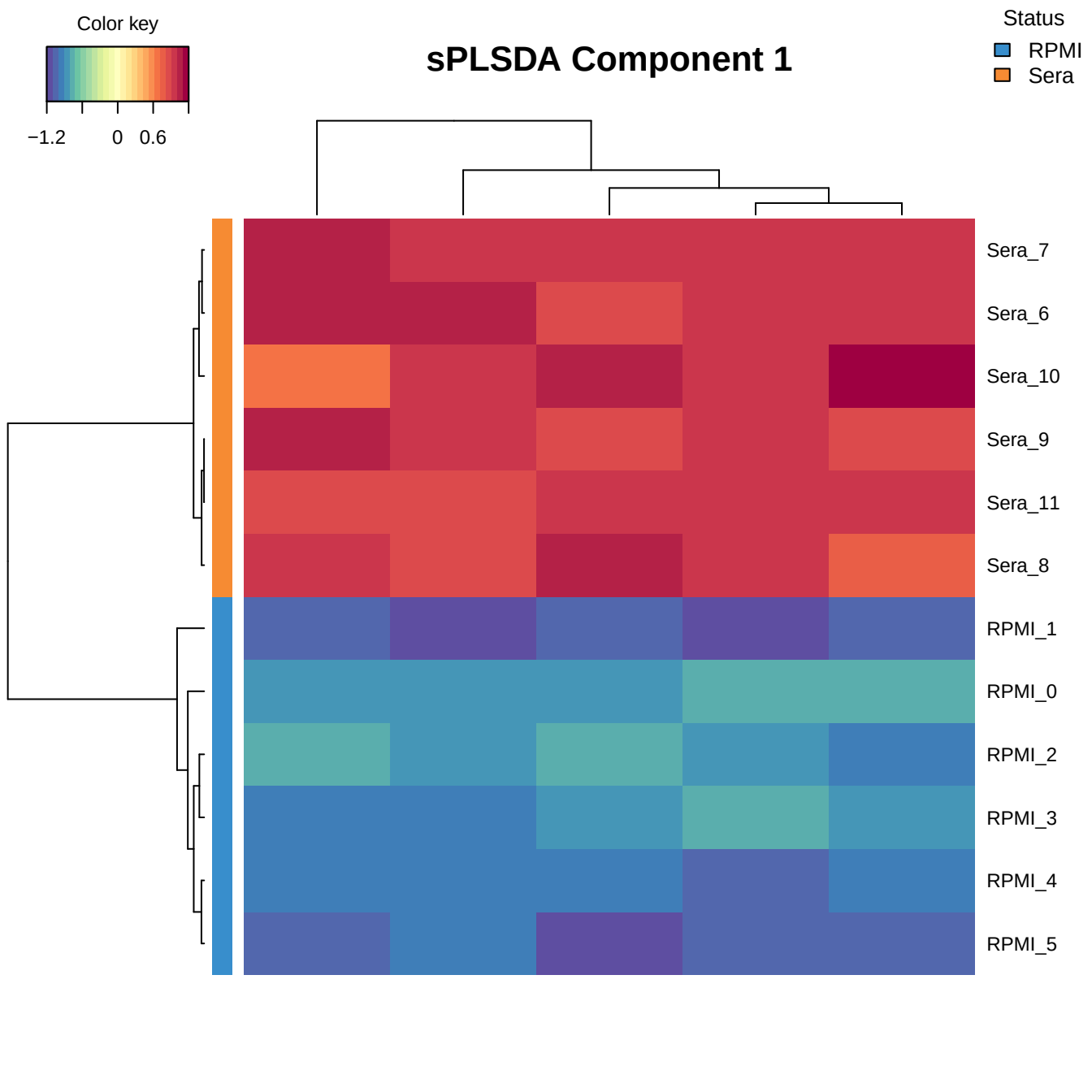

Contribution on comp 1
WP_000159905.1
WP_001229077.1
WP_001019324.1
WP_129760469.1
WP_001041586.1
−0.8
−0.6
−0.4
−0.2
0.0
0.2
Outcome
RPMI
Sera


overall
BER
max.dist
centroids.dist
mahalanobis.dist
Classification error rate
1.0
0.5
0.0
−0.5
−1.0
1
Component

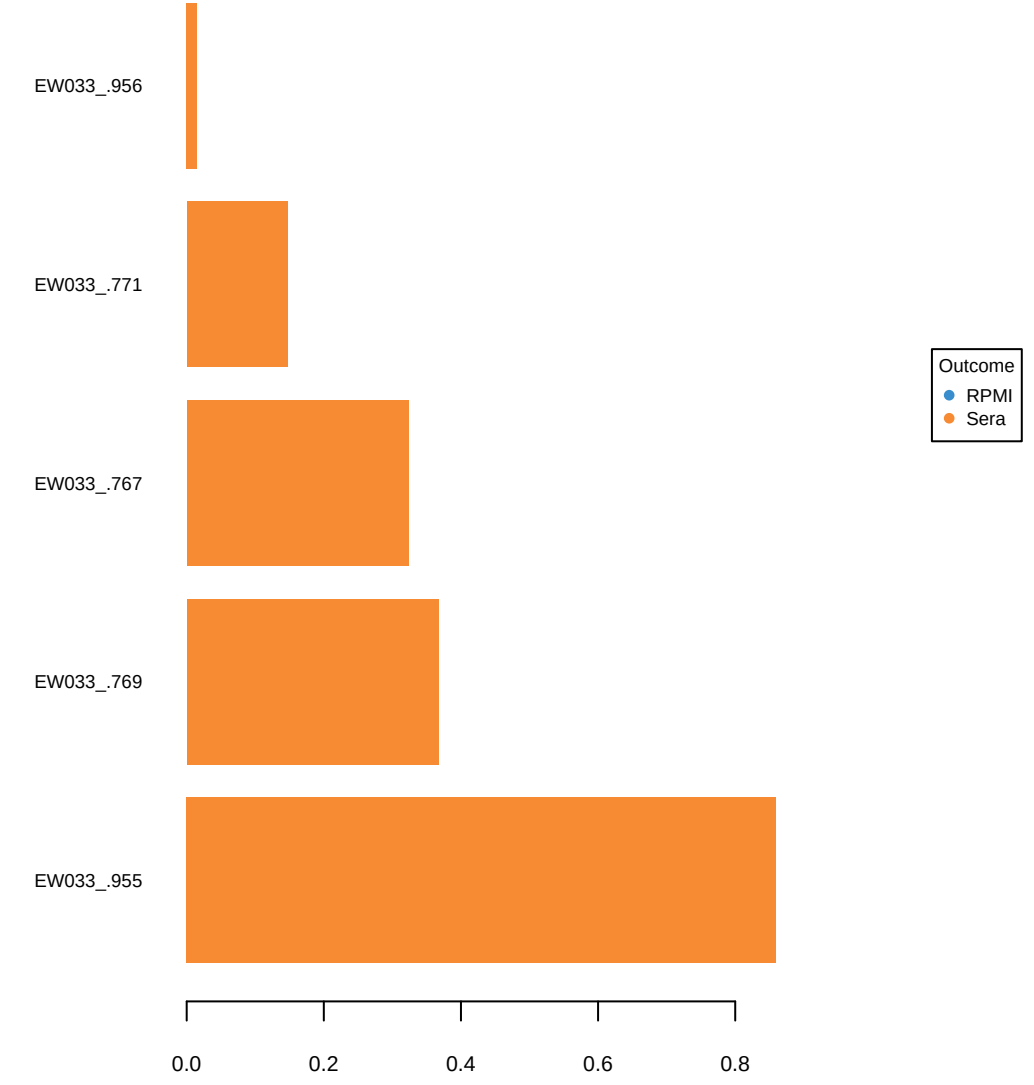

Comp 1
1.0
0.8
0.6
0.4
0.2
0.0
Stability
Features


ROC Curve Comp 1
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1

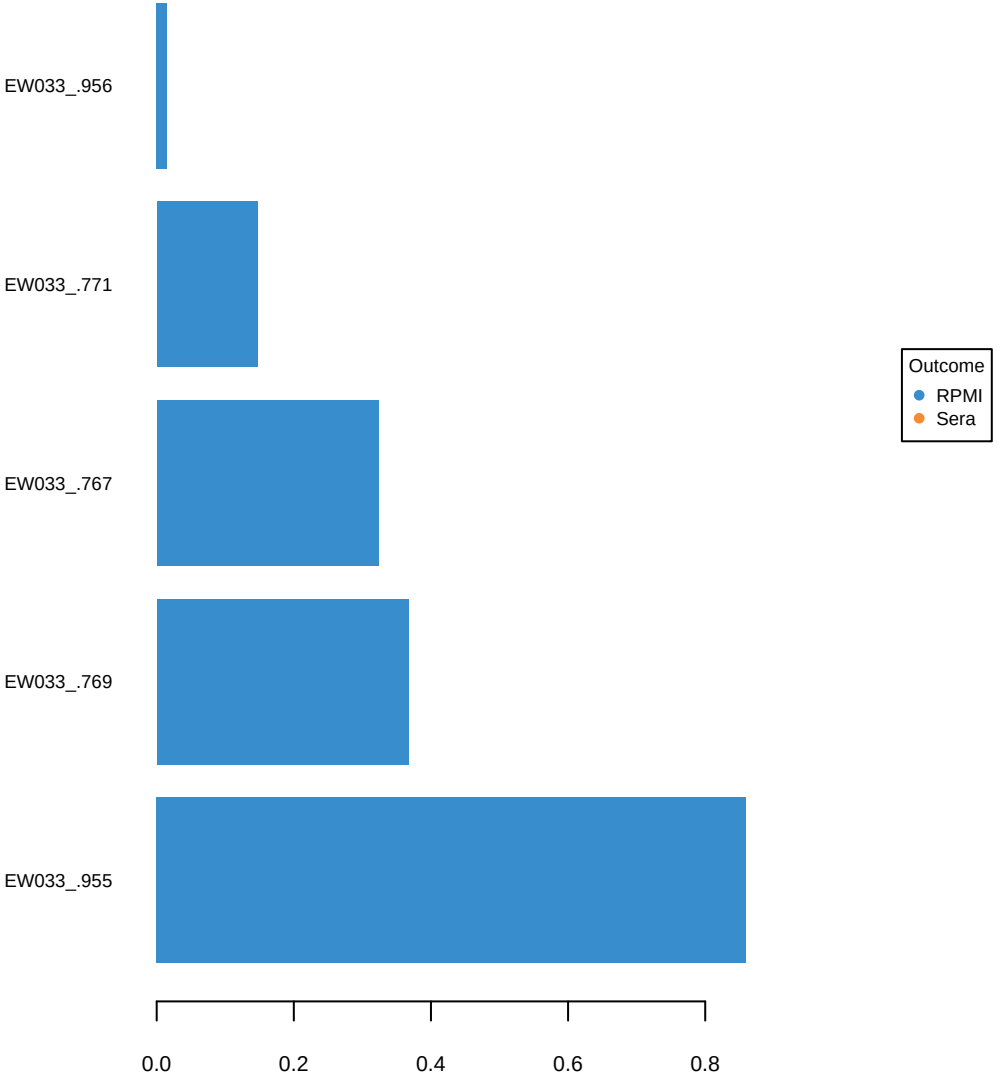

sPLSDA
Color key
−1.2
0
0.6
Status
RPMI
Sera
Sera_7
Sera_6
Sera_10
Sera_9
Sera_11
Sera_8
RPMI_1
RPMI_0
RPMI_2
RPMI_3
RPMI_4
RPMI_5

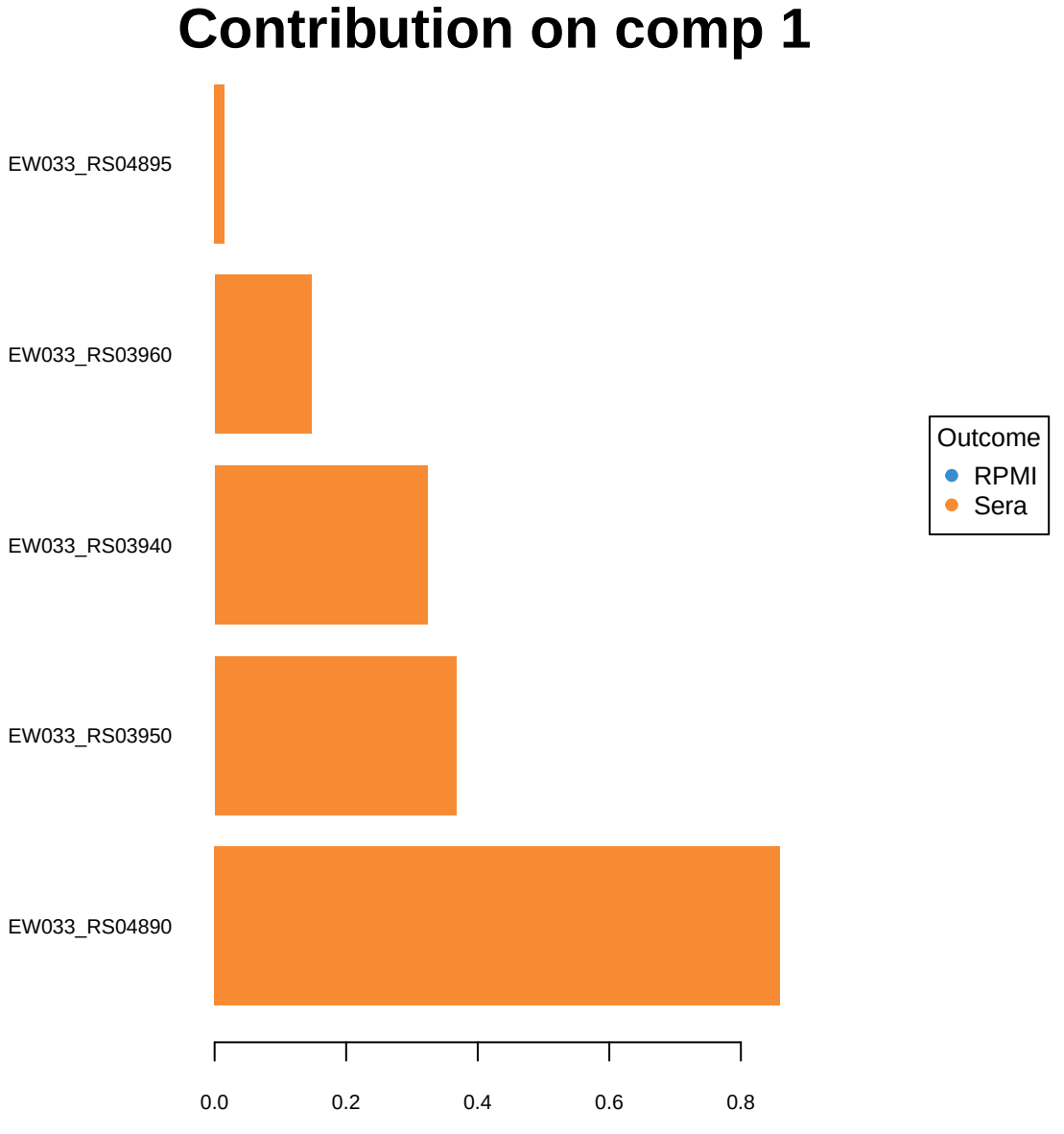

Color key
−1.2
0
0.6
sPLSDA Component 1
Status
RPMI
Sera
Sera_7
Sera_6
Sera_10
Sera_9
Sera_11
Sera_8
RPMI_1
RPMI_0
RPMI_2
RPMI_3
RPMI_4
RPMI_5

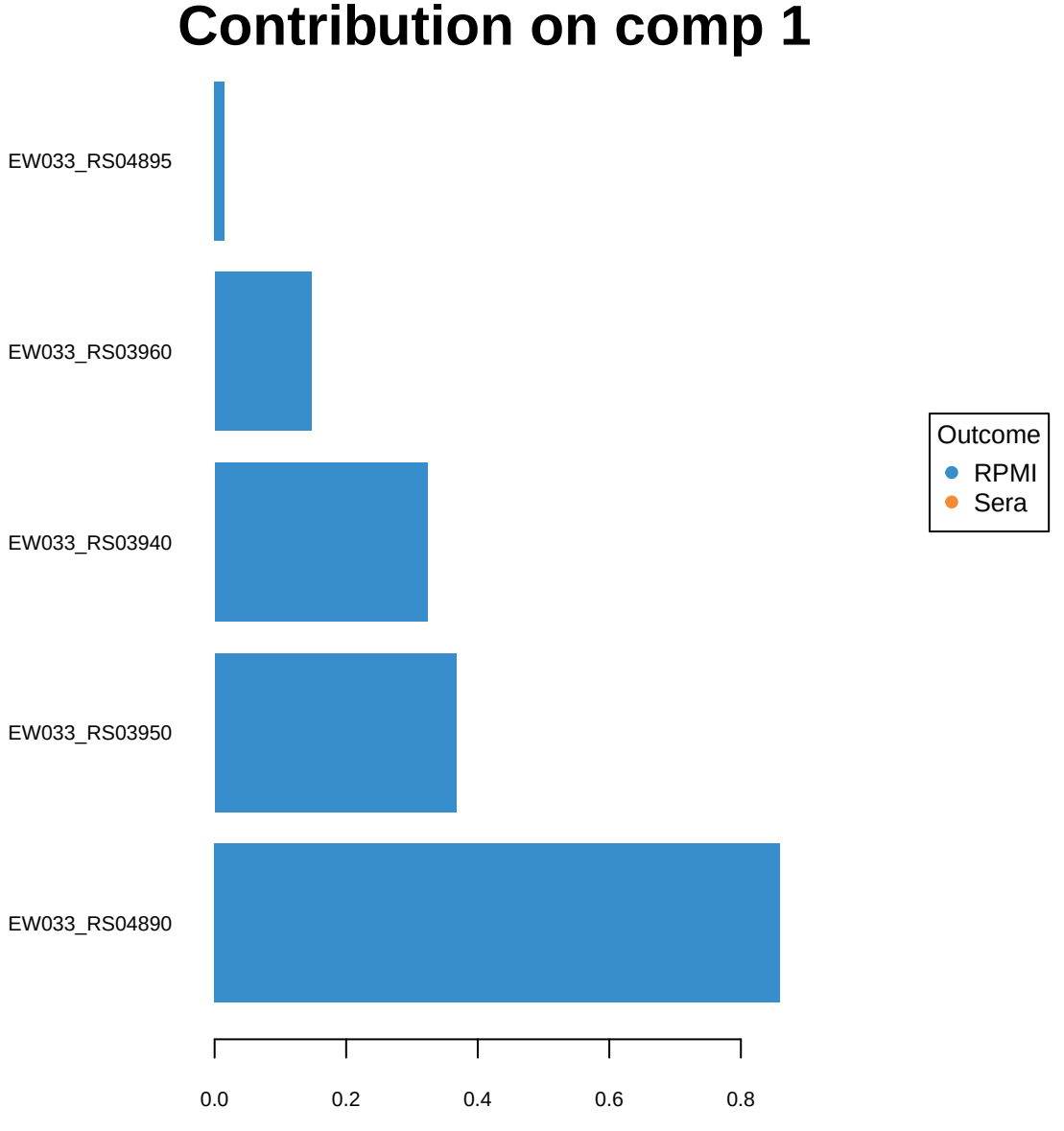
RNA_Seq 1 sPLSDA max loadi

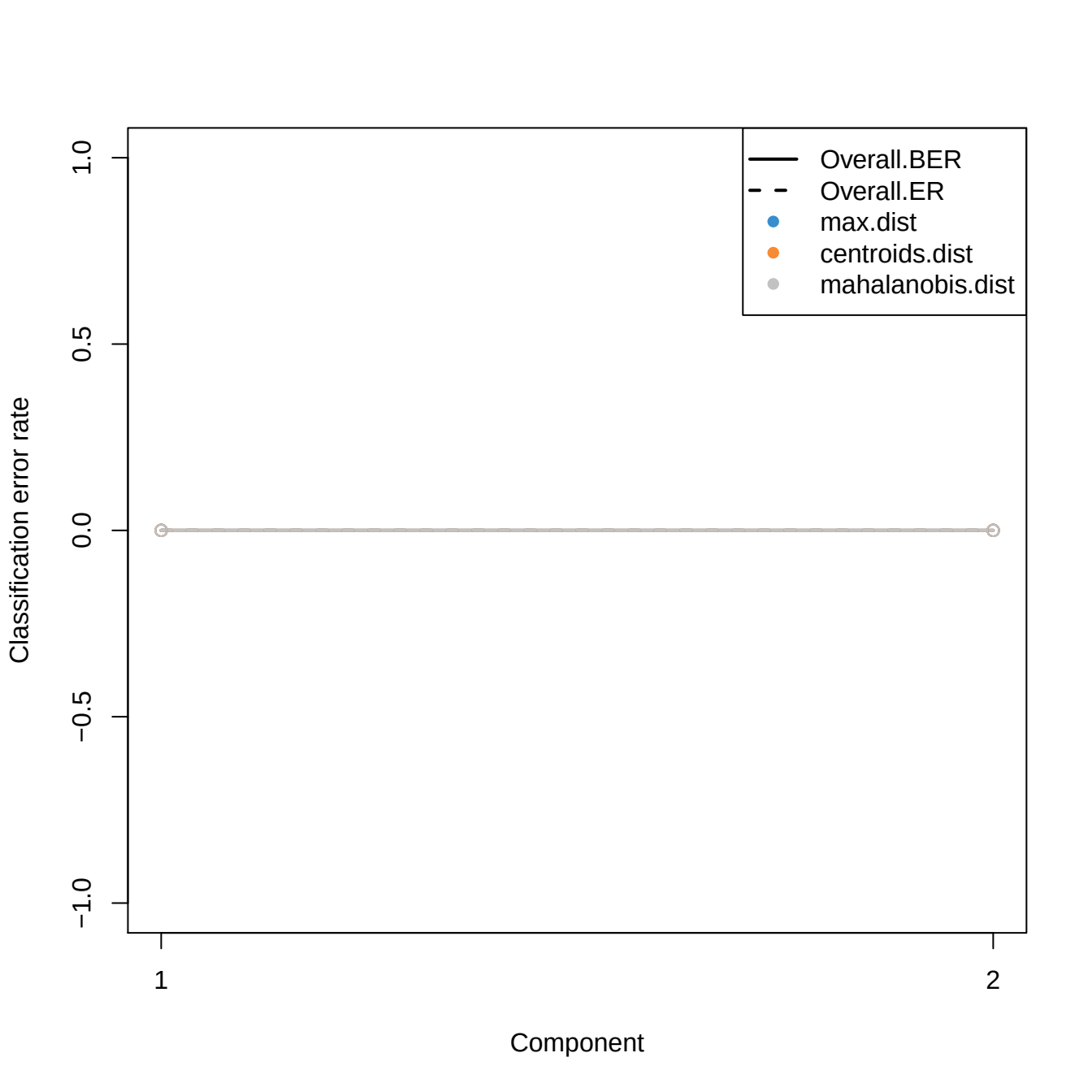


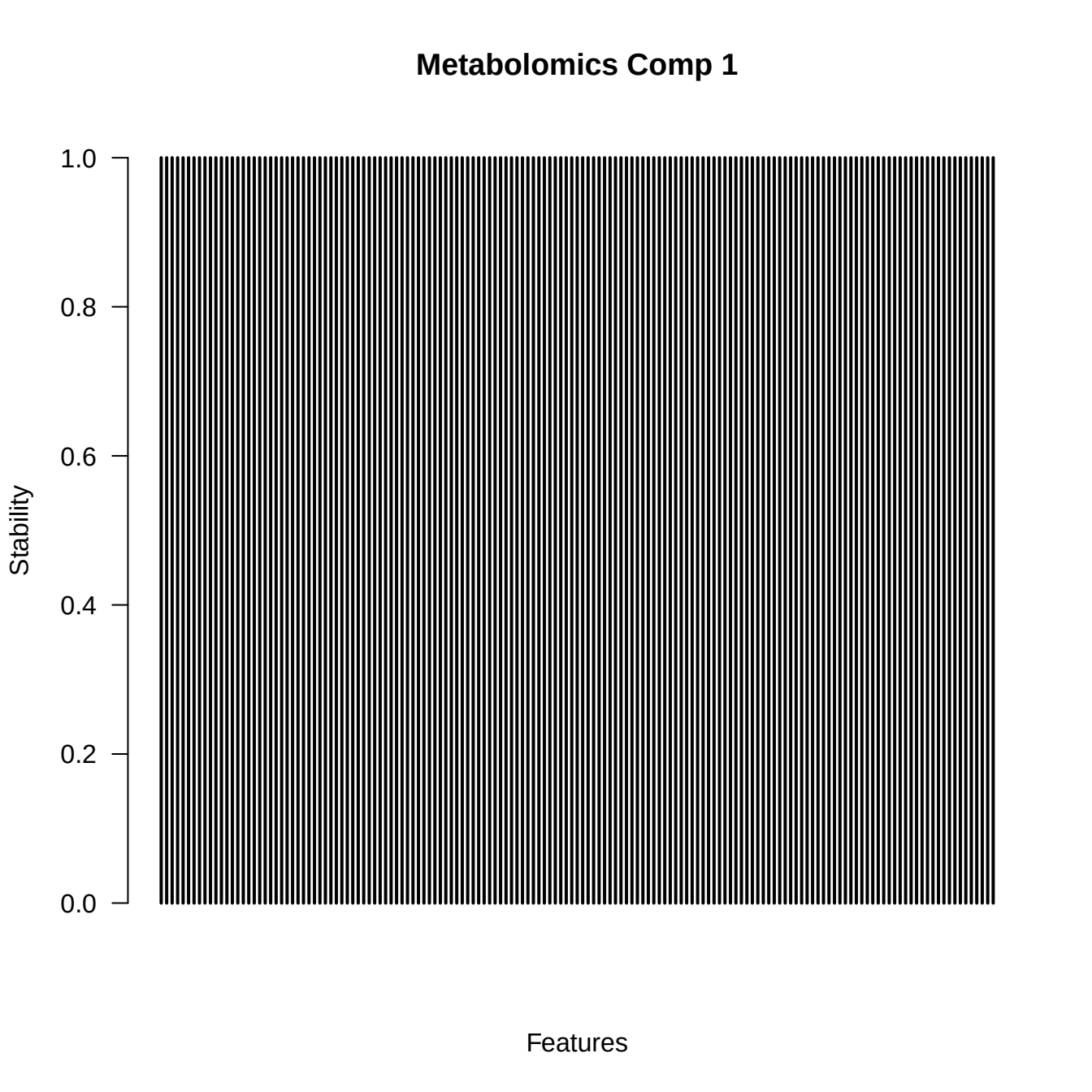
RNA_Seq 1 sPLSDA min loadi

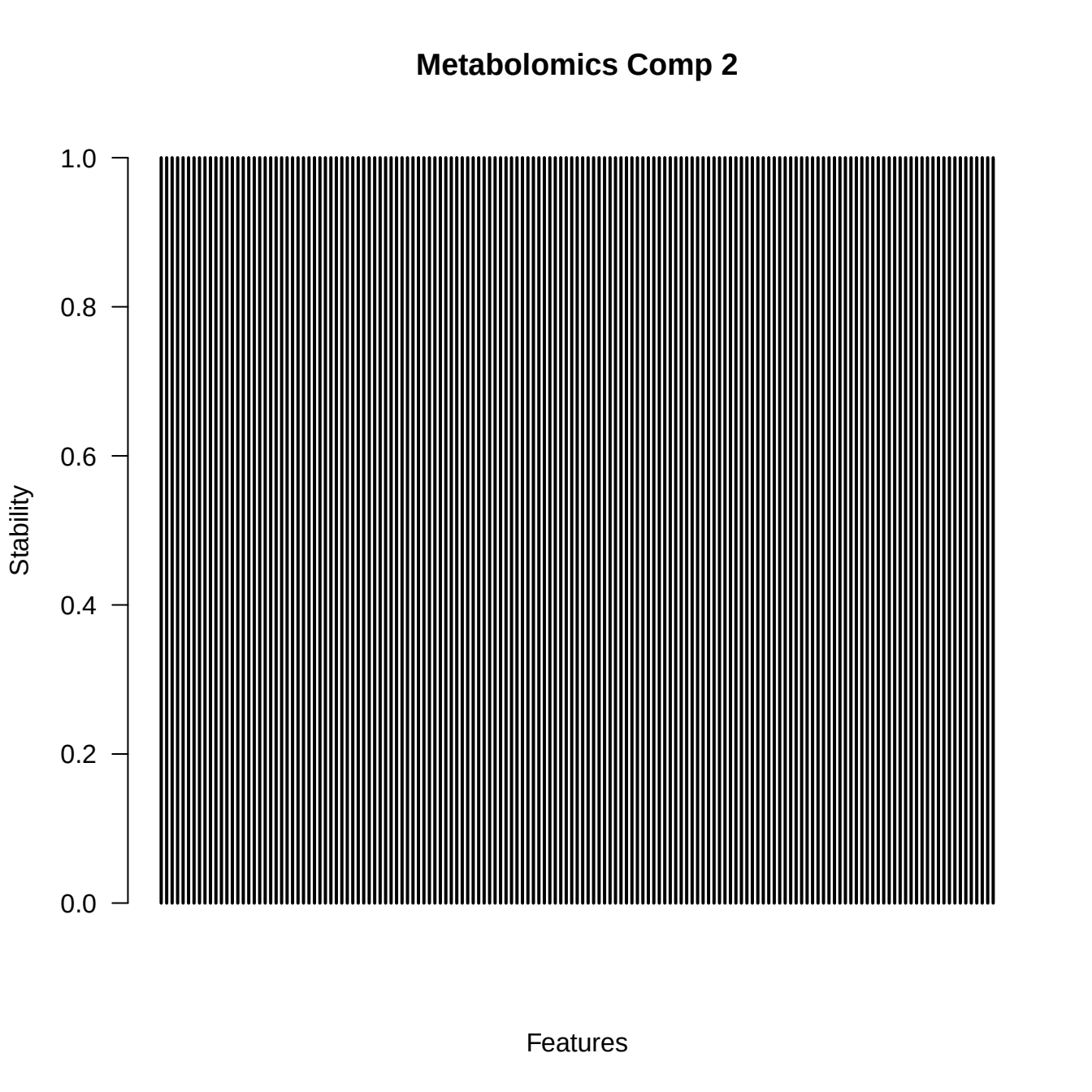


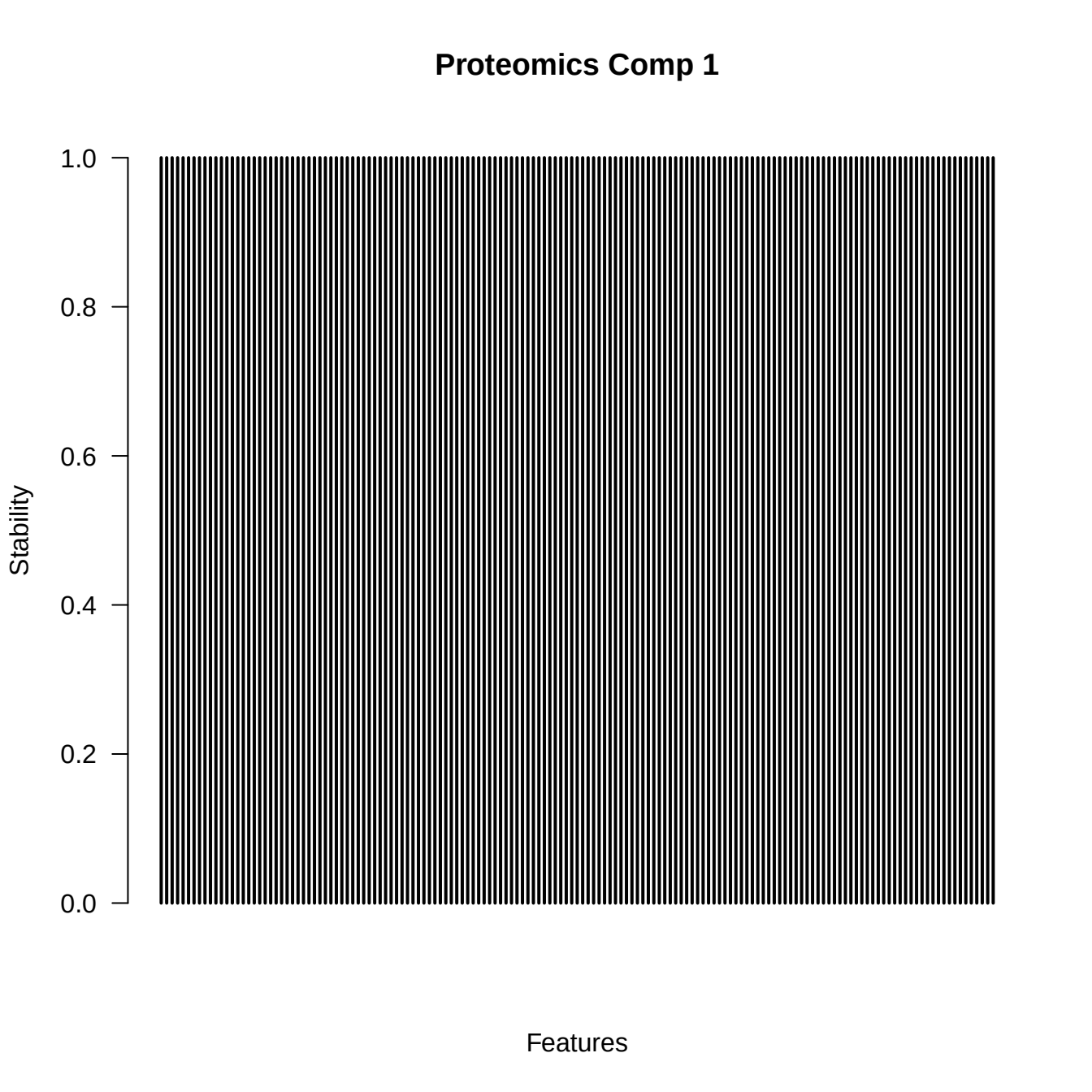

Contribution on comp 1
EW033_RS04895
EW033_RS03960
EW033_RS03940
EW033_RS03950
EW033_RS04890
0.0
0.2
0.4
0.6
0.8
Outcome
RPMI
Sera


Contribution on comp 1
EW033_RS04895
EW033_RS03960
EW033_RS03940
EW033_RS03950
EW033_RS04890
0.0
0.2
0.4
0.6
0.8
Outcome
RPMI
Sera


Overall.BER
Overall.ER
max.dist
centroids.dist
mahalanobis.dist
Classification error rate
1.0
0.5
0.0
−0.5
−1.0
1
2
Component


Metabolomics Comp 1
1.0
0.8
0.6
0.4
0.2
0.0
Stability
Features


Metabolomics Comp 2
1.0
0.8
0.6
0.4
0.2
0.0
Stability
Features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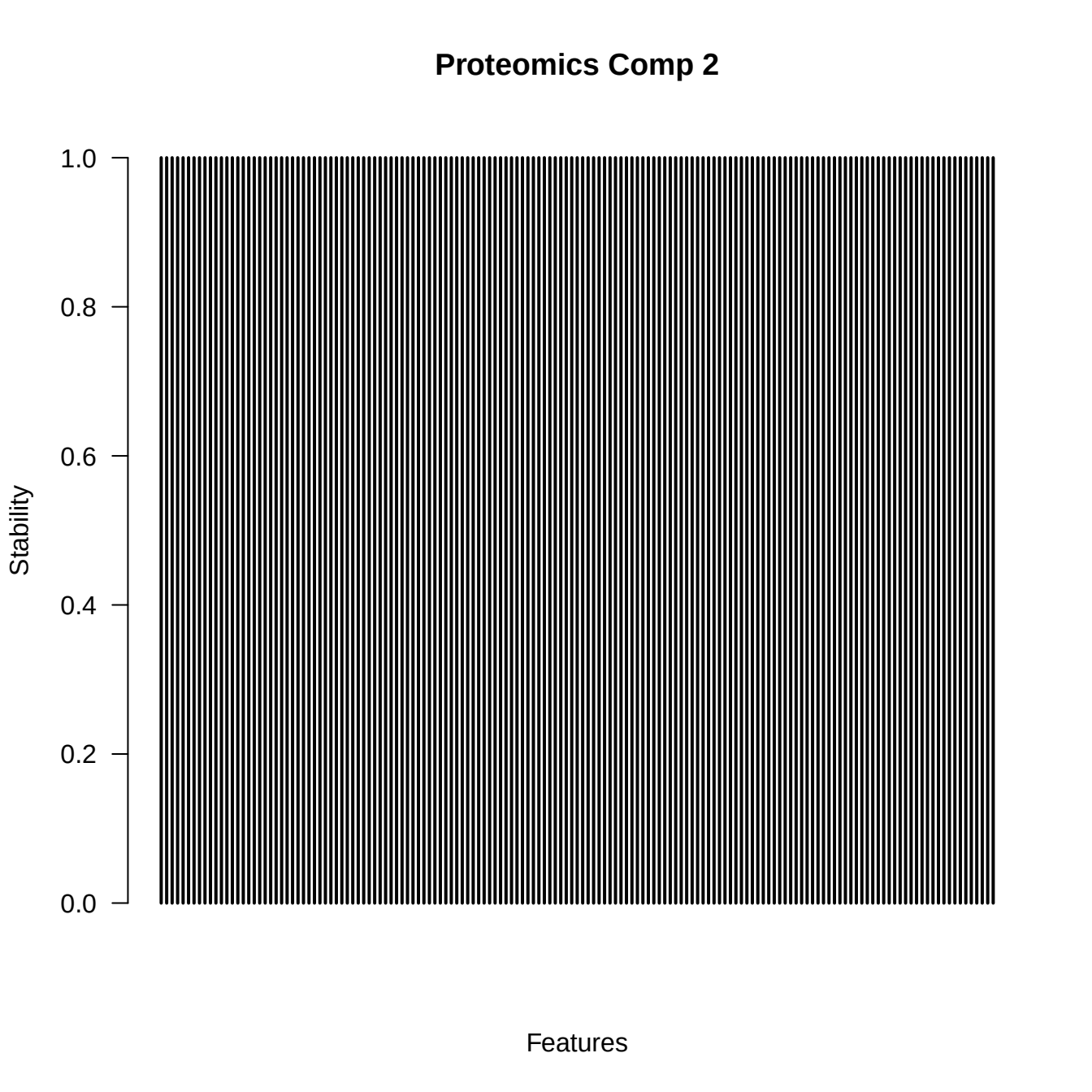
Stability
Features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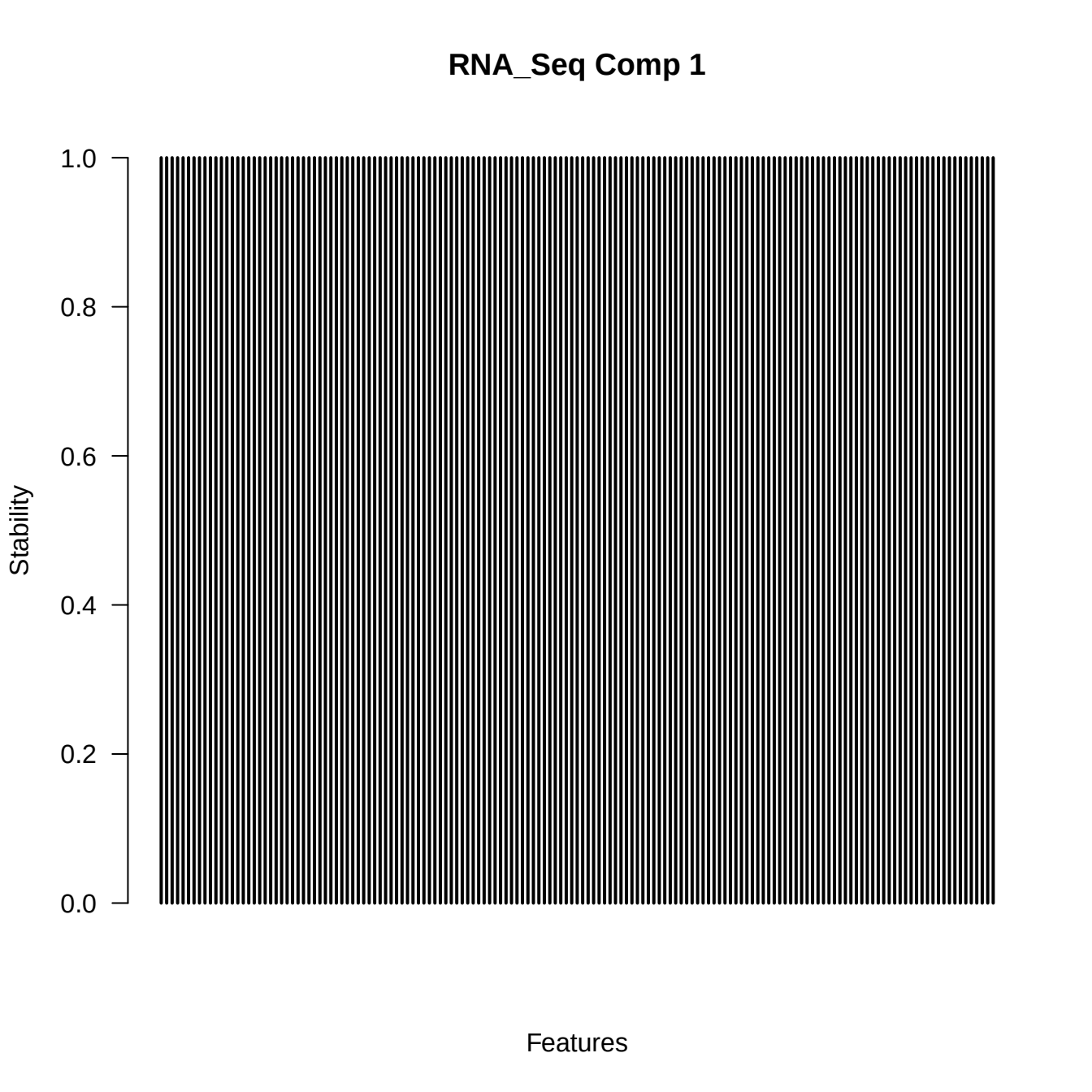
Features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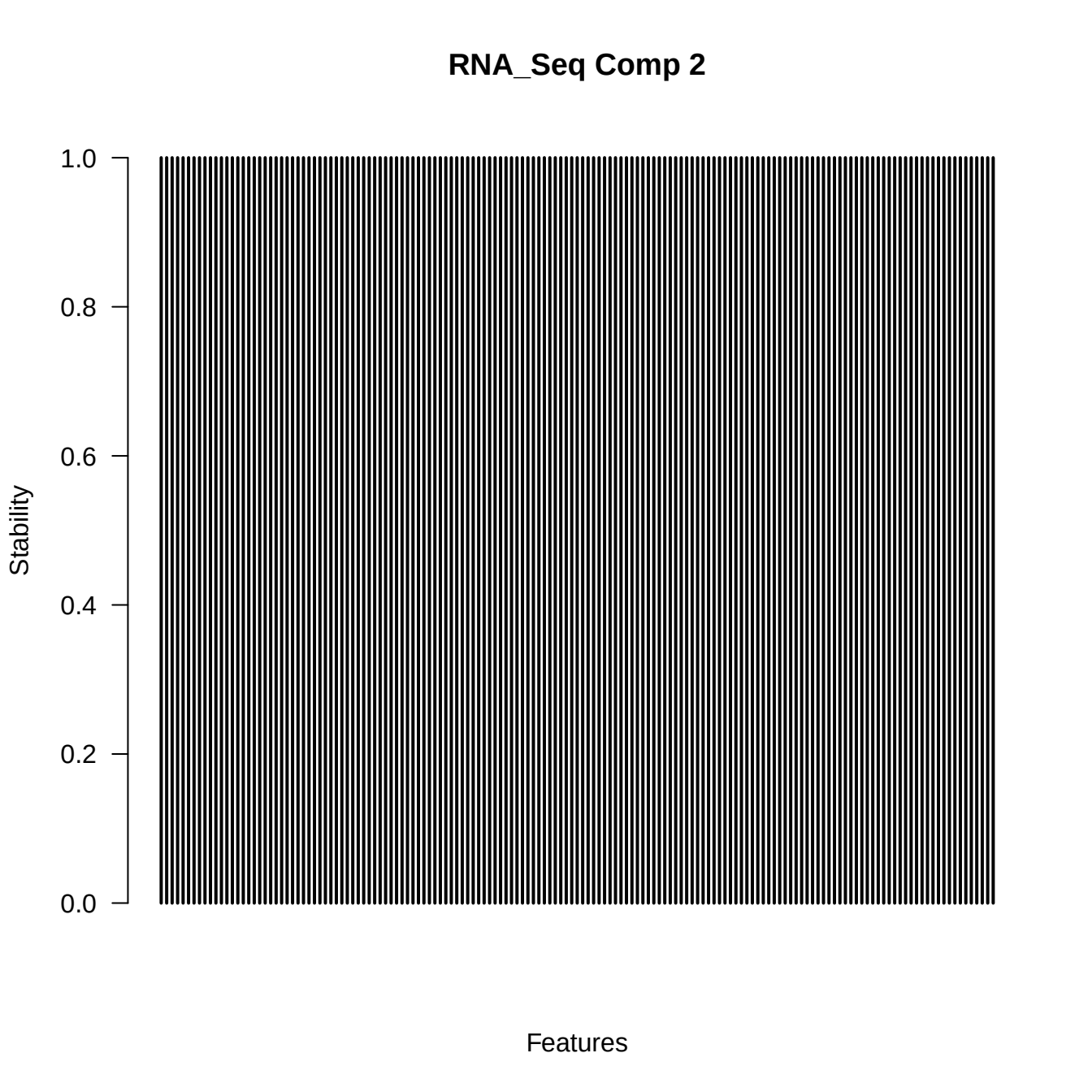
Stability
Features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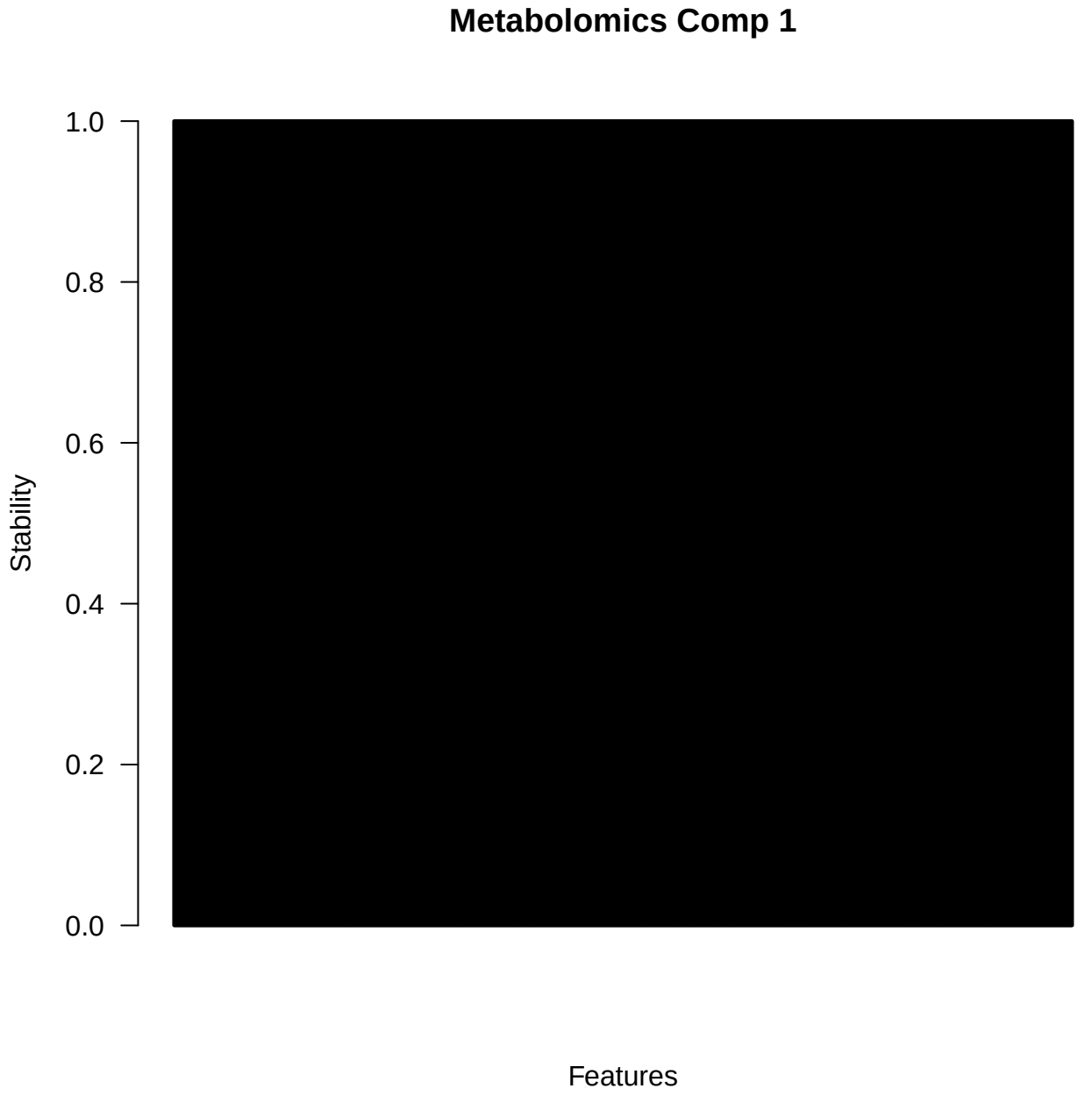
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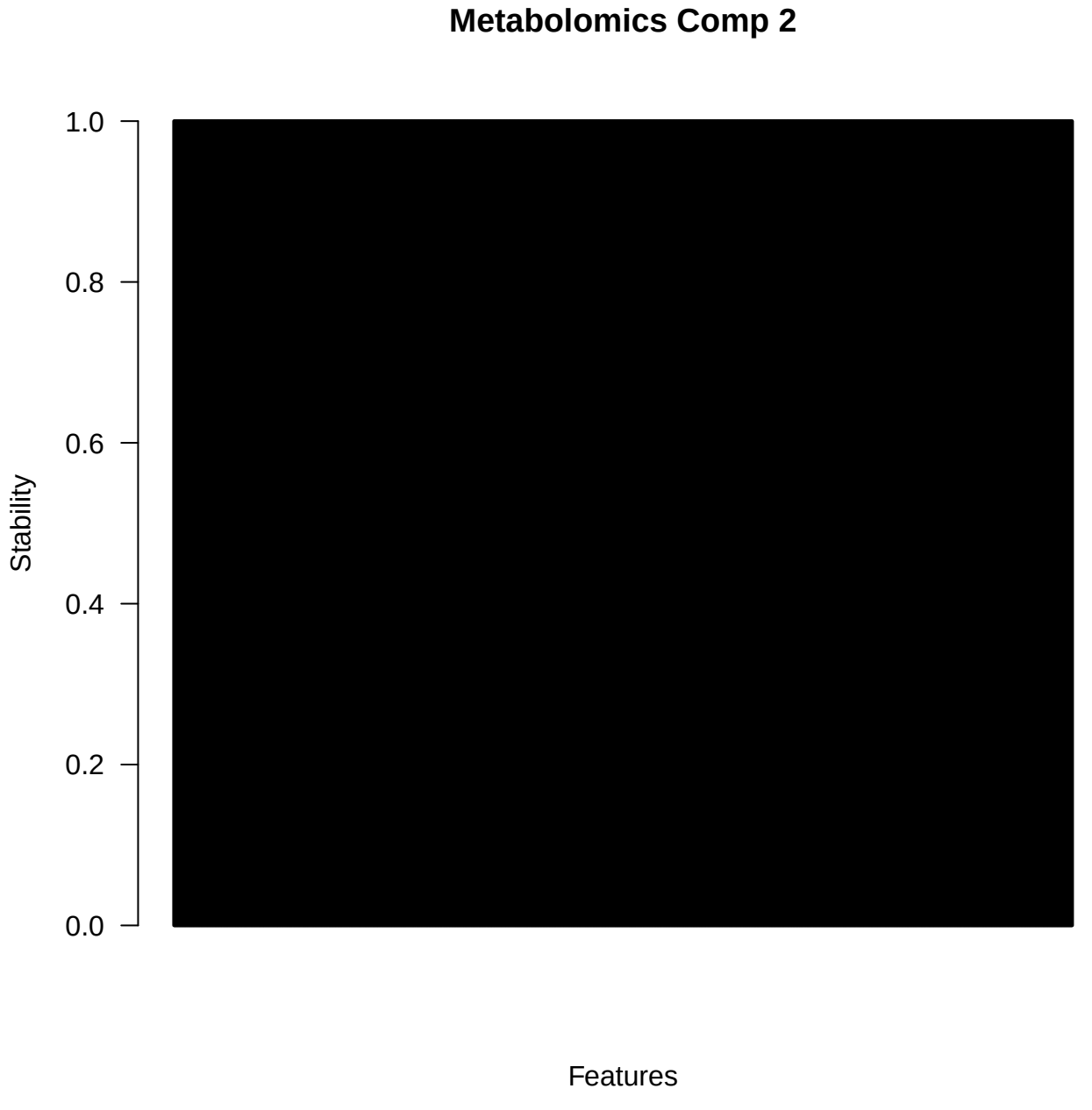
Stability
Features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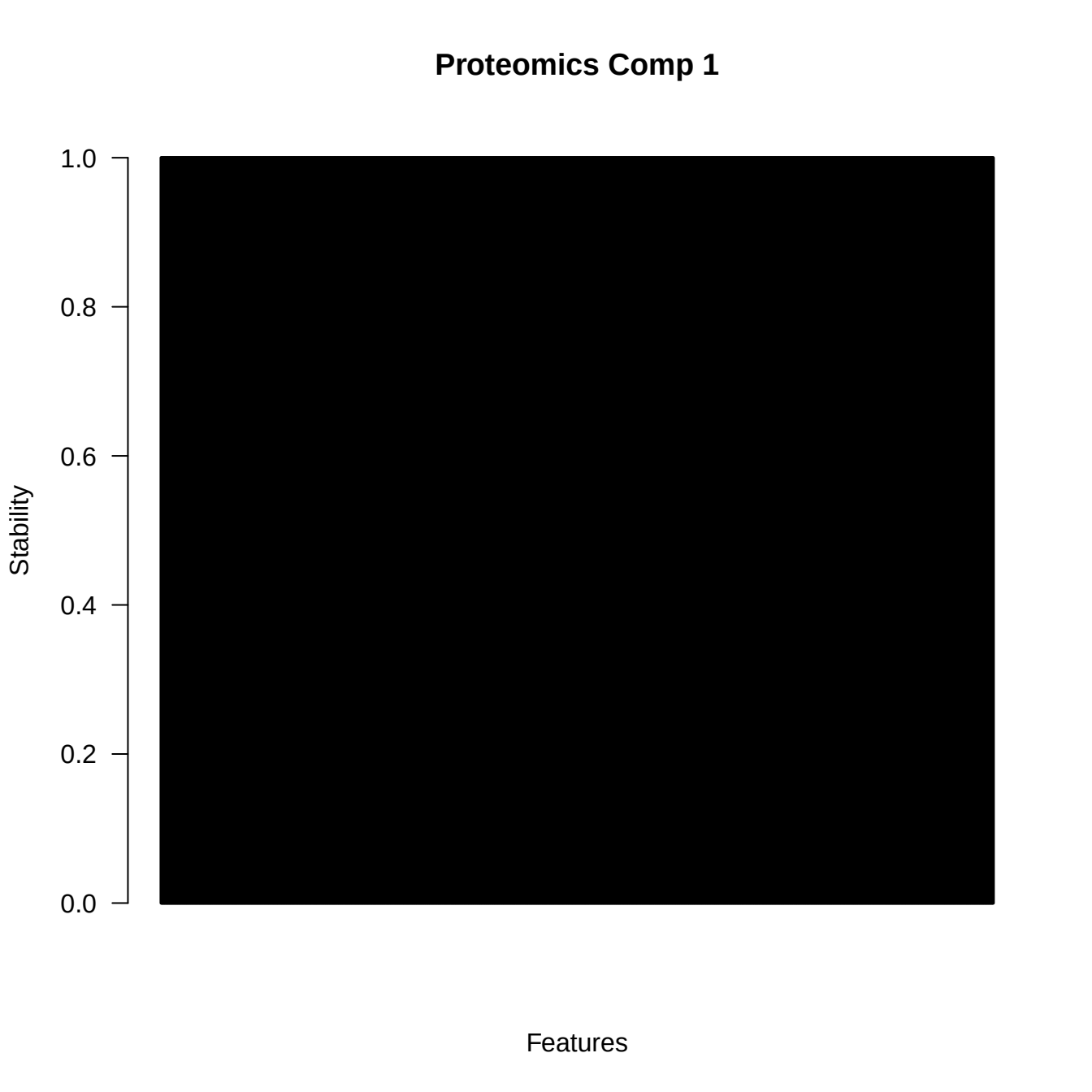
Stability
Features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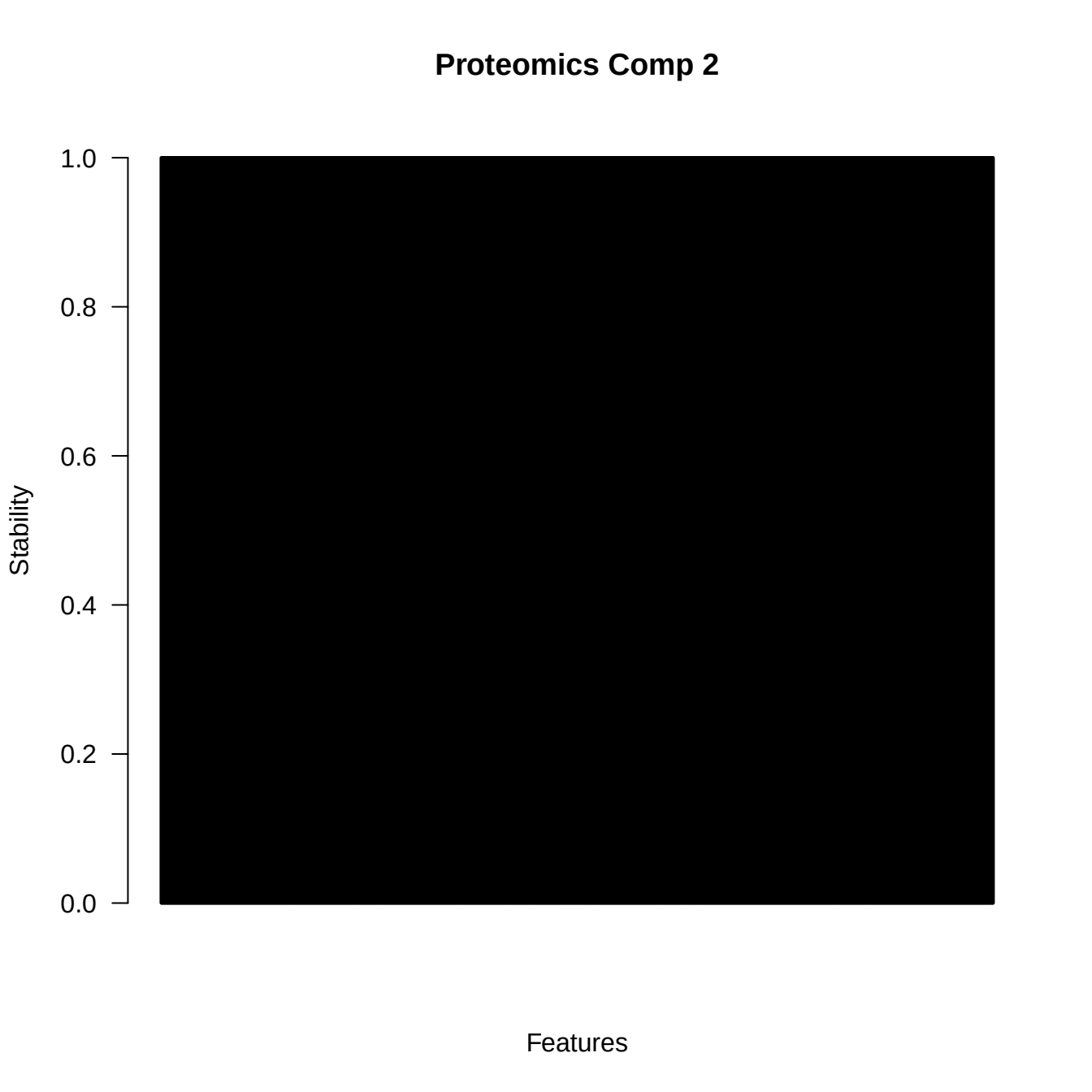
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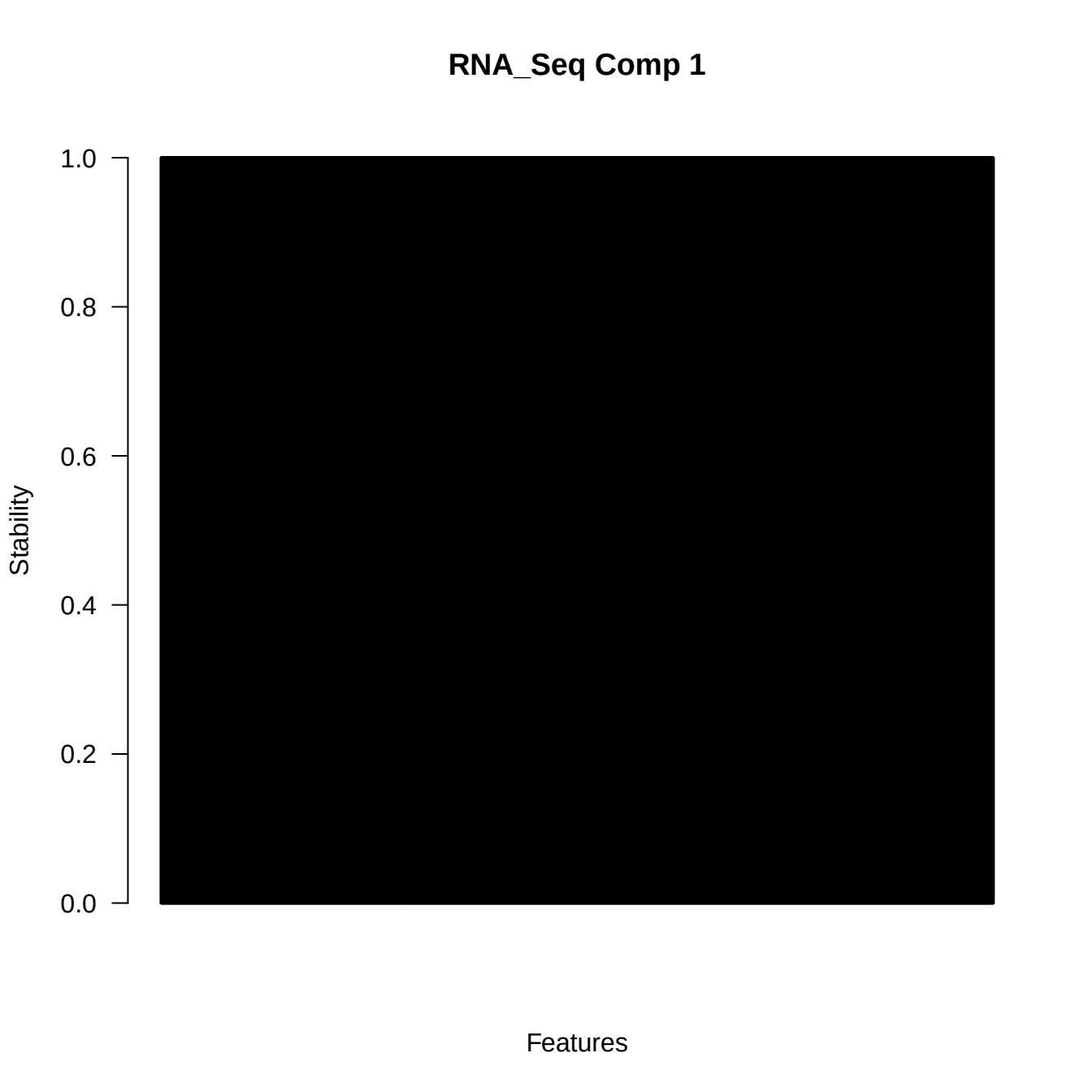
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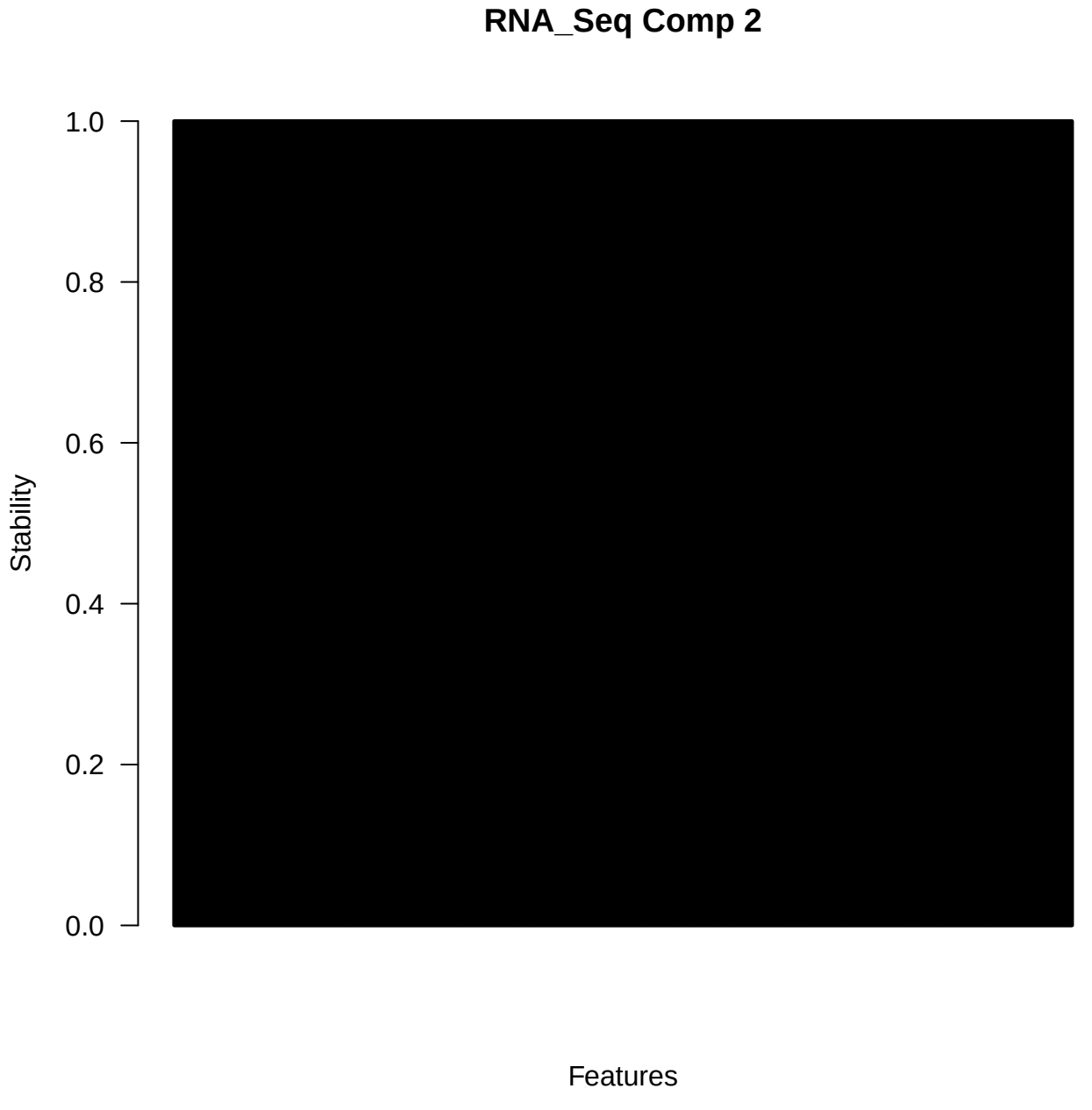
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Stability
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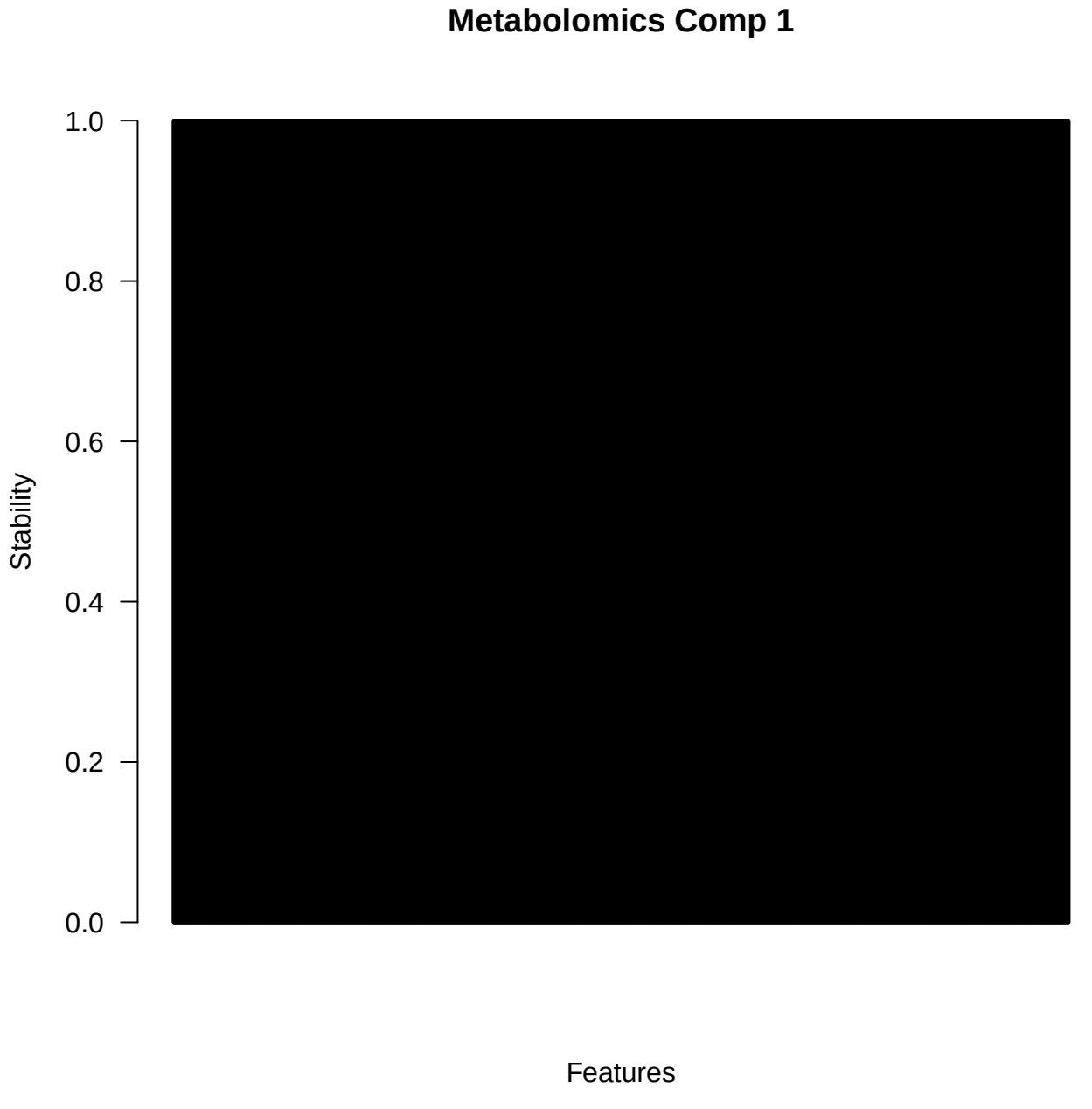
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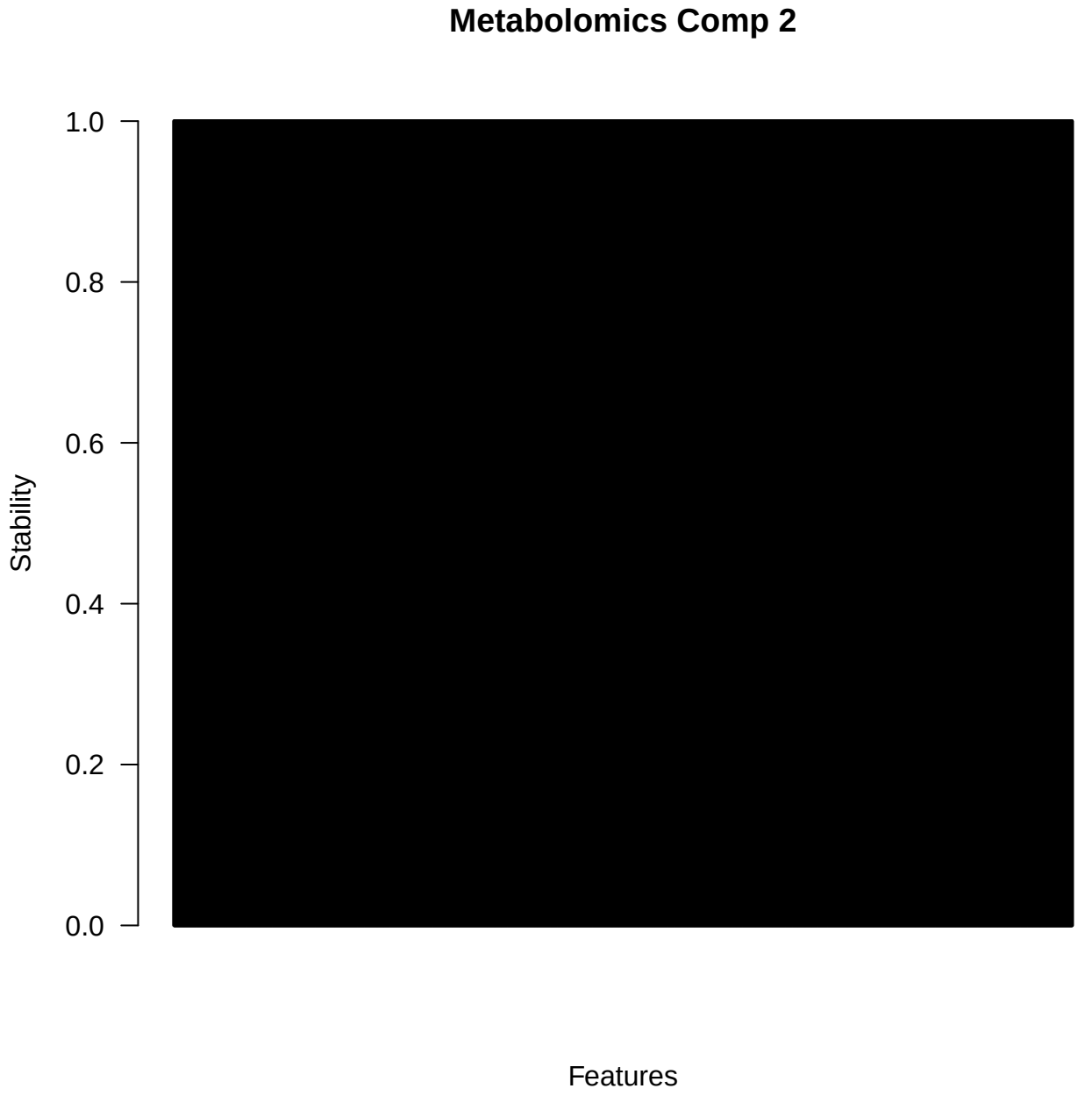
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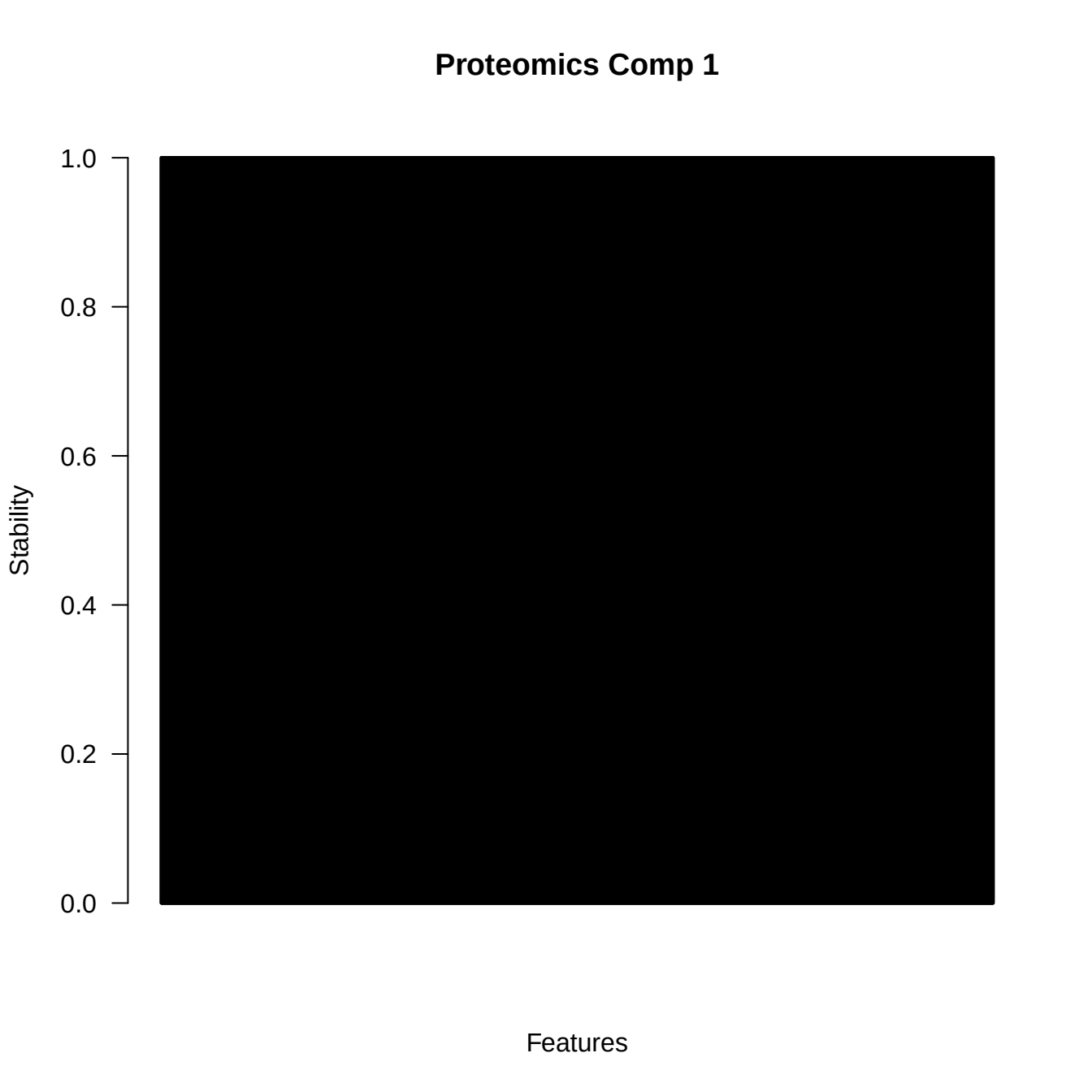
Stability
Features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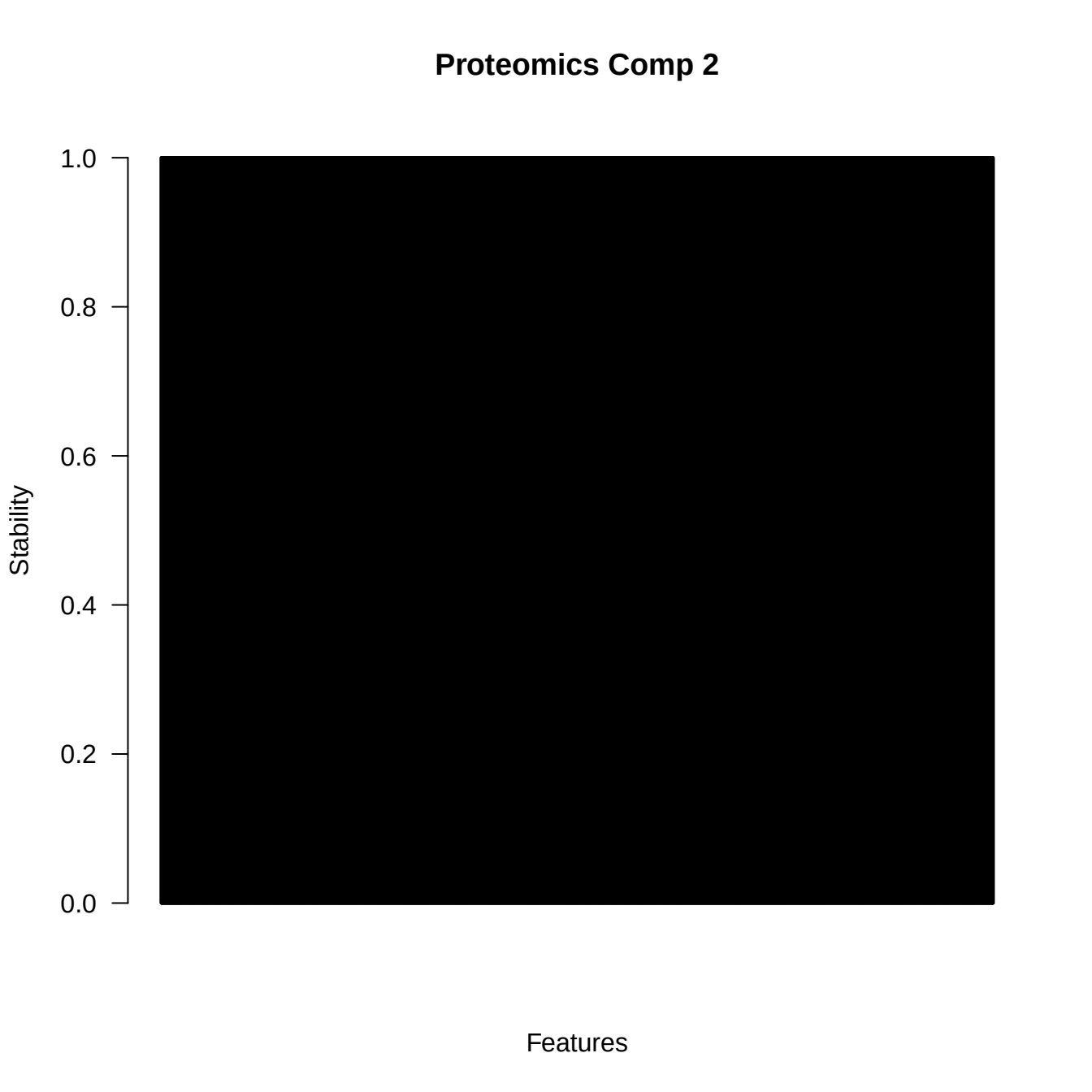
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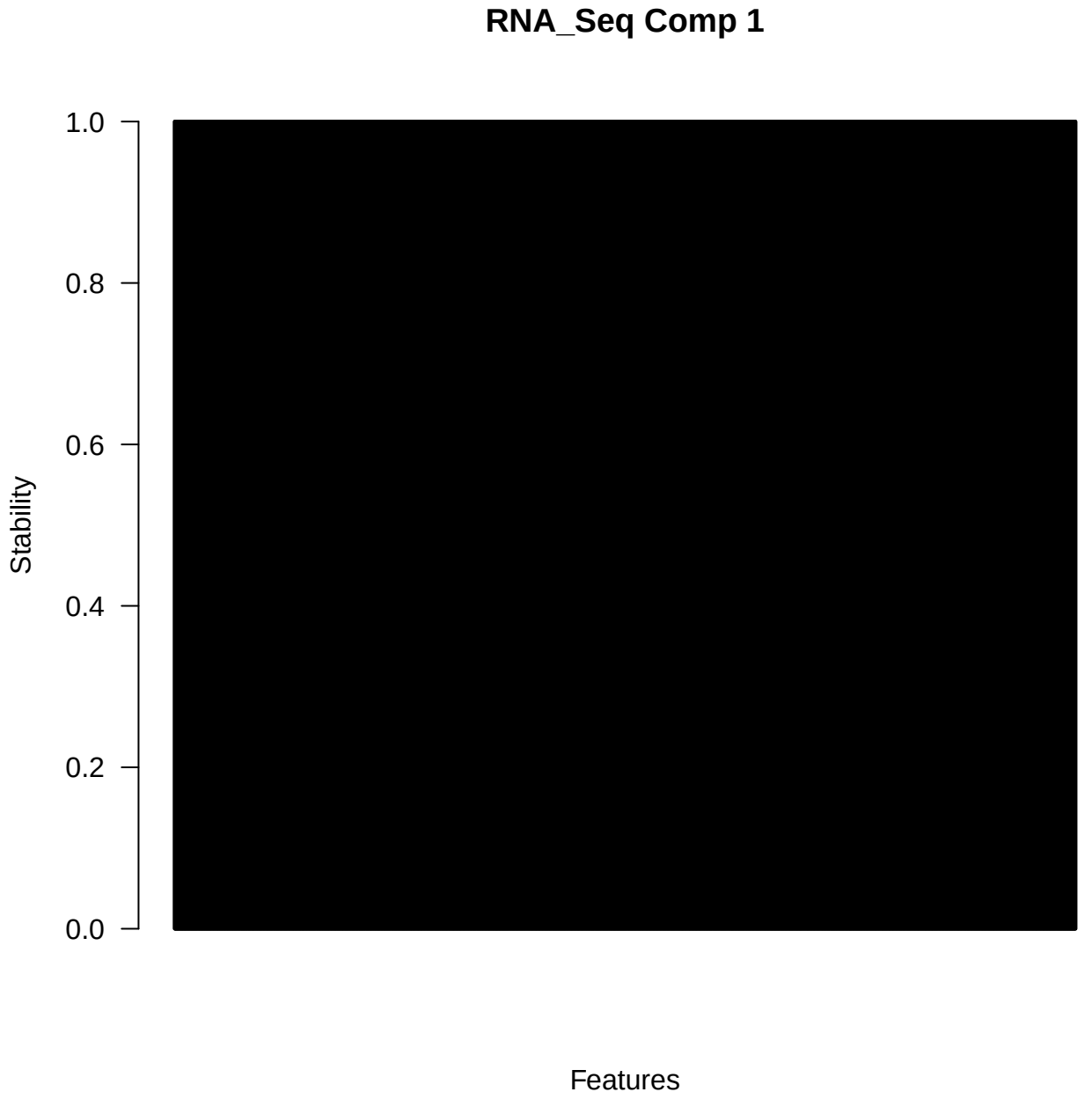
Stability
Features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0.4
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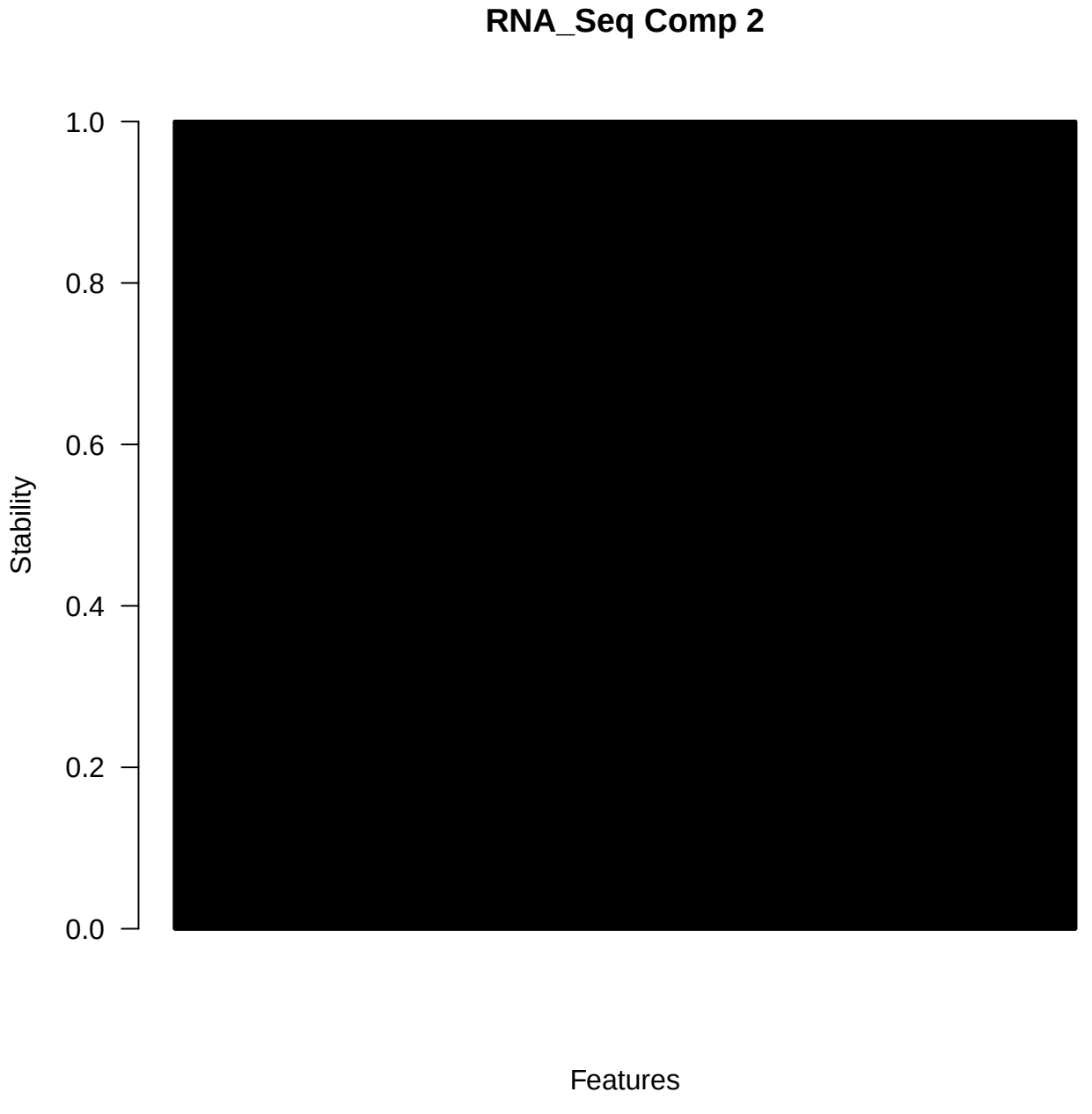
Stability
Features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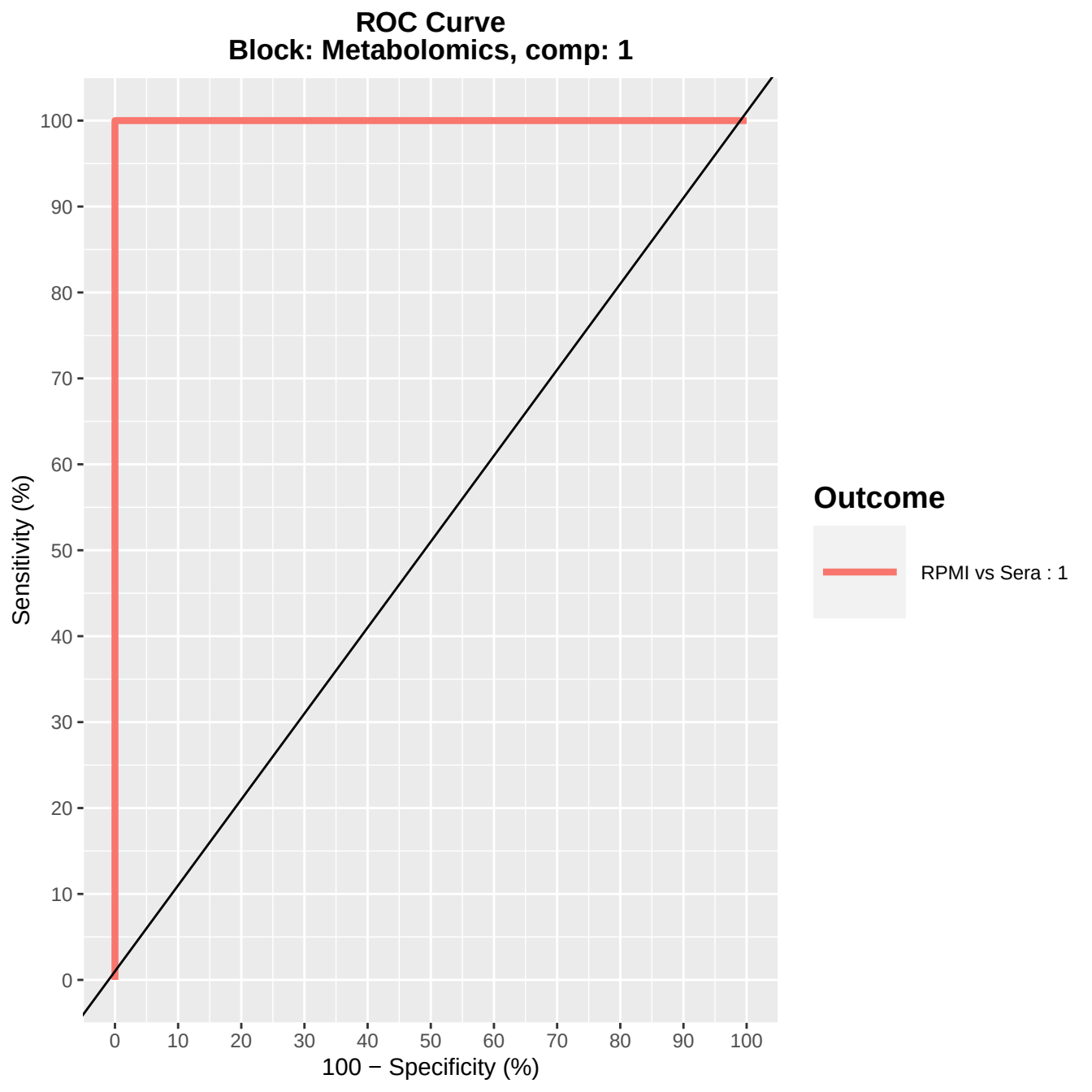
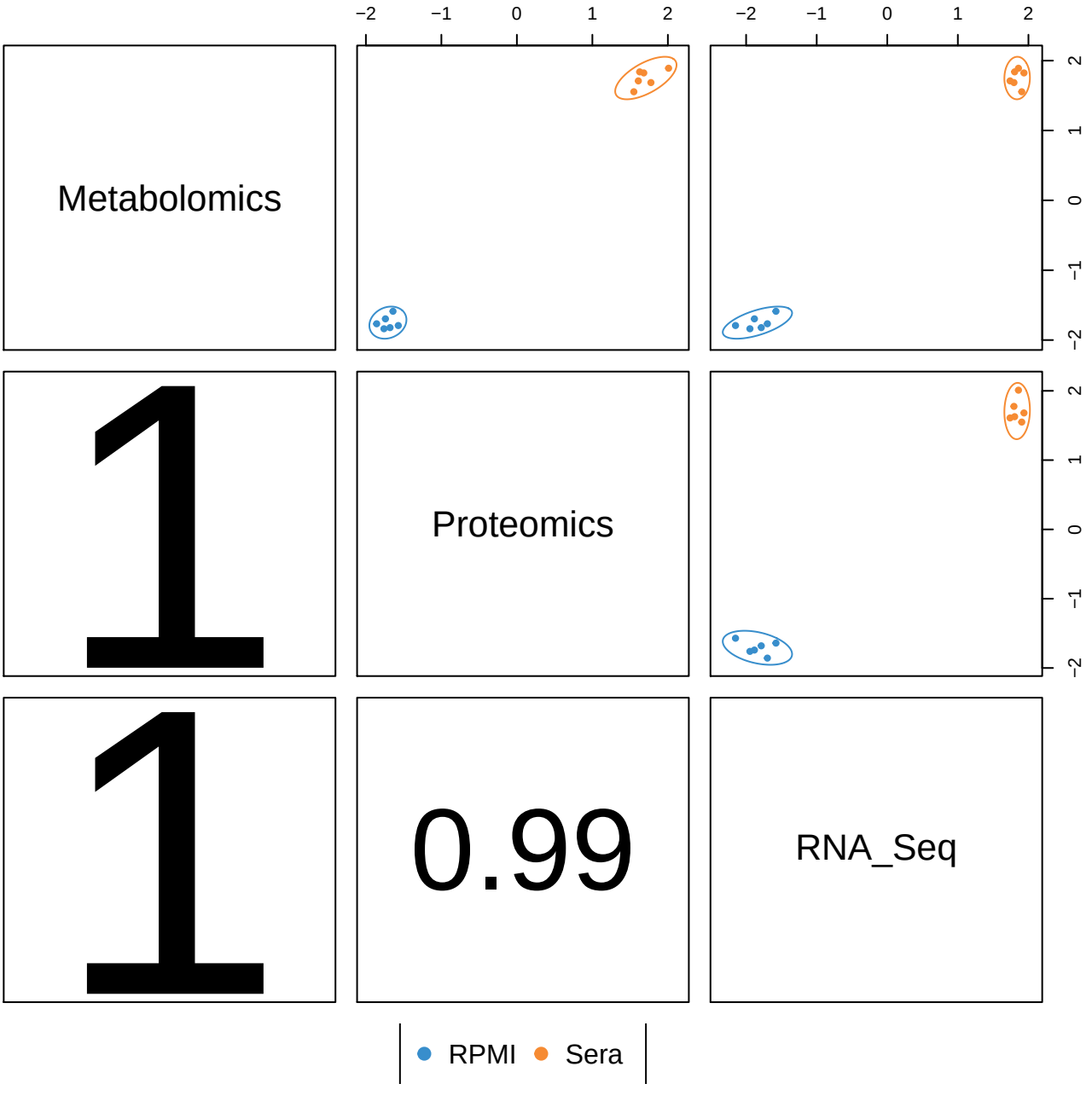
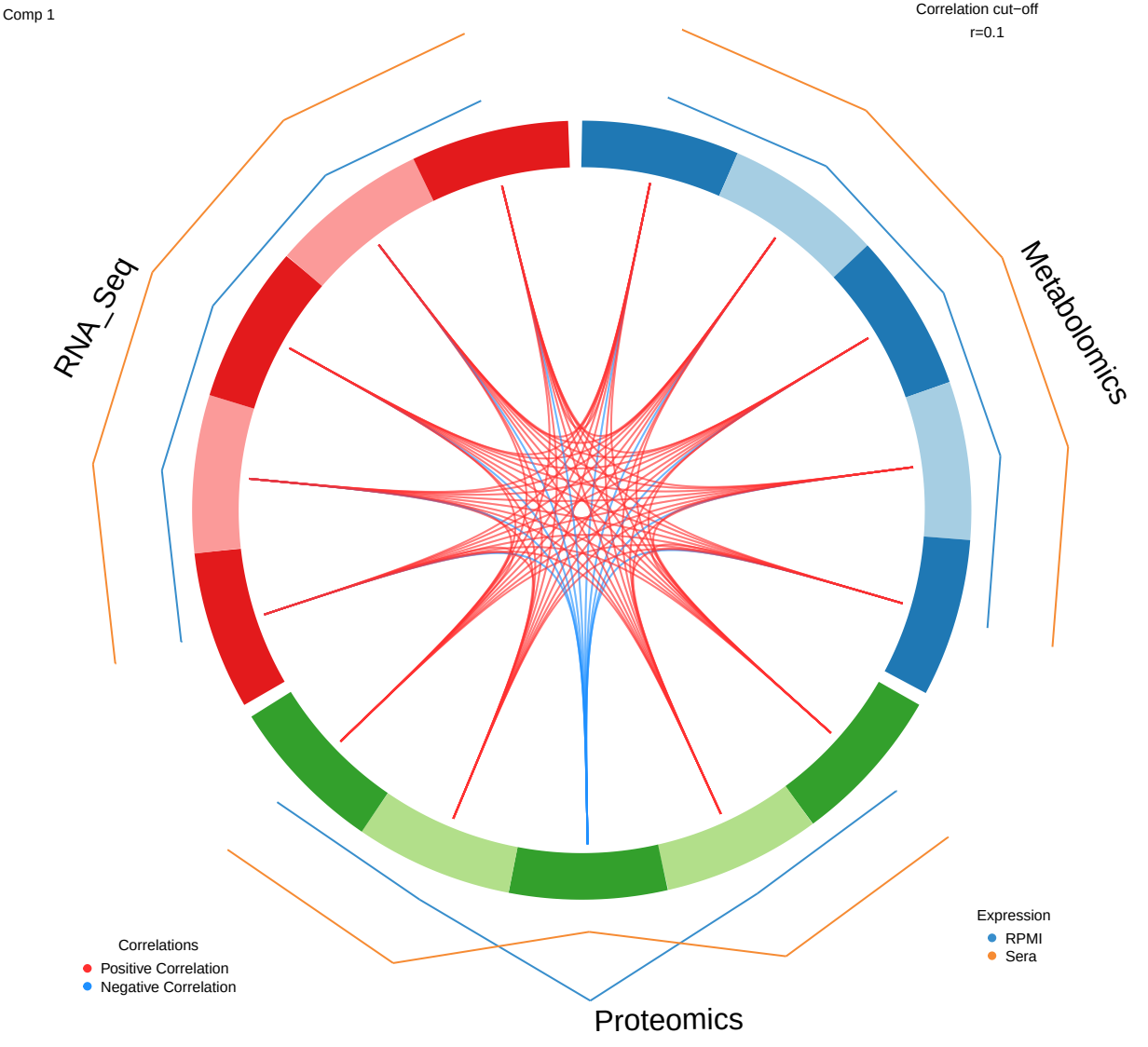
Stability
Features


ROC Curve
Block: Metabolomics, comp: 1
Sensitivity (%)
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
100 − Specificity (%)
Outcome
RPMI vs Sera : 1


Metabolomics
Proteomics
RNA_Seq
1
1
0.99
1
−2
−1
0
1
2
RPMI
Sera


Comp 1
Correlation cut−off
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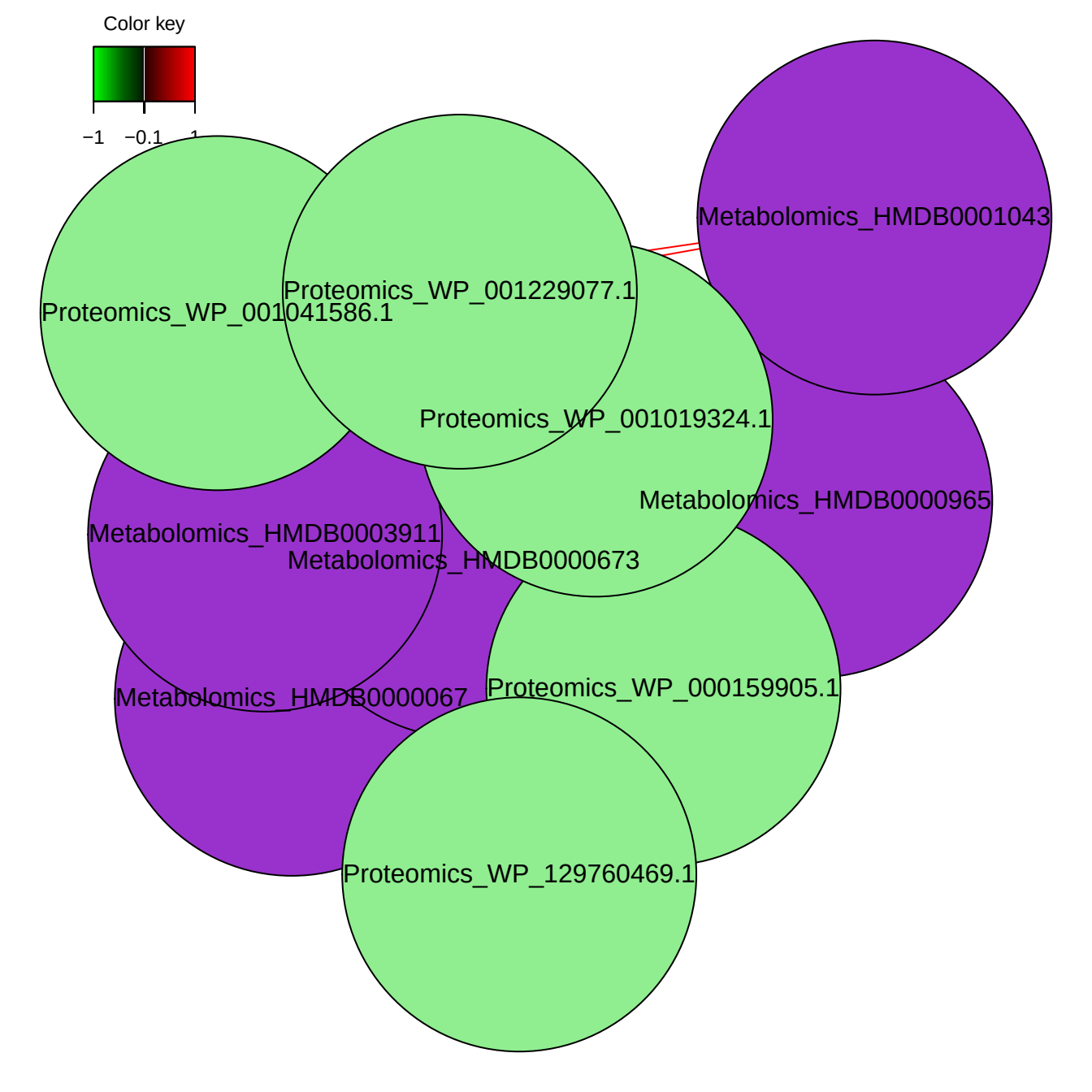
RNA_Seq
Metabolomics
Proteomics
Correlations
Positive Correlation
Negative Correlation
Expression
RPMI
Sera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Metabolomics_HMDB0000965
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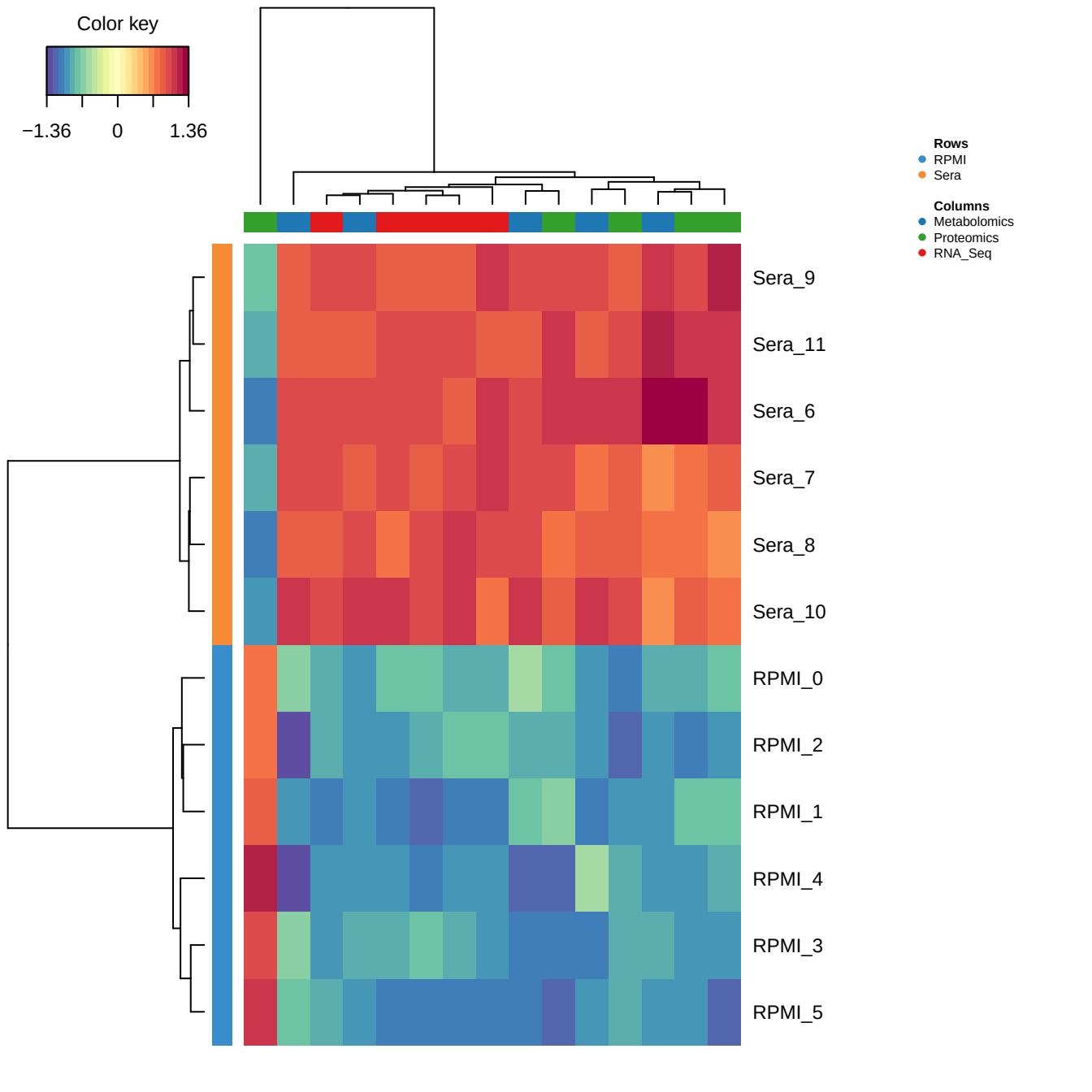
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RPMI
Sera
Columns
Metabolomics
Proteomics
RNA_Seq
Sera_9
Sera_11
Sera_6
Sera_7
Sera_8
Sera_10
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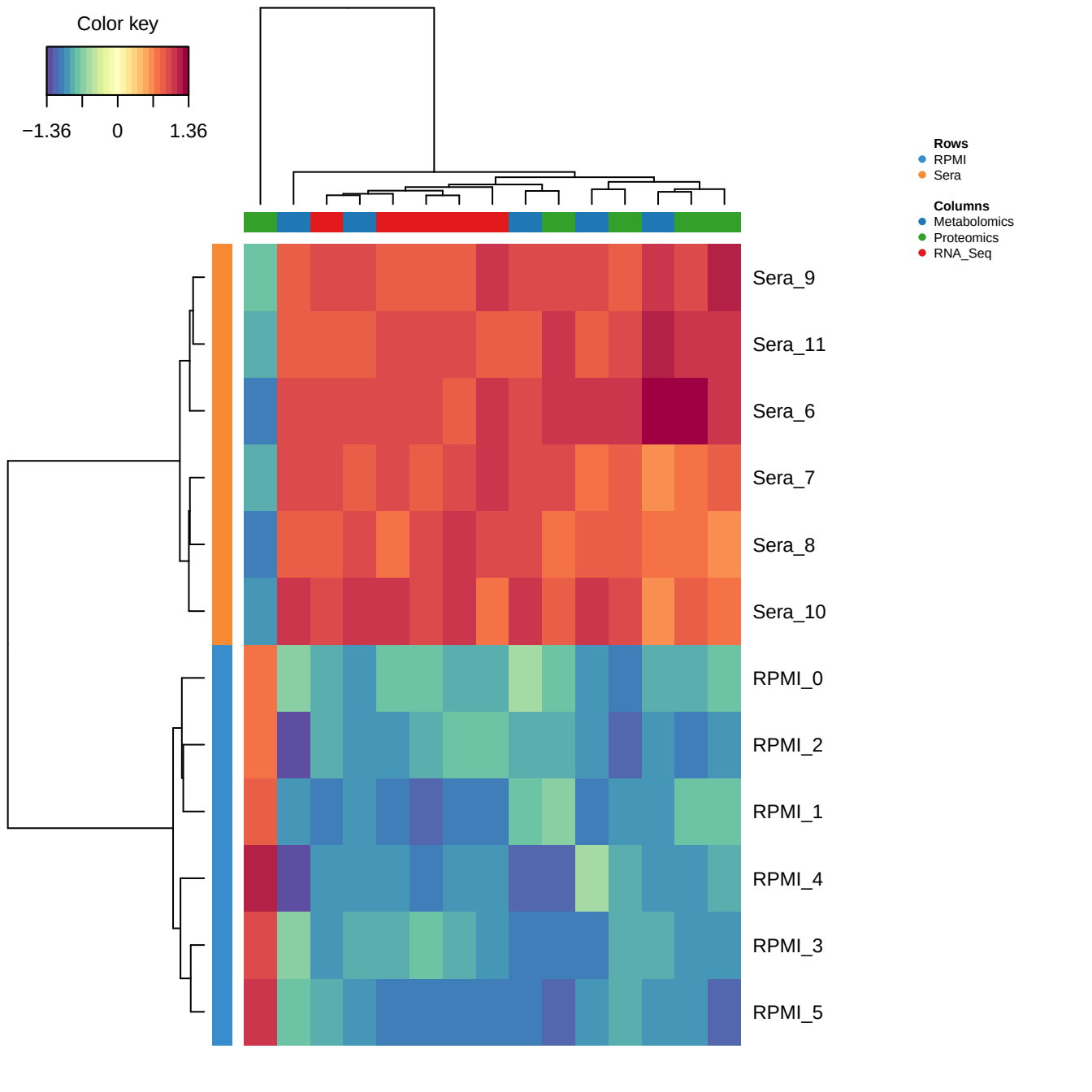
RPMI_2
RPMI_1
RPMI_4
RPMI_3
RPMI_5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RPMI
Sera
Columns
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Proteomics
RNA_Seq
Sera_9
Sera_11
Sera_6
Sera_7
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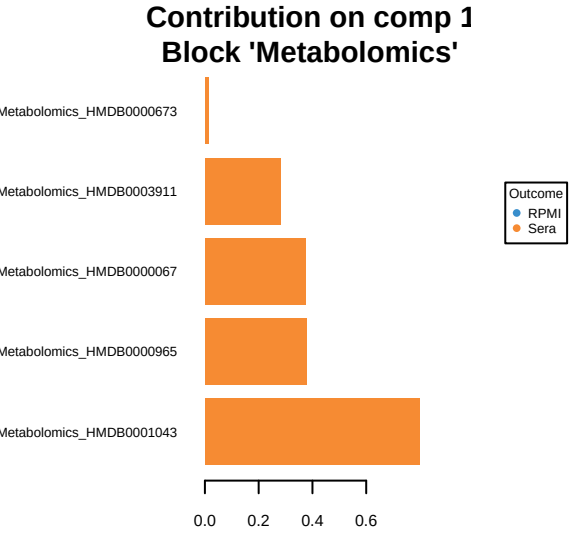
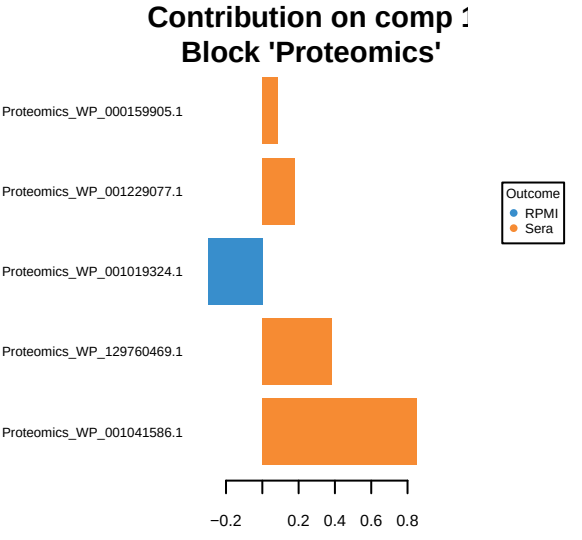
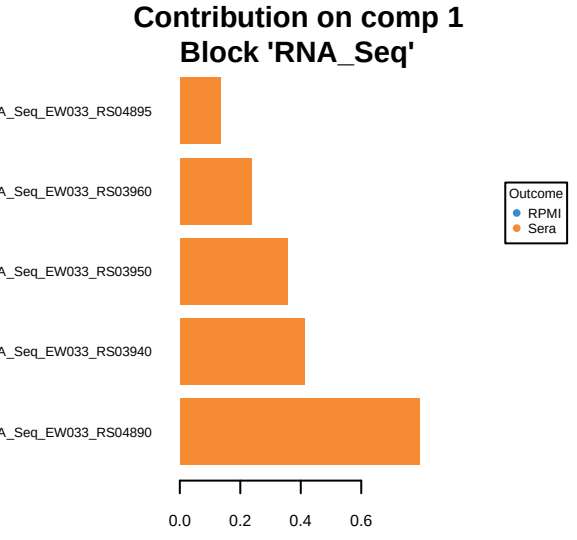
RPMI_0
RPMI_2
RPMI_1
RPMI_4
RPMI_3
RPMI_5

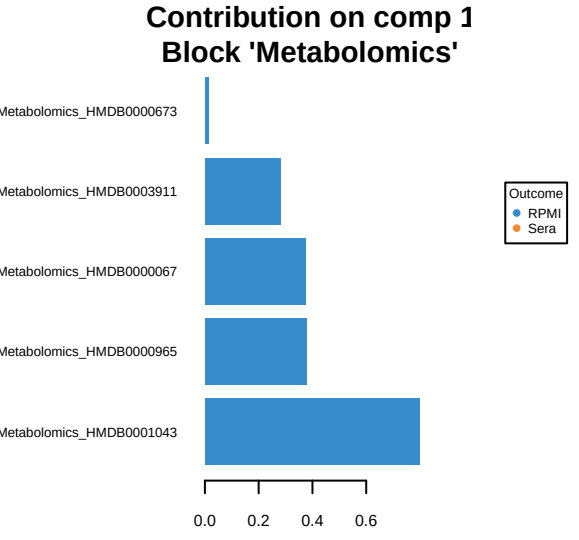
1 DIABLO max loadings

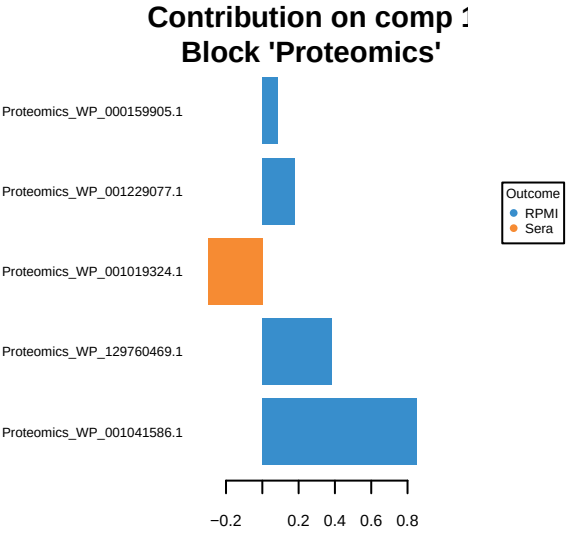


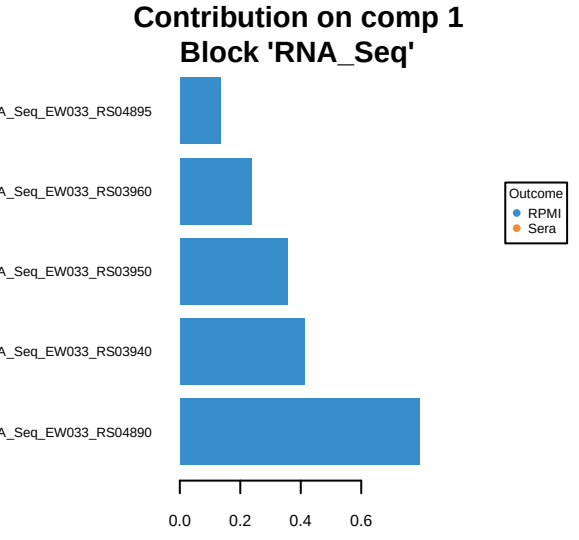




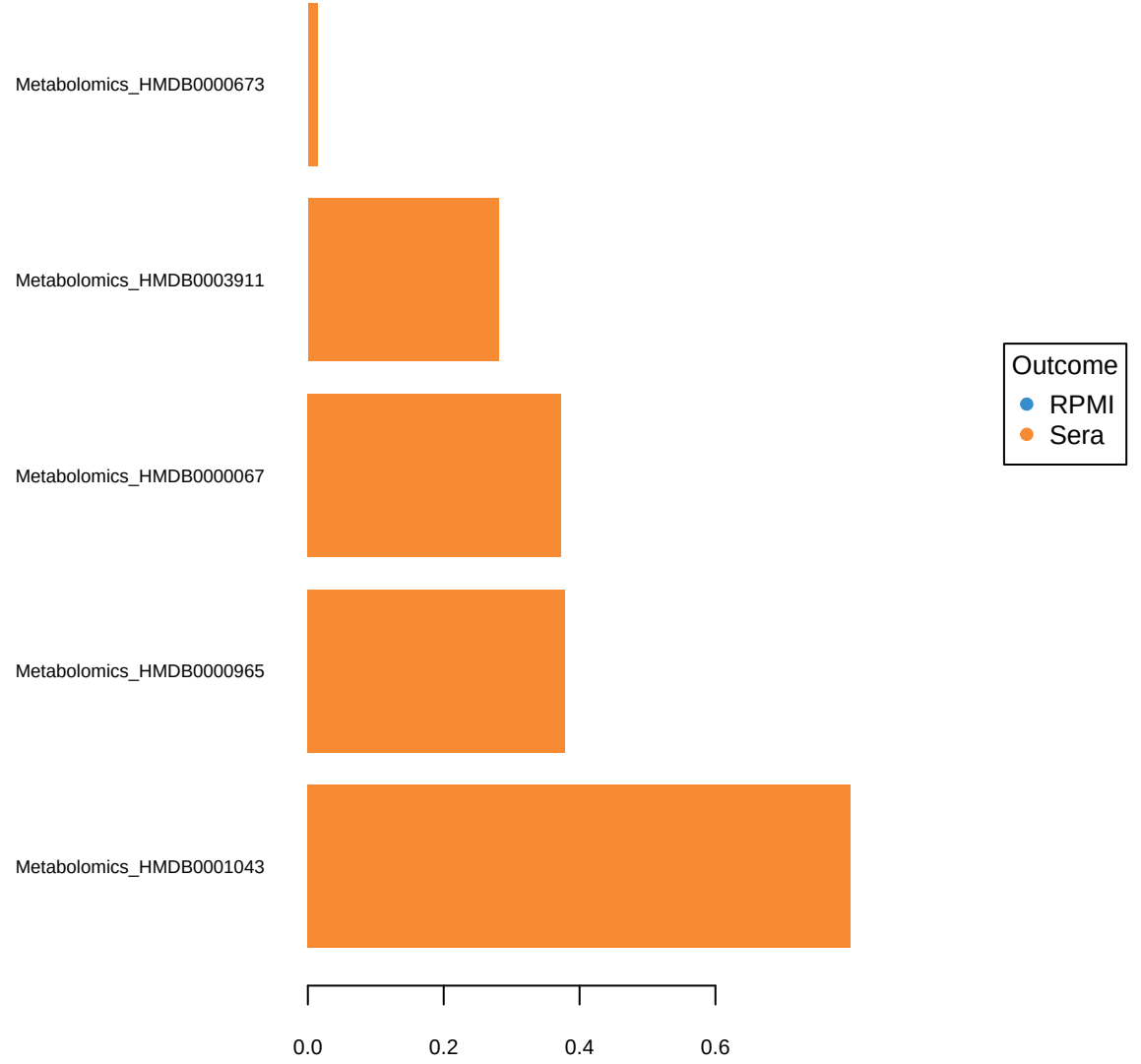
1 DIABLO min loadings



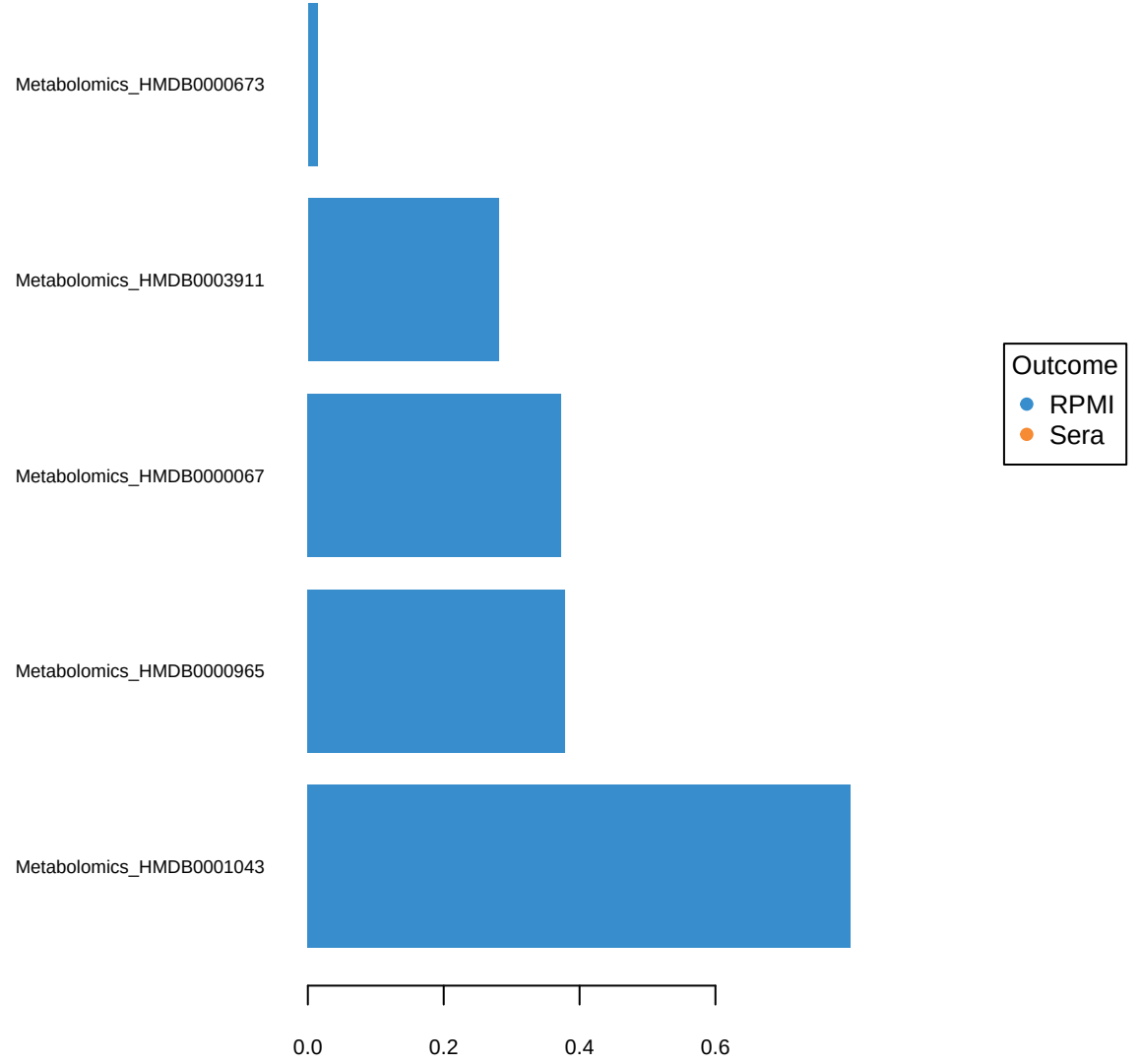


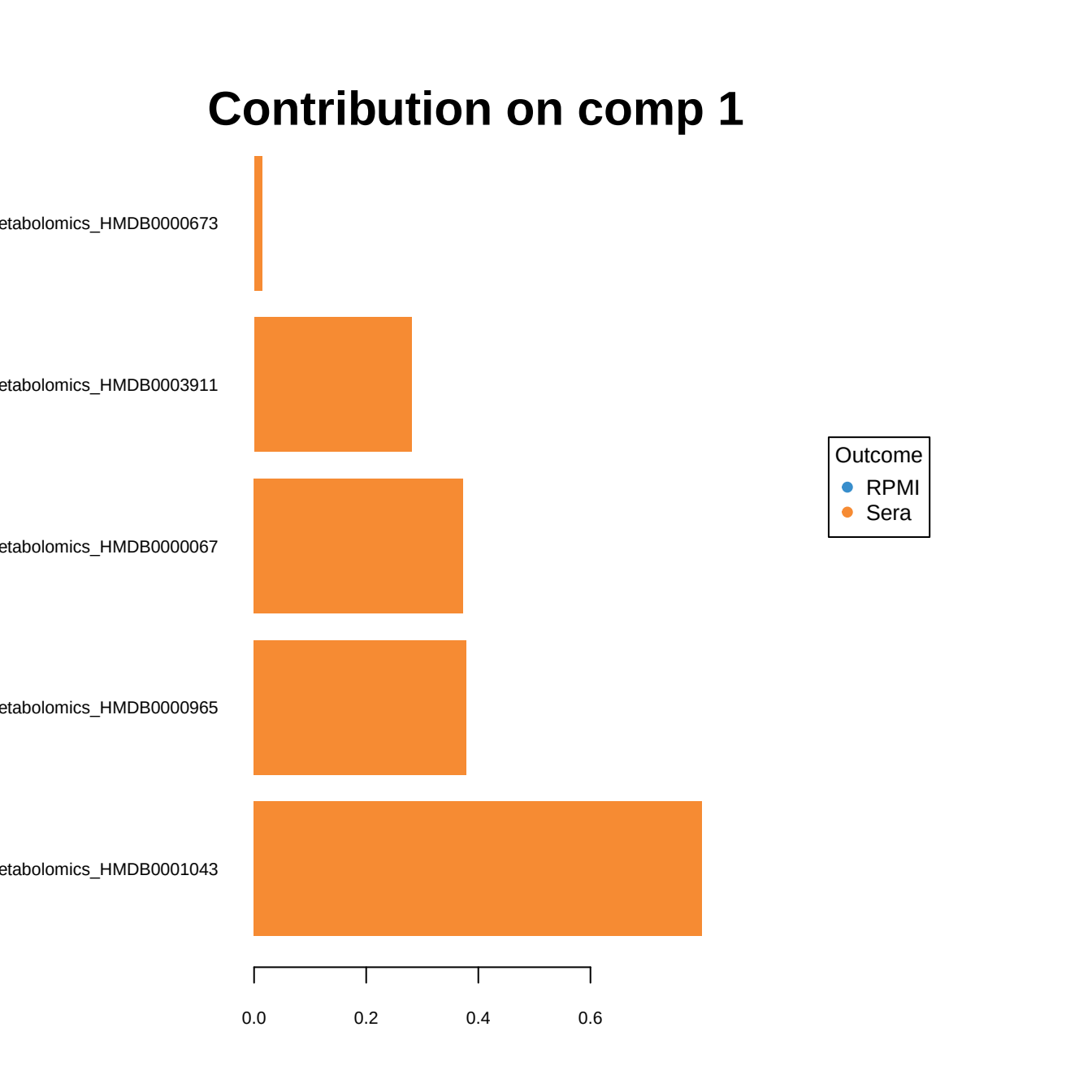


1 Metabolomics DIABLO max loa



1 Metabolomics DIABLO min loa

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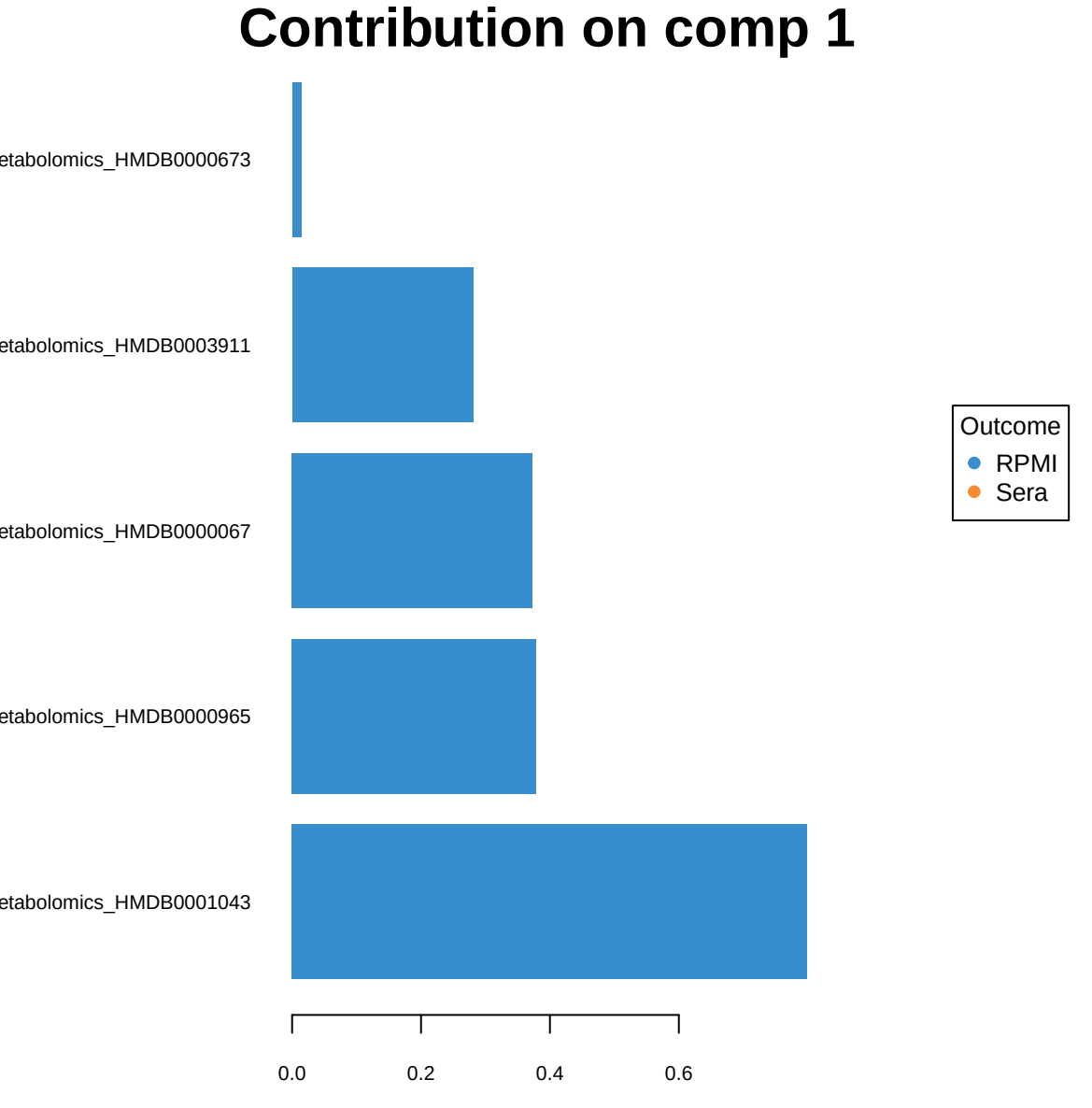
0.4
0.6
Outcome
RPMI
Sera


Contribution on comp 1
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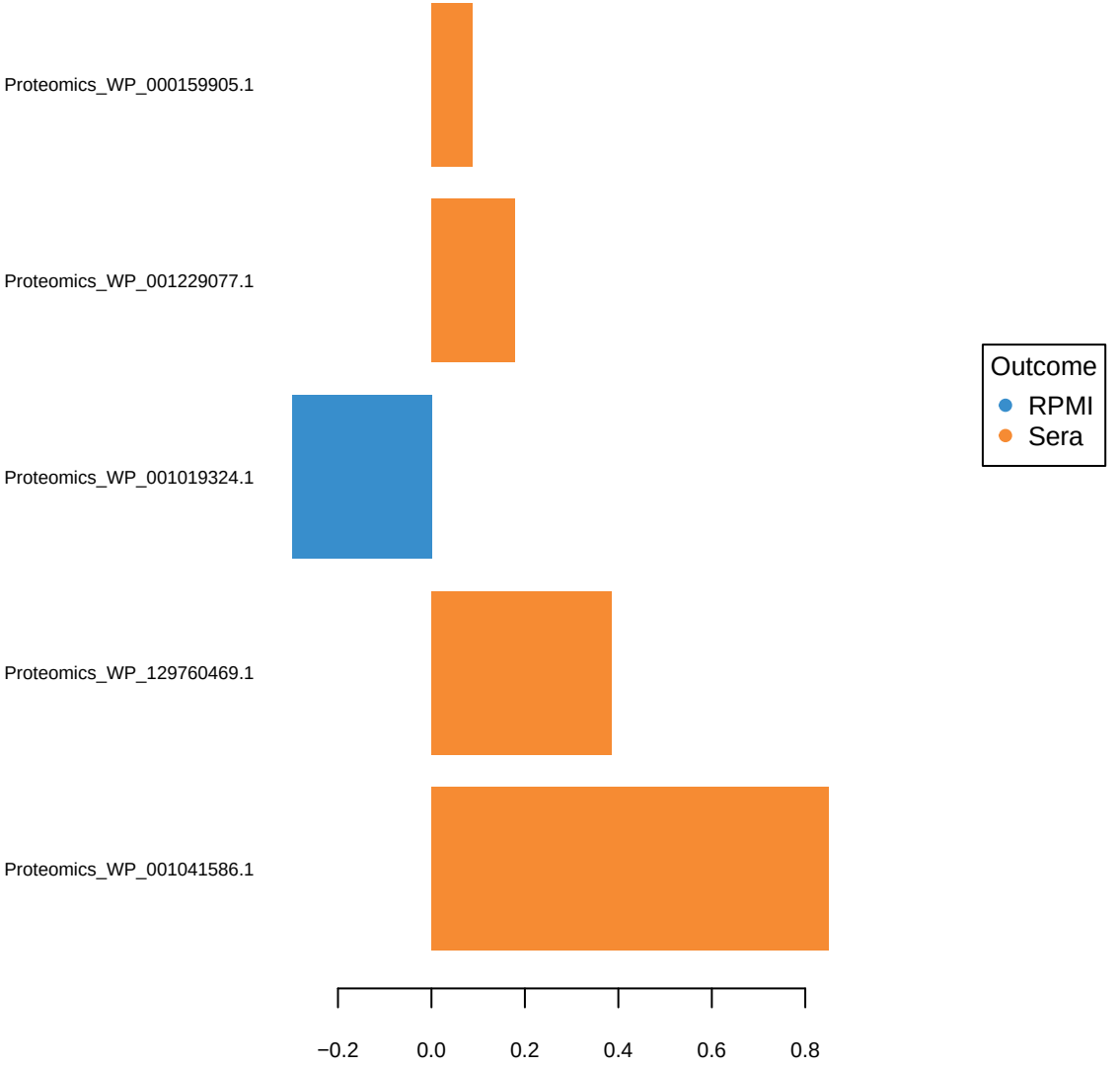
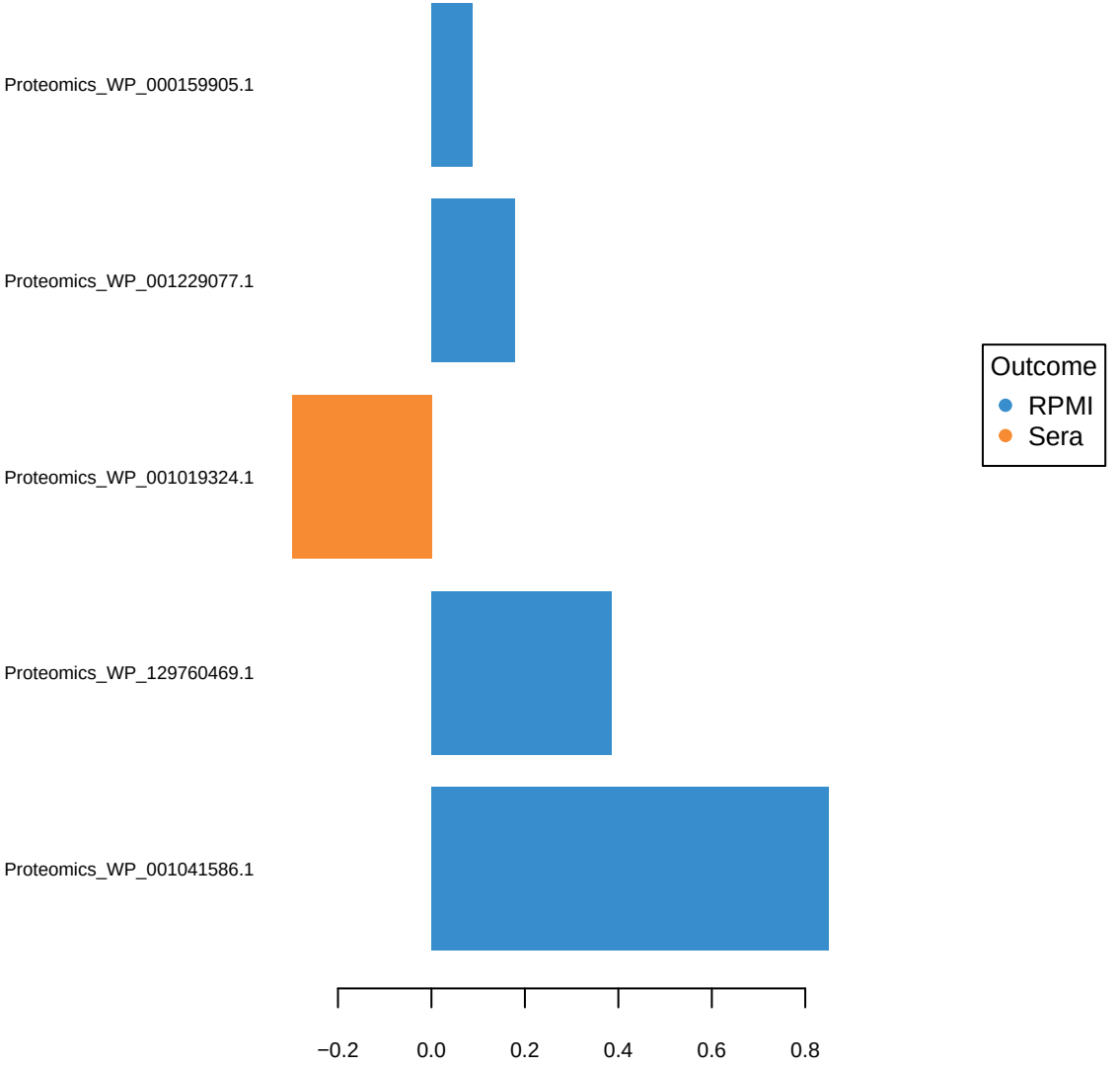
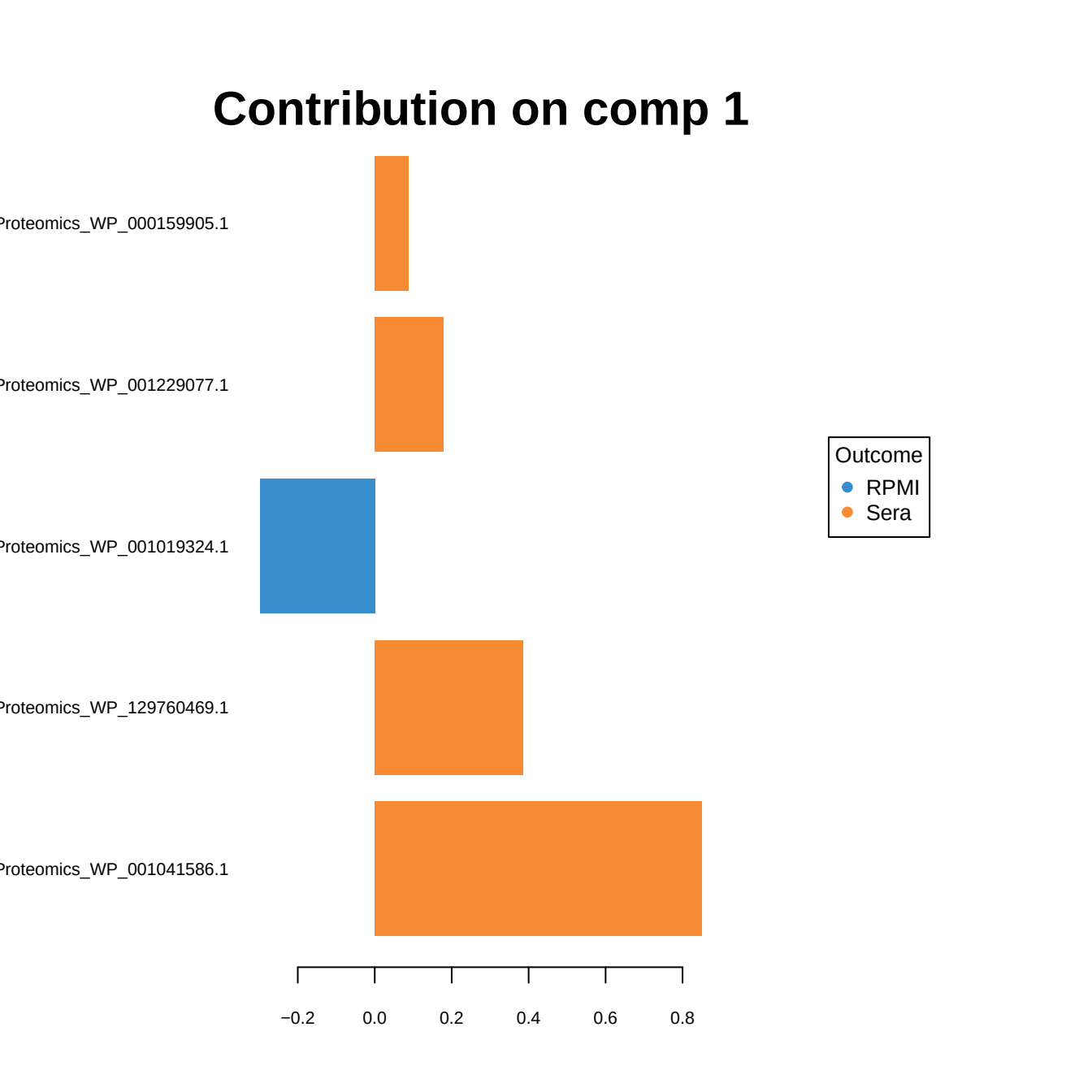
0.2
0.4
0.6
Outcome
RPMI
Sera

1 Proteomics DIABLO max loa



1 Proteomics DIABLO min loa

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Outcome
RPMI
Sera
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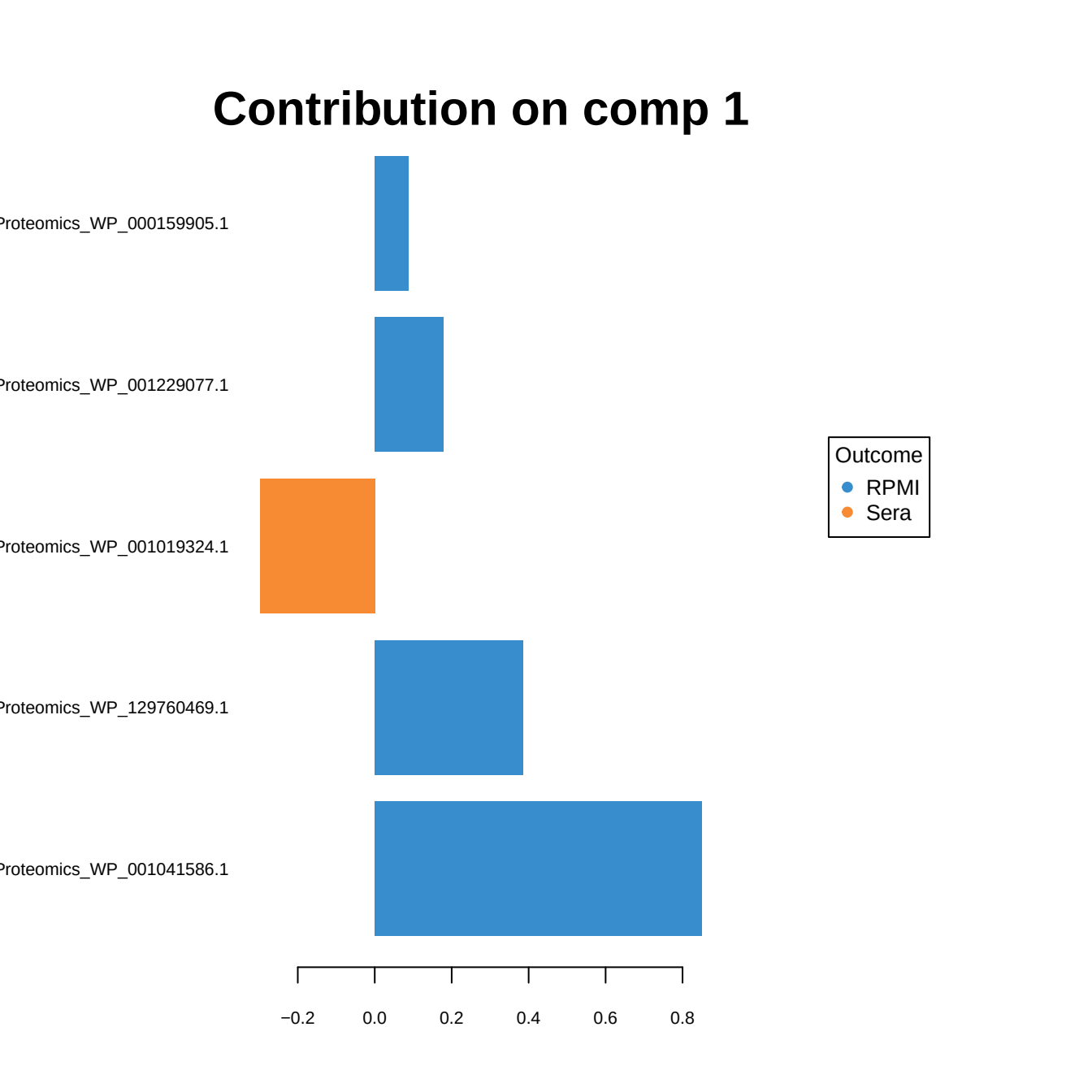
0.4
0.6
0.8


Contribution on comp 1
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Proteomics_WP_001019324.1
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Outcome
RPMI
Sera
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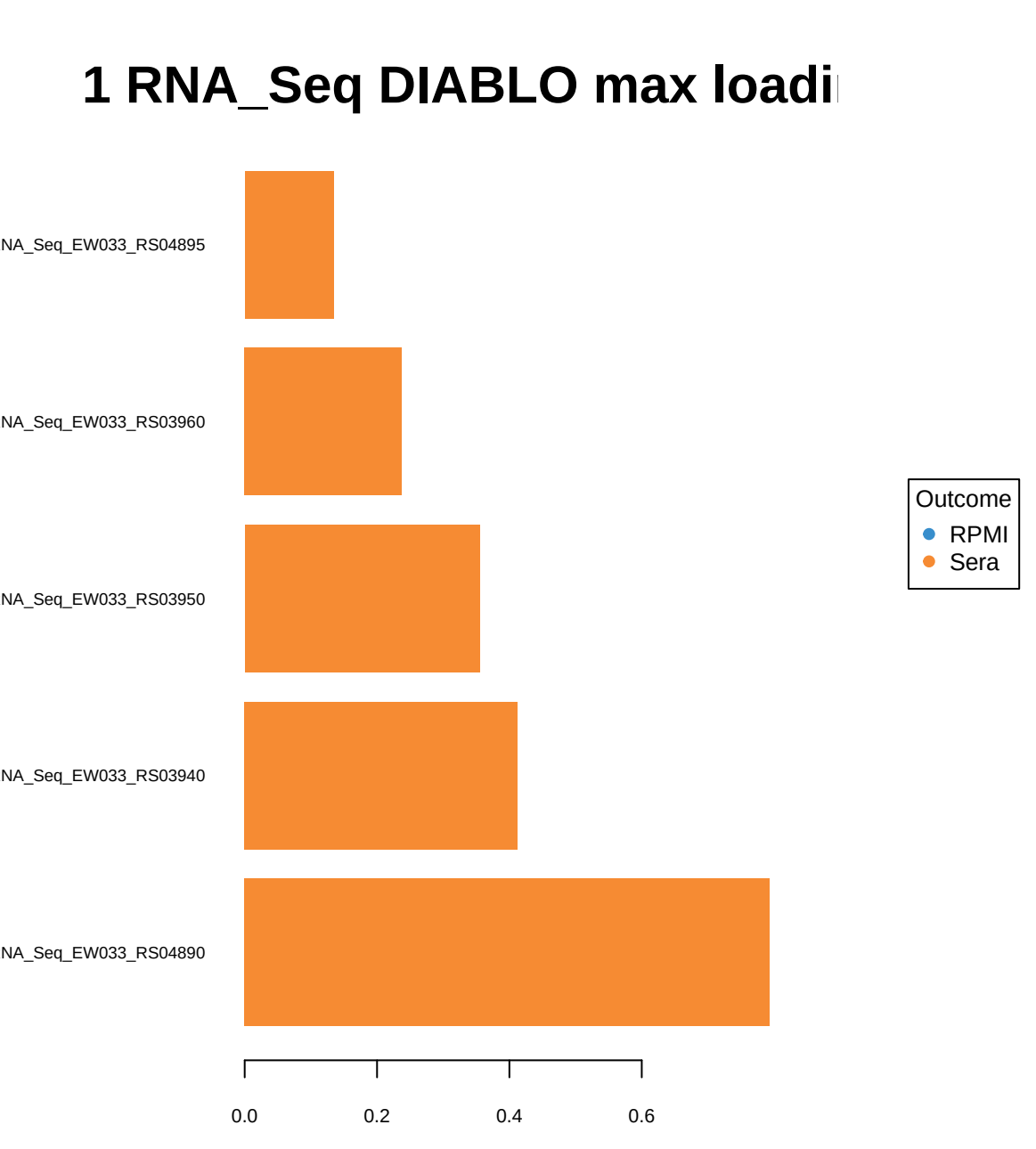
0.4
0.6
0.8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NA_Seq_EW033_RS03960
NA_Seq_EW033_RS03950
NA_Seq_EW033_RS03940
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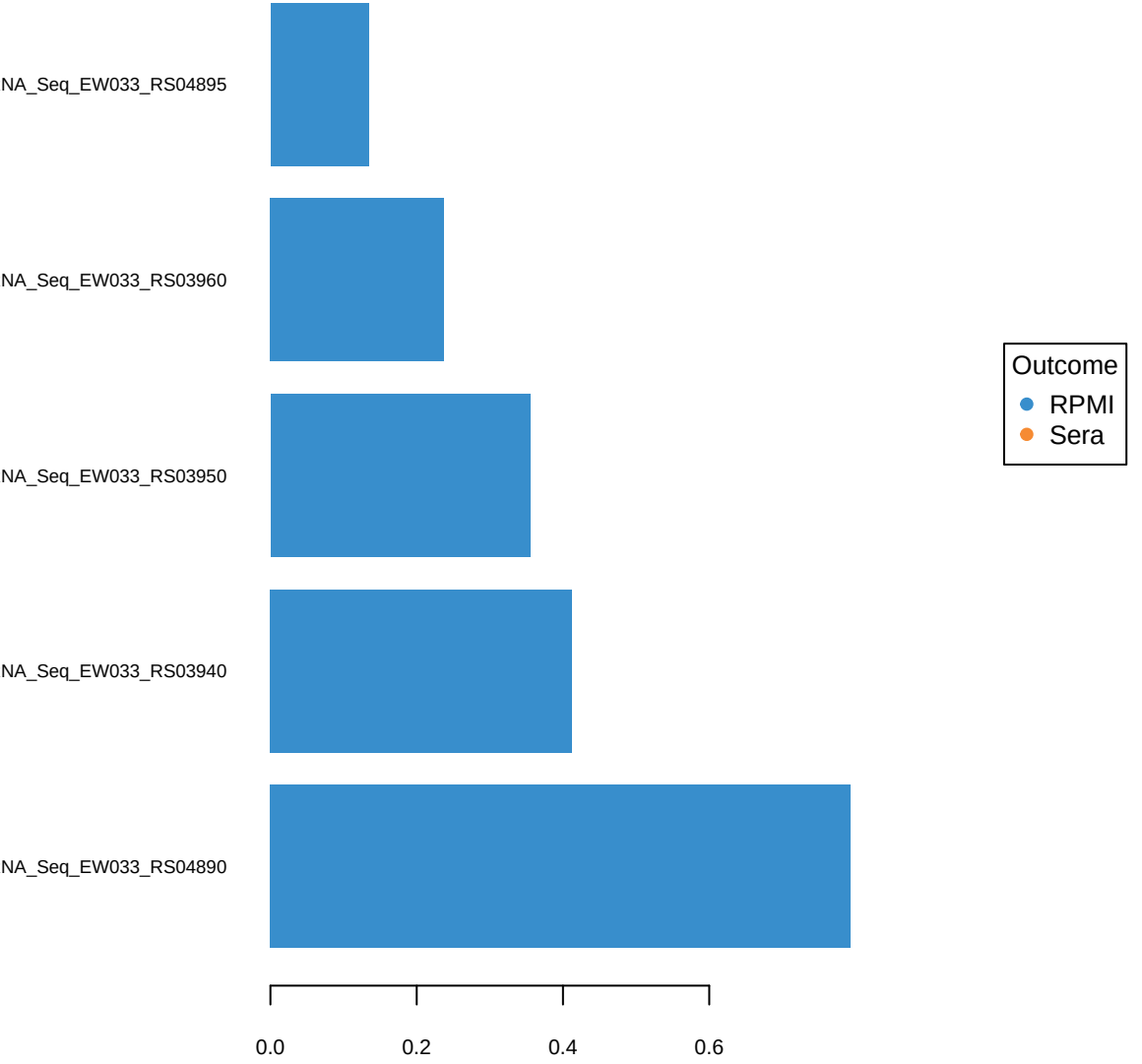
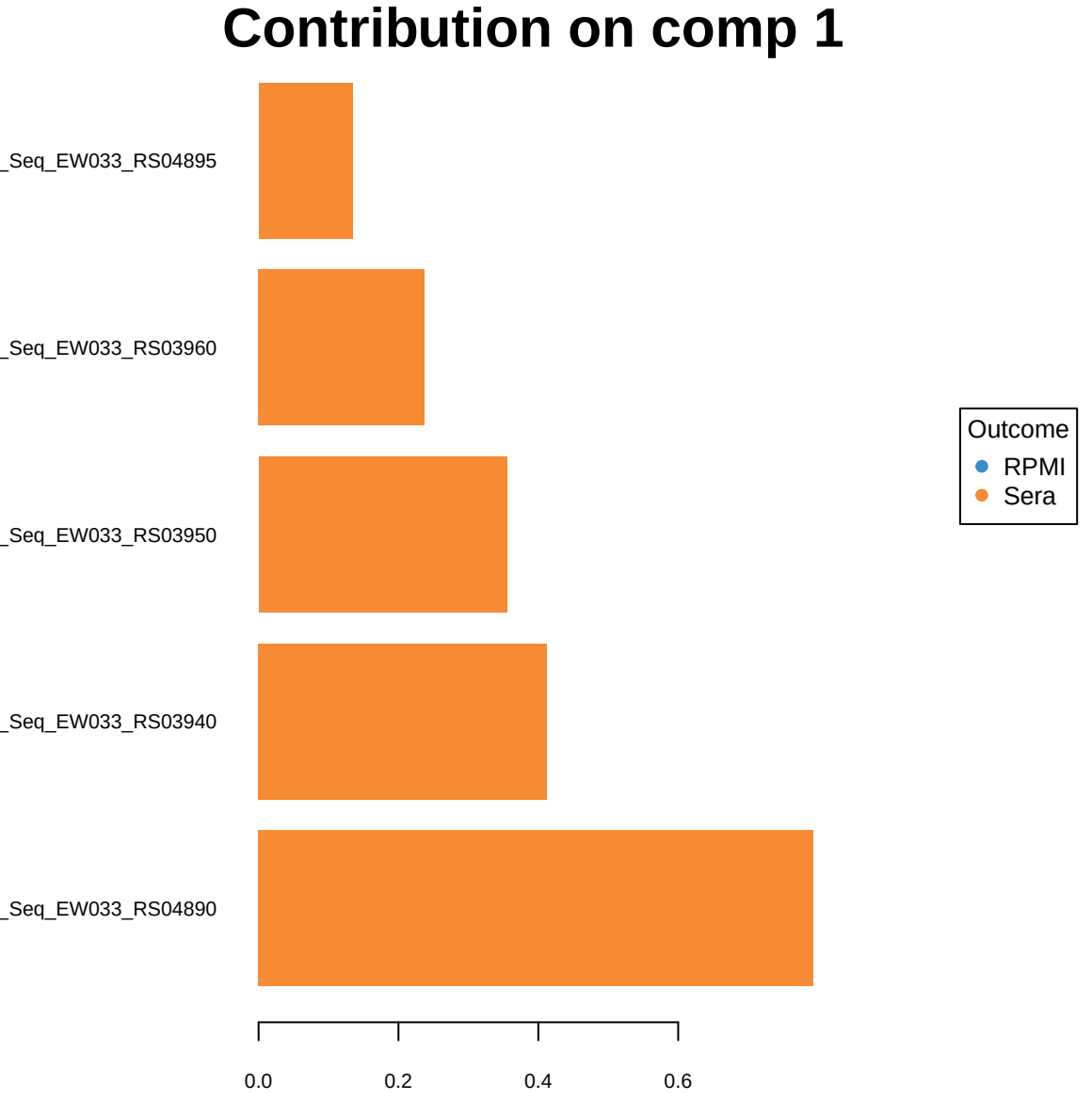
0.0
0.2
0.4
0.6
Outcome
RPMI
Sera

1 RNA_Seq DIABLO min loadi

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_Seq_EW033_RS03960
_Seq_EW033_RS03950
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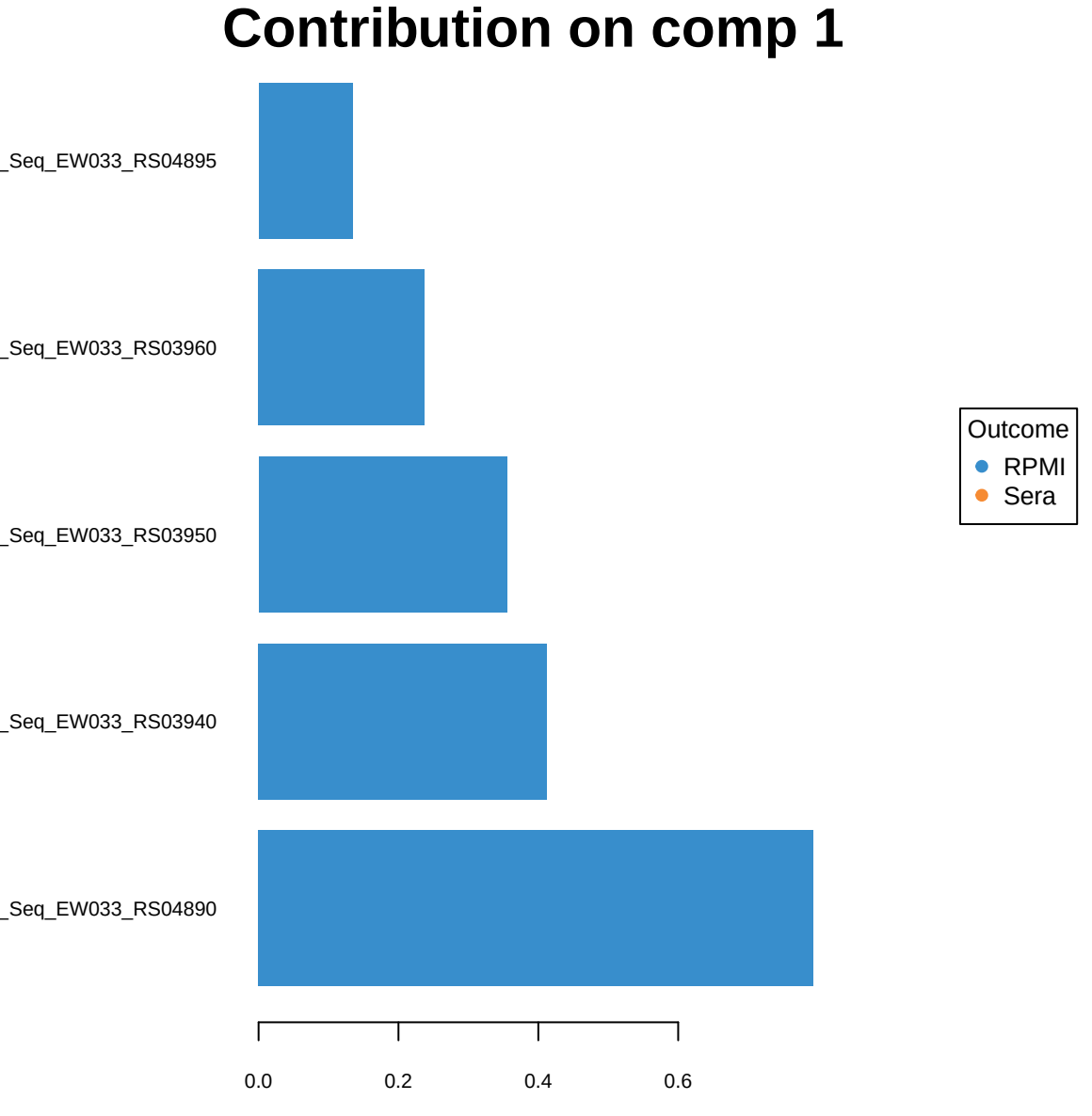
0.4
0.6
Outcome
RPMI
Sera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_Seq_EW033_RS03950
_Seq_EW033_RS03940
_Seq_EW033_RS04890
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0.2
0.4
0.6
Outcome
RPMI
Sera