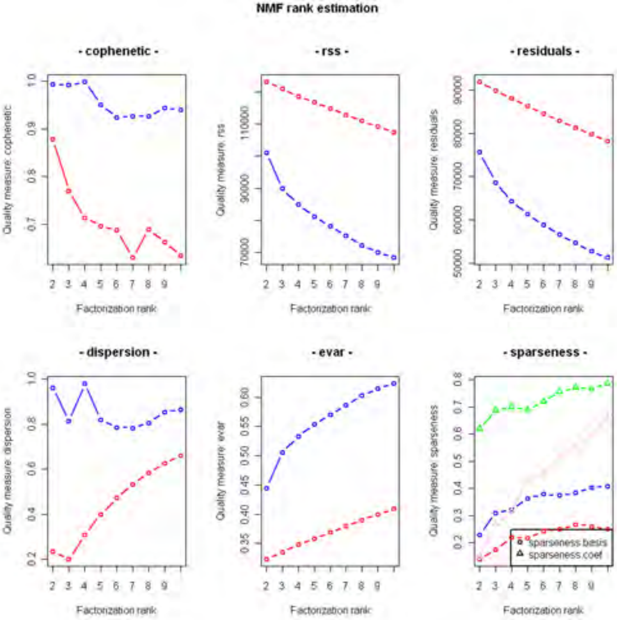
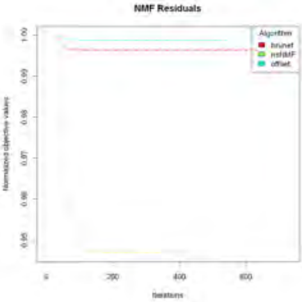
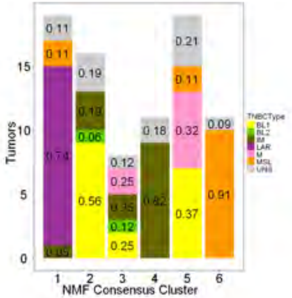
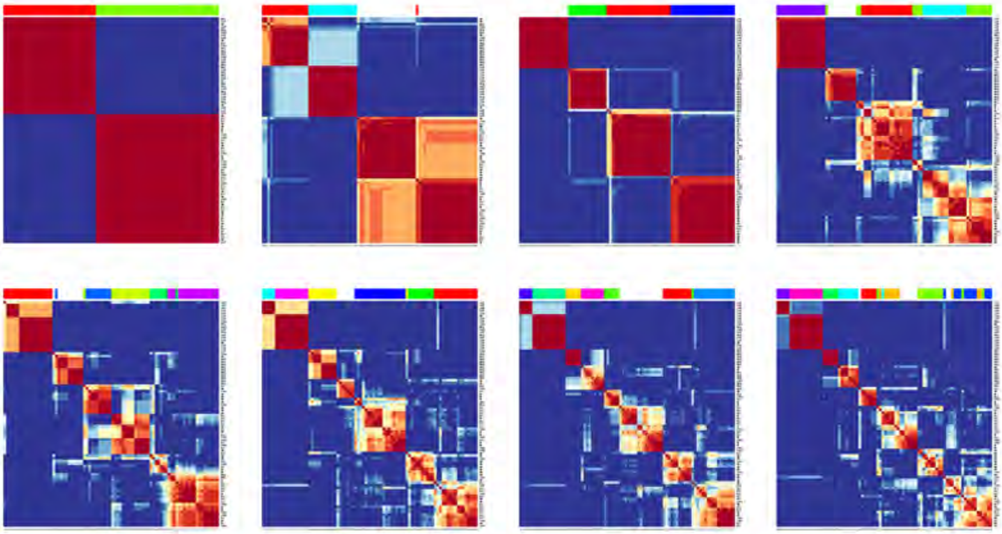
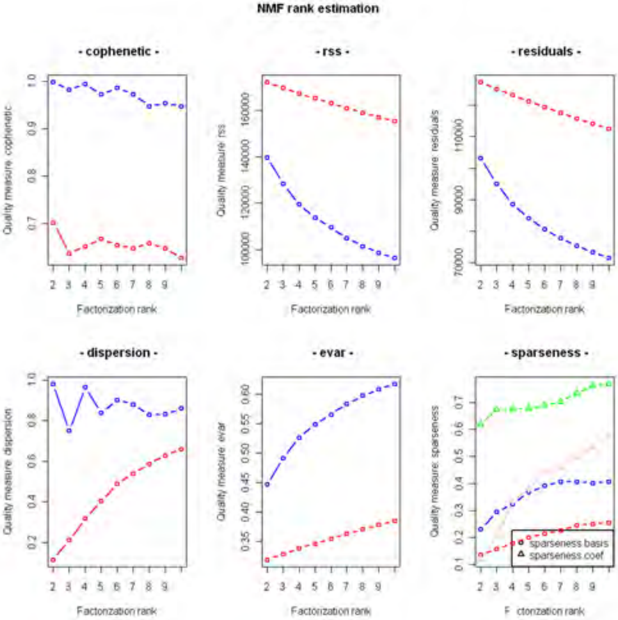
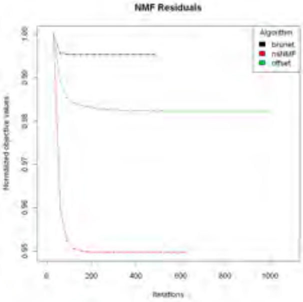

NMF rank estimation
- cophenetic -
Quality measure: cophenetic
1.0
0.9
0.8
0.7
- rss -
Quality measure: rss
110000
90000
70000
- residuals -
Quality measure: residuals
90000
80000
70000
60000
50000
- dispersion -
Quality measure: dispersion
1.0
0.8
0.6
0.4
0.2
- evar -
Quality measure: evar
0.60
0.55
0.50
0.45
0.40
0.35
- sparseness -
Quality measure: sparseness
0.8
0.7
0.6
0.5
0.4
0.3
0.2
sparseness basis
sparseness coef
2 3 4 5 6 7 8 9
Factorization rank

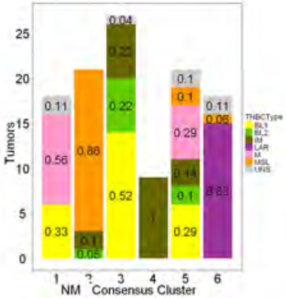

NMF Residuals
Algorithm
brunet
nsNMF
offset
Normalized objective values
1.00
0.99
0.98
0.97
0.96
0.95
0
200
400
600
Iterations

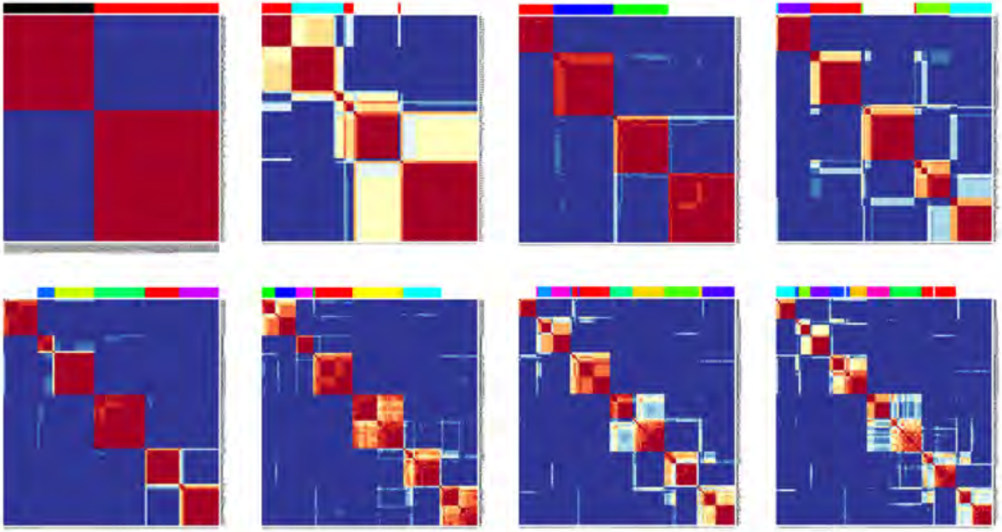

Tumors
0
5
10
15
0.11
0.11
0.74
0.05
0.19
0.19
0.06
0.56
0.12
0.25
0.35
0.12
0.25
0.18
0.82
0.21
0.11
0.32
0.37
0.09
0.91
1
2
3
4
5
6
NMF Consensus Cluster
TNBCType
BL1
BL2
IM
LAR
M
MSL
UNS

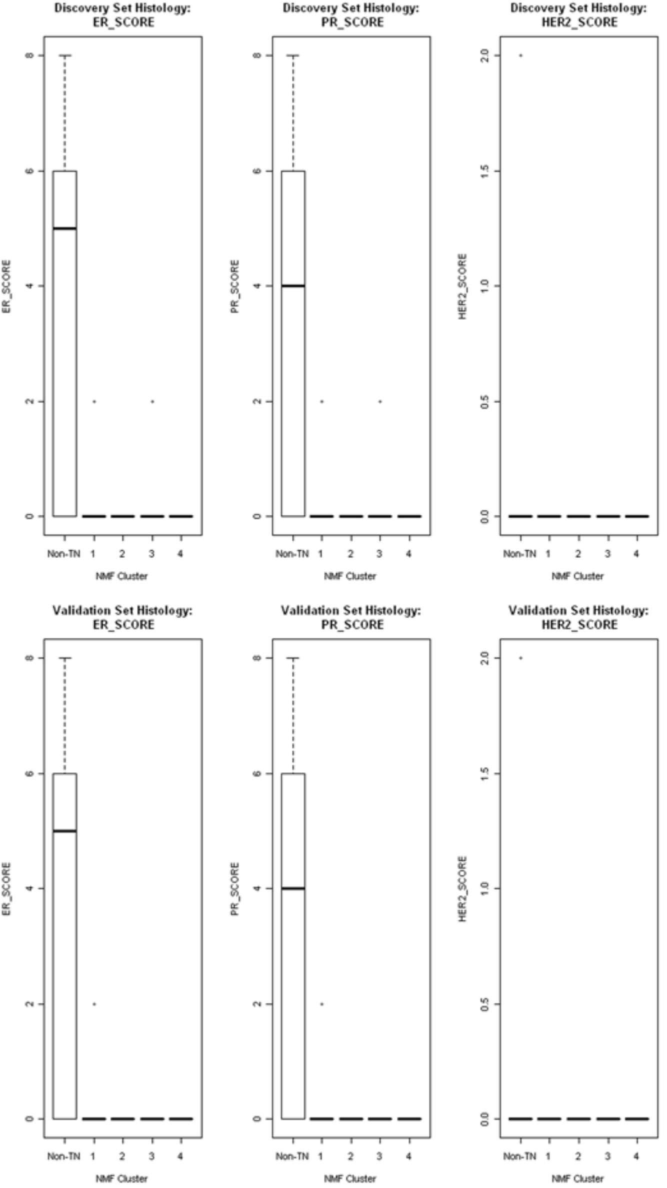


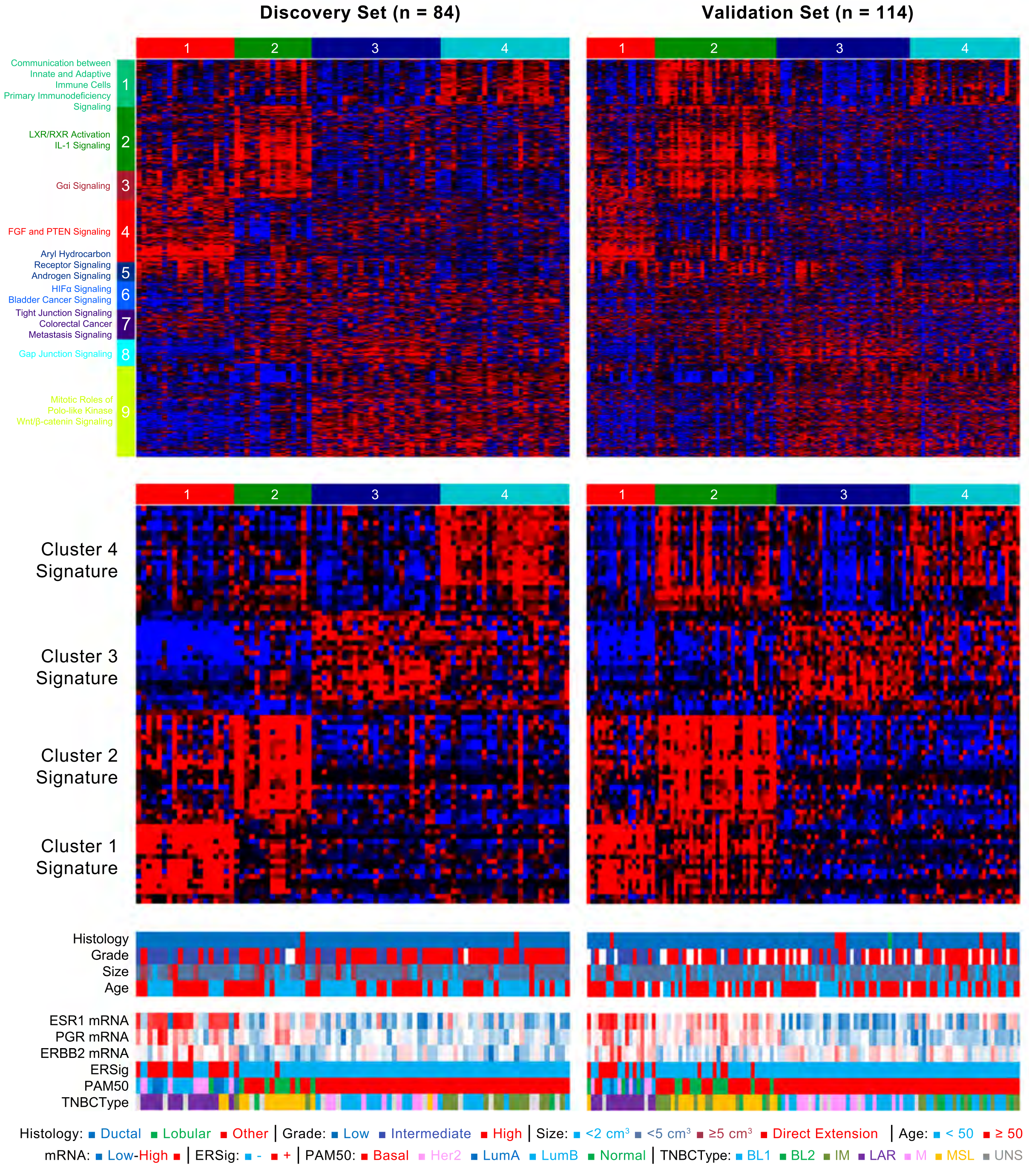

NMF rank estimation
- cophenetic -
- rss -
- residuals -
- dispersion -
- evar -
- sparseness -
Quality measure: cophenetic
Quality measure: rss
Quality measure: residuals
Quality measure: dispersion
Quality measure: evar
Quality measure: sparseness
Factorization rank
2 3 4 5 6 7 8 9
1.0 0.9 0.8 0.7
100000 120000 140000 160000
70000 90000 110000
0.2 0.4 0.6 0.8 1.0
0.35 0.40 0.45 0.50 0.55 0.60
0.1 0.2 0.3 0.4 0.5 0.6 0.7
sparseness basis
sparseness coef
F ctorization rank

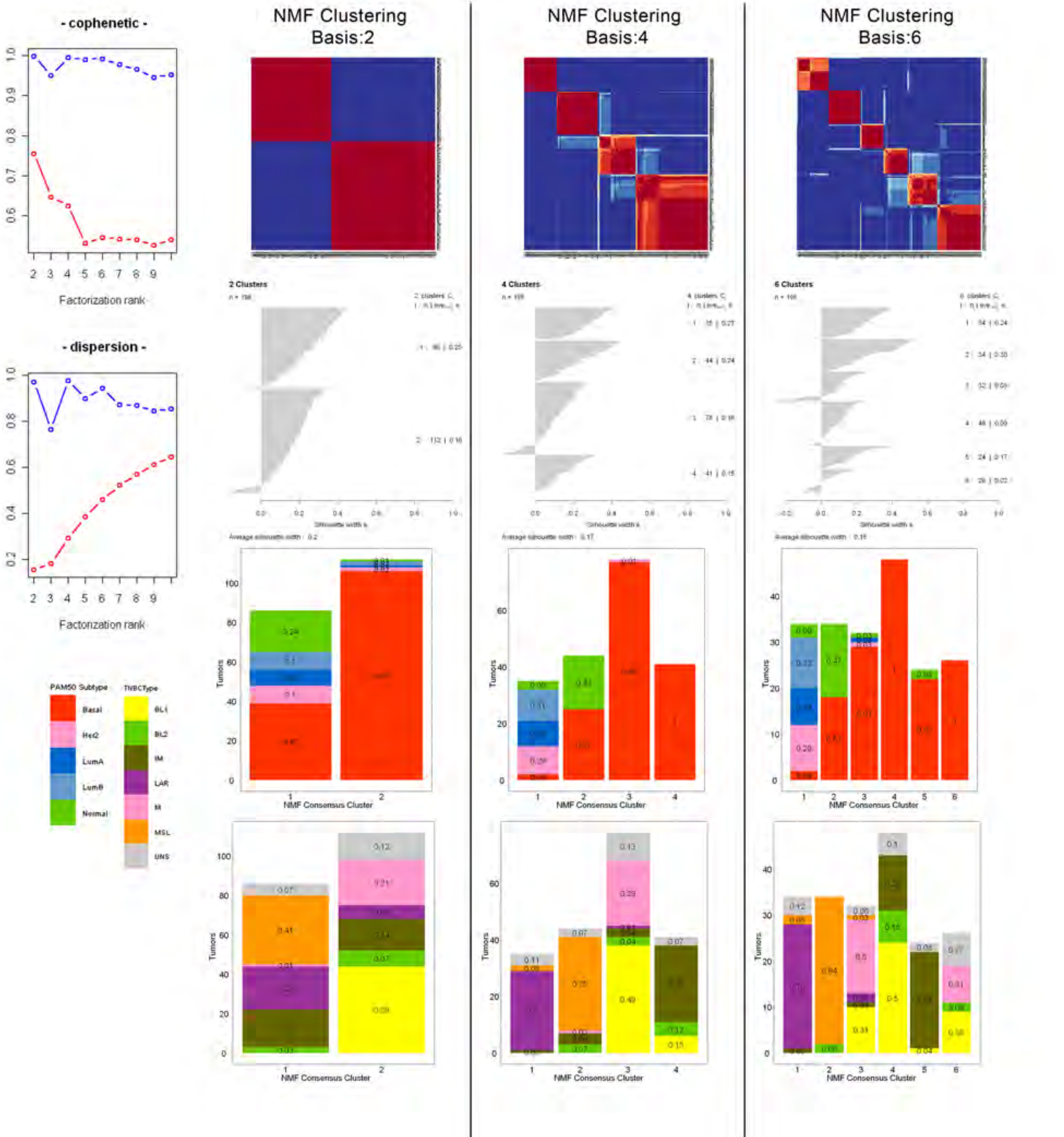

NMF Residuals
Algorithm
brunet
nsNMF
offset
Normalized objective values
1.00 0.99 0.98 0.97 0.96 0.95
0 200 400 600 800 1000
Iterations


Tumors
0 5 10 15 20 25
0.11
0.56
0.33
0.86
0.1
0.05
0.04
0.22
0.22
0.52
1
0.1
0.1
0.29
0.14
0.1
0.29
0.11
0.06
0.83
THBCType
BL1
BL2
IM
LAR
M
MSL
UNS
1 2 3 4 5 6
NM Consensus Cluster

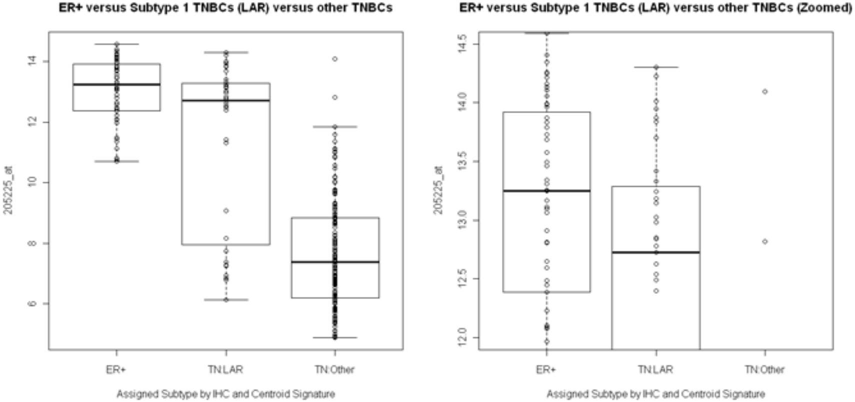



Discovery Set Histology: ER_SCORE
Discovery Set Histology: PR_SCORE
Discovery Set Histology: HER2_SCORE
Validation Set Histology: ER_SCORE
Validation Set Histology: PR_SCORE
Validation Set Histology: HER2_SCORE
ER_SCORE
PR_SCORE
HER2_SCORE
0
2
4
6
8
0.0
0.5
1.0
1.5
2.0
Non-TN
1
2
3
4
NMF Cluster

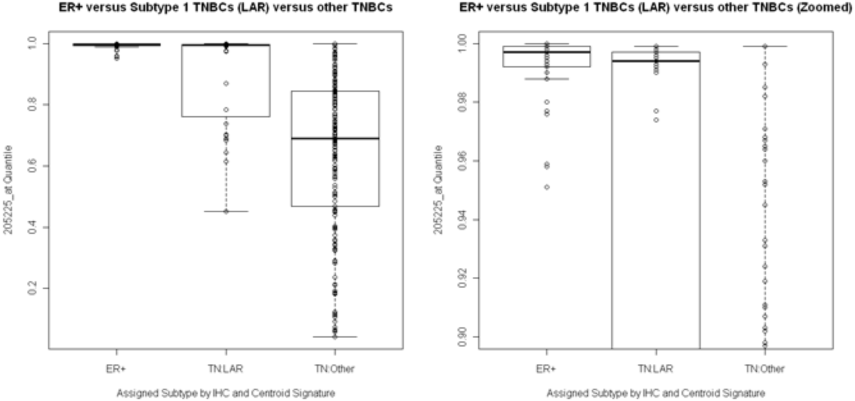

Discovery Set (n = 84)
Validation Set (n = 114)
1
2
3
4
Communication between Innate and Adaptive Immune Cells
Primary Immunodeficiency Signaling
LXR/RXR Activation
IL-1 Signaling
Gαi Signaling
FGF and PTEN Signaling
Aryl Hydrocarbon Receptor Signaling
Androgen Signaling
HIFα Signaling
Bladder Cancer Signaling
Tight Junction Signaling
Colorectal Cancer Metastasis Signaling
Gap Junction Signaling
Mitotic Roles of Polo-like Kinase
Wnt/β-catenin Signaling
1
2
3
4
5
6
7
8
9
Cluster 4 Signature
Cluster 3 Signature
Cluster 2 Signature
Cluster 1 Signature
Histology
Grade
Size
Age
ESR1 mRNA
PGR mRNA
ERBB2 mRNA
ERSig
PAM50
TNBCType
Histology: ■ Ductal ■ Lobular ■ Other | Grade: ■ Low ■ Intermediate ■ High | Size: ■ <2 cm^3 ■ <5 cm^3 ■ ≥5 cm^3 ■ Direct Extension | Age: ■ < 50 ■ ≥ 50
mRNA: ■ Low-High ■ | ERSig: ■ - ■ + | PAM50: ■ Basal ■ Her2 ■ LumA ■ LumB ■ Normal | TNBCType: ■ BL1 ■ BL2 ■ IM ■ LAR ■ M ■ MSL ■ UNS

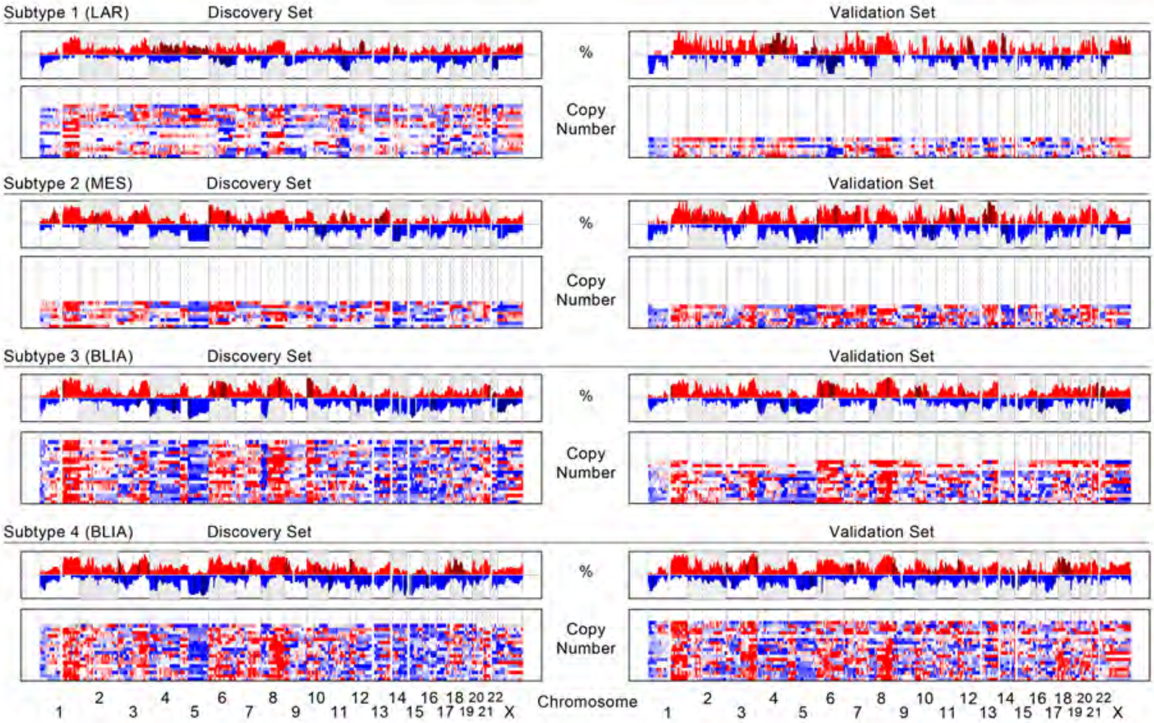

- cophenetic -
- dispersion -
Factorization rank
PAM50 Subtype
Basal
Her2
LumA
LumB
Normal
TNBCType
BL1
BL2
IM
LAR
M
MSL
UNS
NMF Clustering Basis:2
NMF Clustering Basis:4
NMF Clustering Basis:6
2 Clusters
4 Clusters
6 Clusters
Silhouette width s_i
Average silhouette width : 0.2
Average silhouette width : 0.17
Average silhouette width : 0.16
Tumors
NMF Consensus Cluster

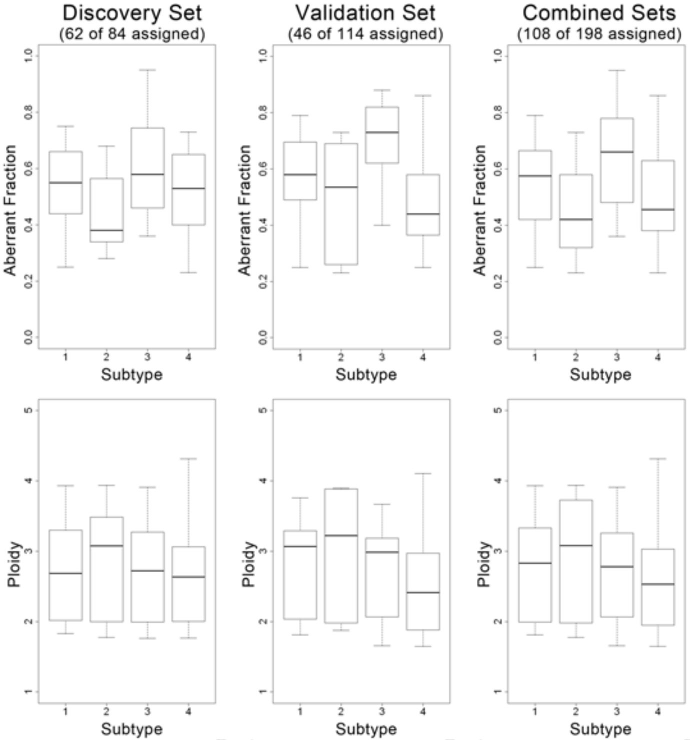
A


ER+ versus Subtype 1 TNBCs (LAR) versus other TNBCs
205225_at
6
8
10
12
14
ER+
TN:LAR
TN:Other
Assigned Subtype by IHC and Centroid Signature
ER+ versus Subtype 1 TNBCs (LAR) versus other TNBCs (Zoomed)
205225_at
12.0
12.5
13.0
13.5
14.0
14.5
ER+
TN:LAR
TN:Other
Assigned Subtype by IHC and Centroid Signature

B

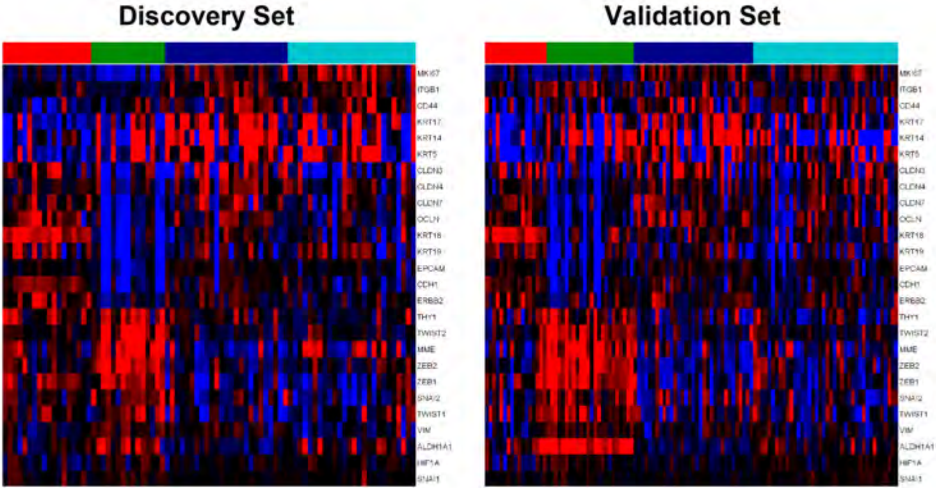

ER+ versus Subtype 1 TNBCs (LAR) versus other TNBCs
205225_at Quantile
0.2
0.4
0.6
0.8
1.0
ER+
TN:LAR
TN:Other
Assigned Subtype by IHC and Centroid Signature
ER+ versus Subtype 1 TNBCs (LAR) versus other TNBCs (Zoomed)
205225_at Quantile
0.90
0.92
0.94
0.96
0.98
1.00
ER+
TN:LAR
TN:Other
Assigned Subtype by IHC and Centroid Signature


Subtype 1 (LAR)
Discovery Set
Validation Set
%
Copy Number
Subtype 2 (MES)
Discovery Set
Validation Set
%
Copy Number
Subtype 3 (BLIA)
Discovery Set
Validation Set
%
Copy Number
Subtype 4 (BLIA)
Discovery Set
Validation Set
%
Copy Number
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 X
Chromosome
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 X



Subtypes: 1 = LAR
2 = MES
3 = BLIS
4 = BLIA

	1	2	3	4	Total	1	2	3	4	Total	1	2	3	4	Total
Assigned Cases with mRNA data:	18	15	25	26	84	17	24	33	40	114	35	39	58	66	198
Assigned Cases with SNP data:	18	15	25	26	84	07	13	13	25	58	25	28	38	51	142
Assigned Cases passing ASCAT:	17	11	20	14	62	07	06	13	20	46	24	17	33	34	108


Discovery Set
MKI67
ITGB1
CD44
KRT17
KRT14
KRT5
CLDN3
CLDN4
CLDN7
OCLN
KRT18
KRT19
EPCAM
CDH1
ERBB2
THY1
TWIST2
MME
ZEB2
ZEB1
SNAI2
TWIST1
VIM
ALDH1A1
HIF1A
SNAI1
Validation Set
MKI67
ITGB1
CD44
KRT17
KRT14
KRT5
CLDN3
CLDN4
CLDN7
OCLN
KRT18
KRT19
EPCAM
CDH1
ERBB2
THY1
TWIST2
MME
ZEB2
ZEB1
SNAI2
TWIST1
VIM
ALDH1A1
HIF1A
SNAI1