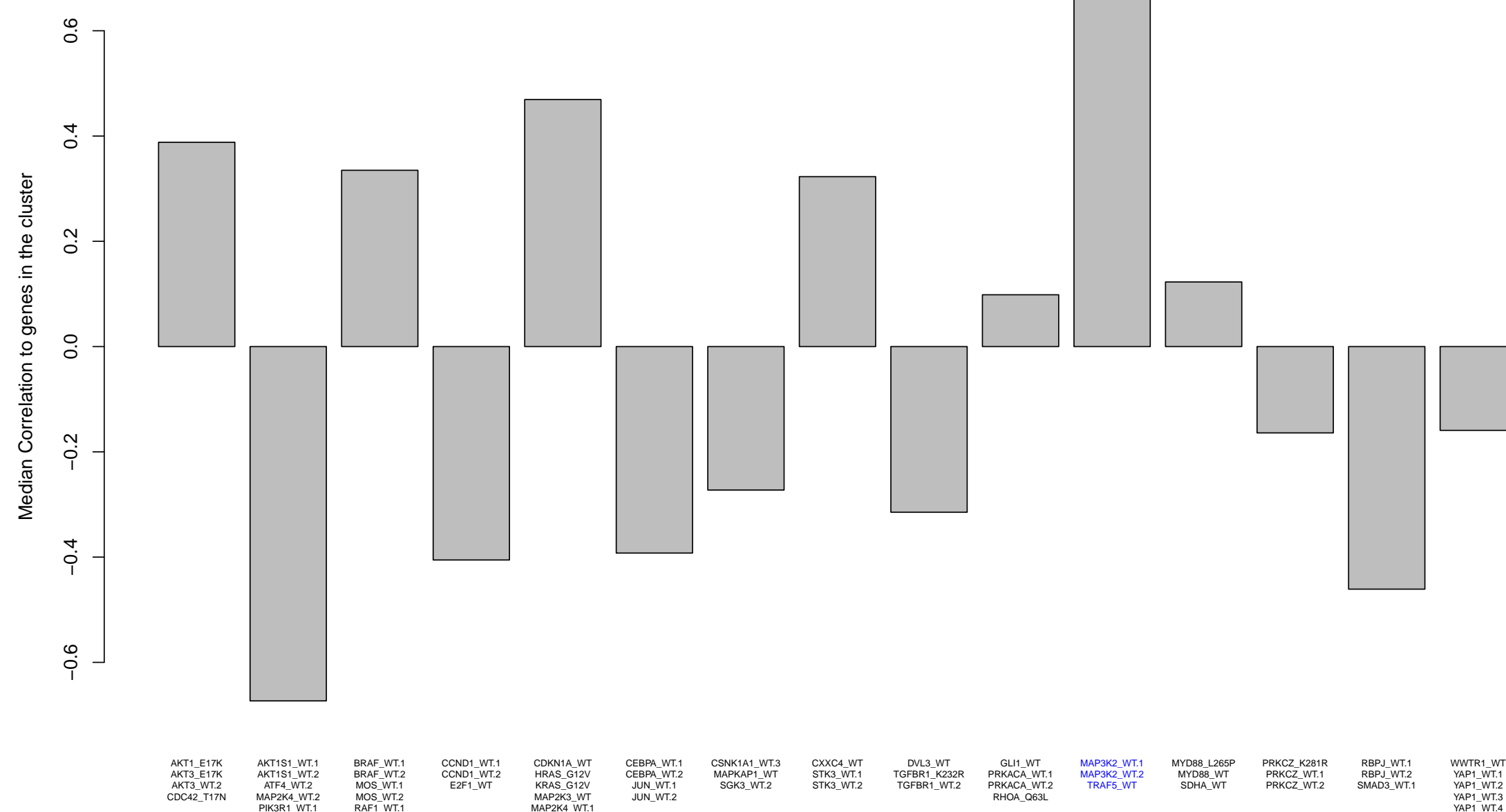
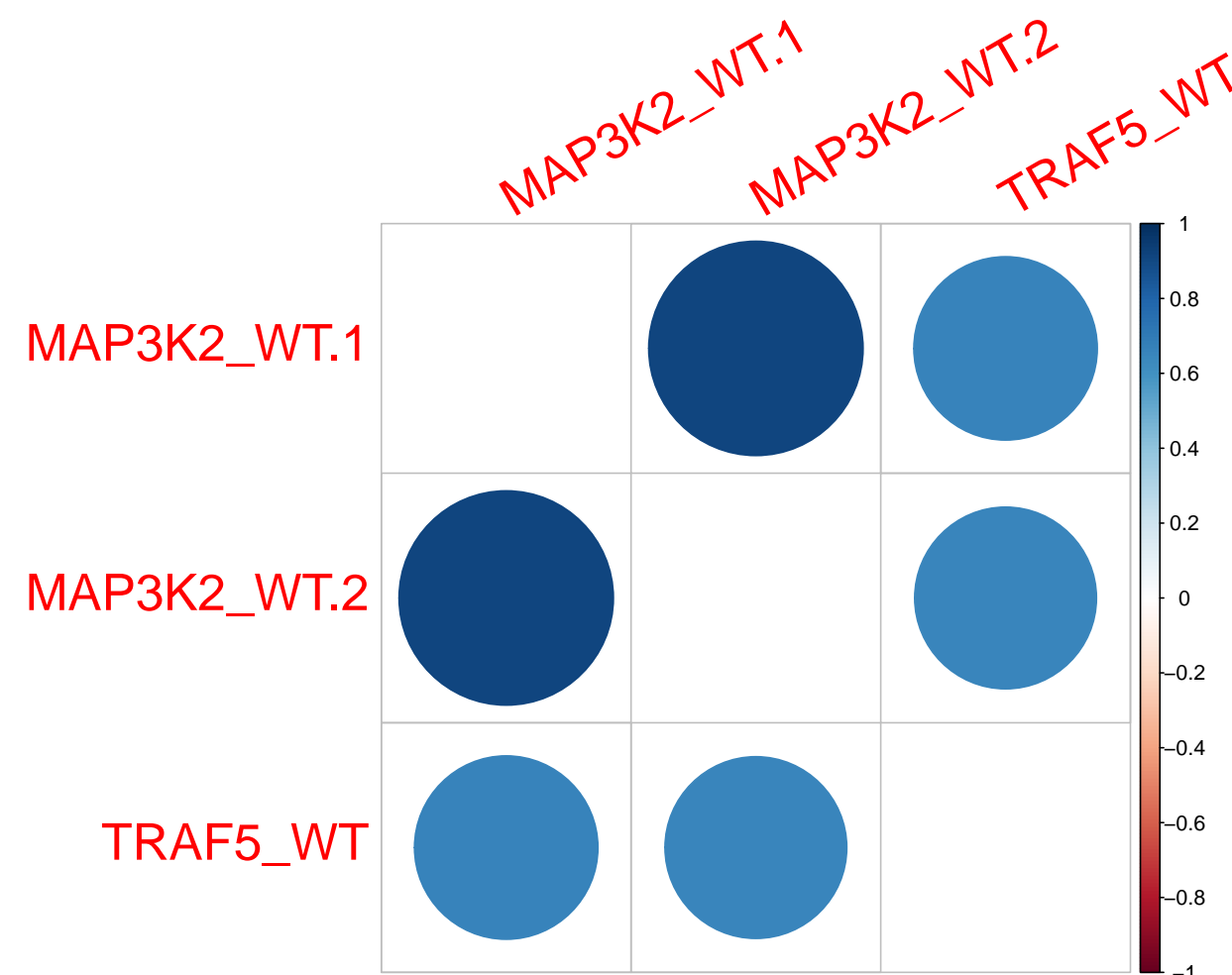
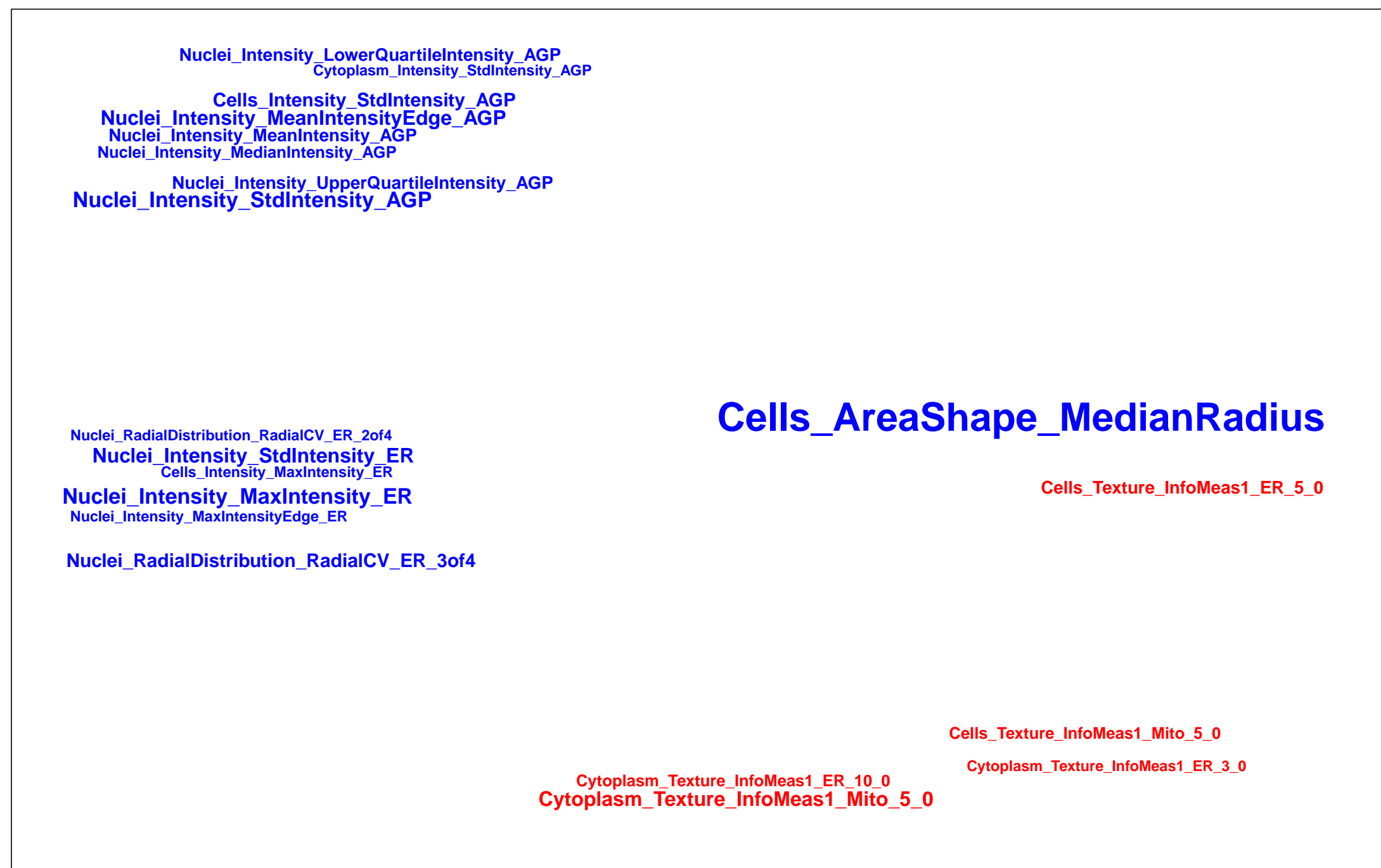
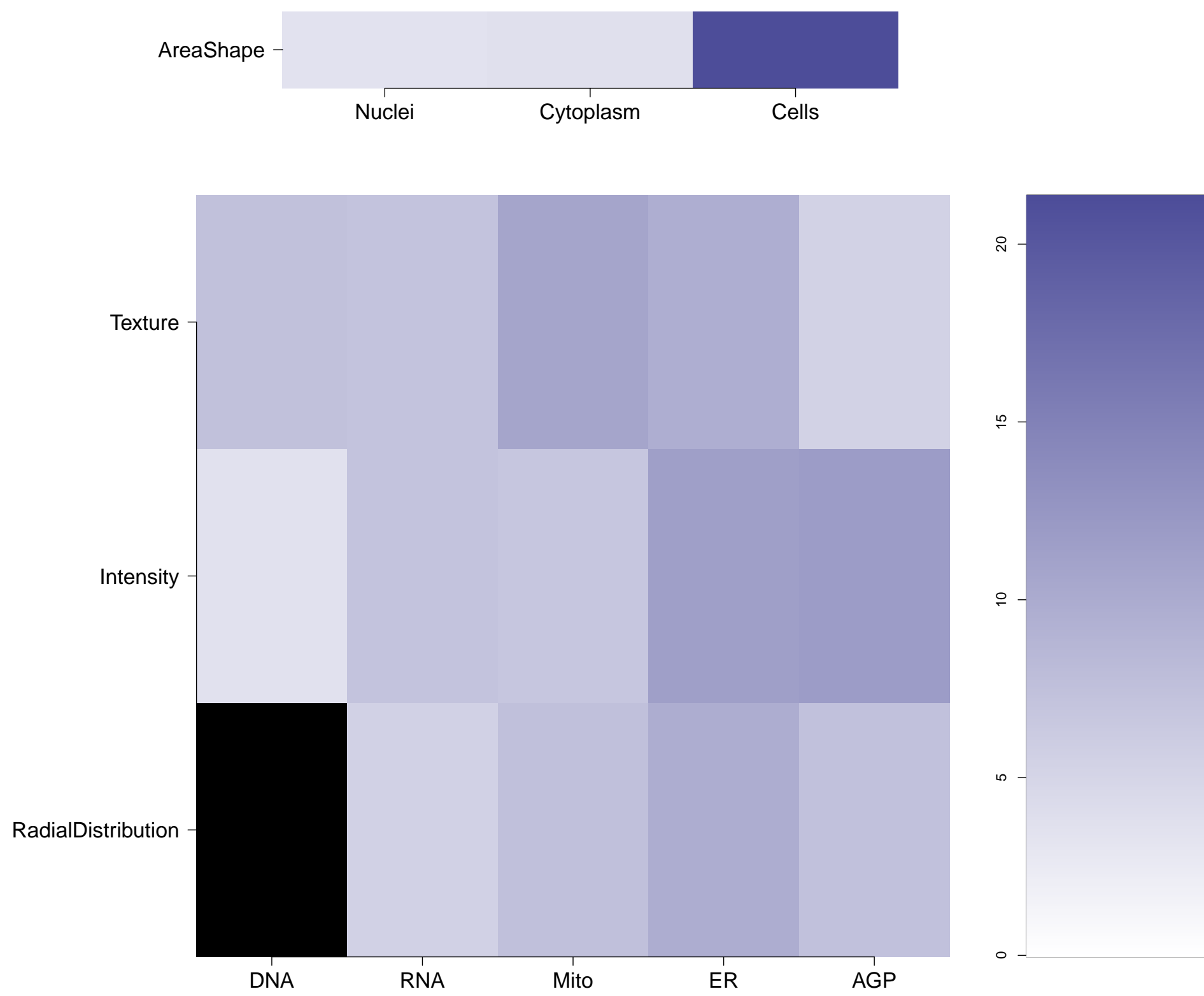


Treatment	Expert Annotation	
	Pathway	Regulation Type
MAP3K2_WT.1	Canonical MAPK	Activator
MAP3K2_WT.2	Canonical MAPK	Activator
TRAF5_WT	Canonical NFkB	Activator



Top 5 genes negatively correlated to the cluster				
Expert Annotation			Mean Correlation	Standard Deviation
Treatment	Pathway	Regulation Type		
MAP2K4.WT.2	Canonical MAPK	Activator	-0.68	0.13
AKT1S1.WT.1	TOR	Inhibitor	-0.67	0.05
PIK3R1.WT.1	Canonical PI3K/AKT	Activator	-0.65	0.07
RBPJ.WT.1	NOTCH	Activator	-0.64	0.10
AKT1S1.WT.2	TOR	Inhibitor	-0.64	0.06

Which individual morphological features are distinguishing in the cluster relative to the untreated samples? Blue/Red means the feature has a positive/negative z-score. Size is proportional to the z-score value.

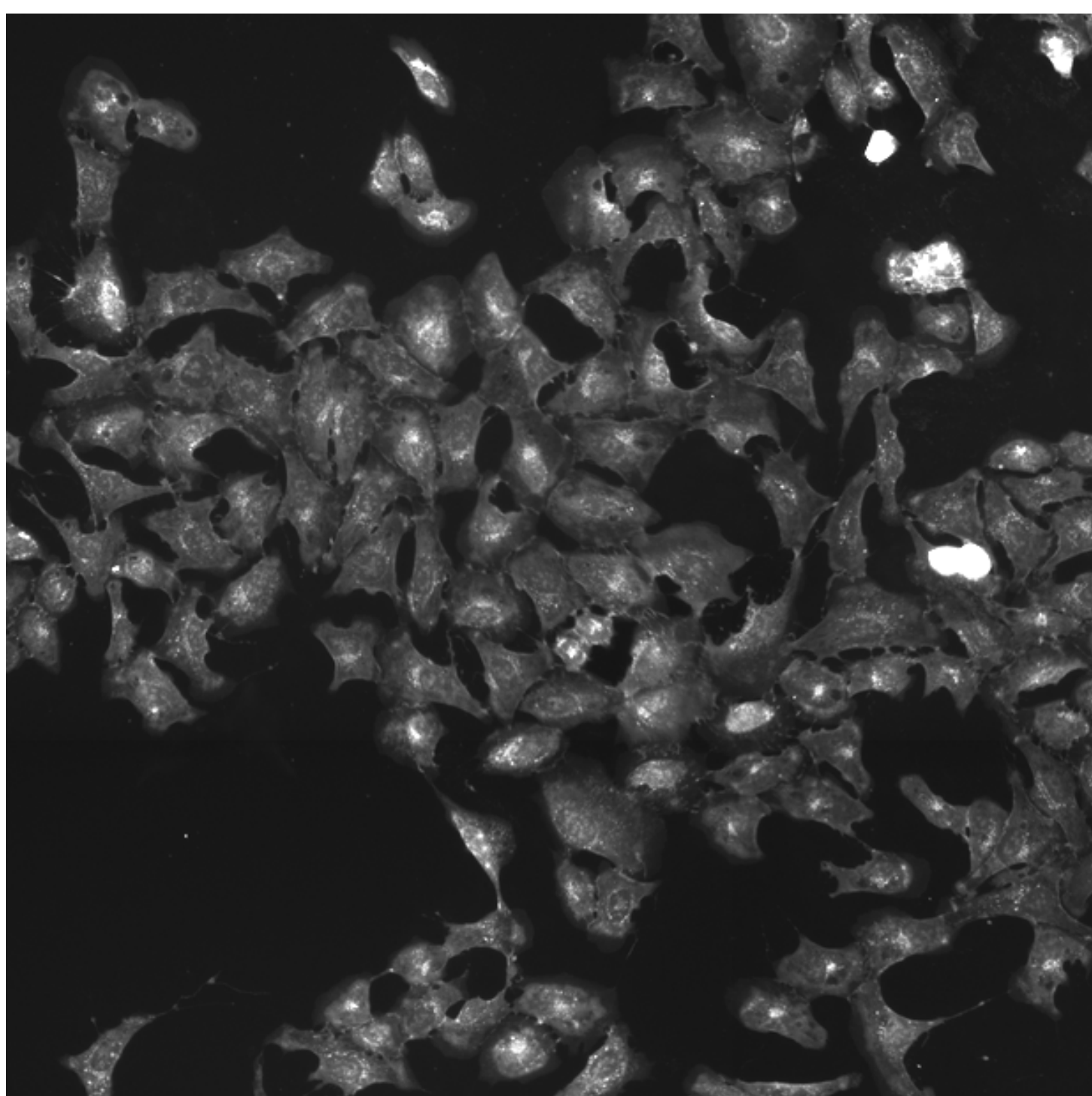
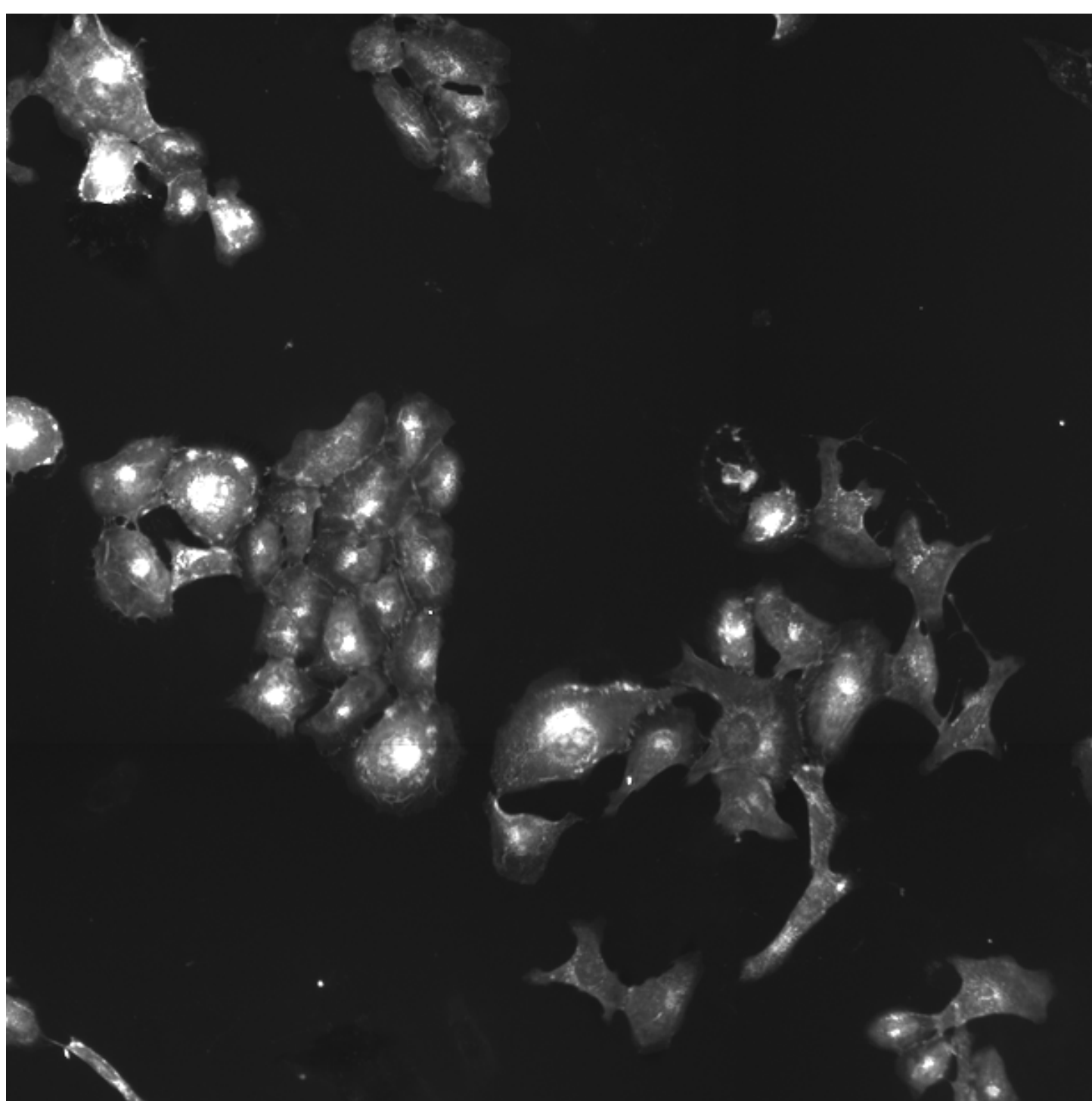
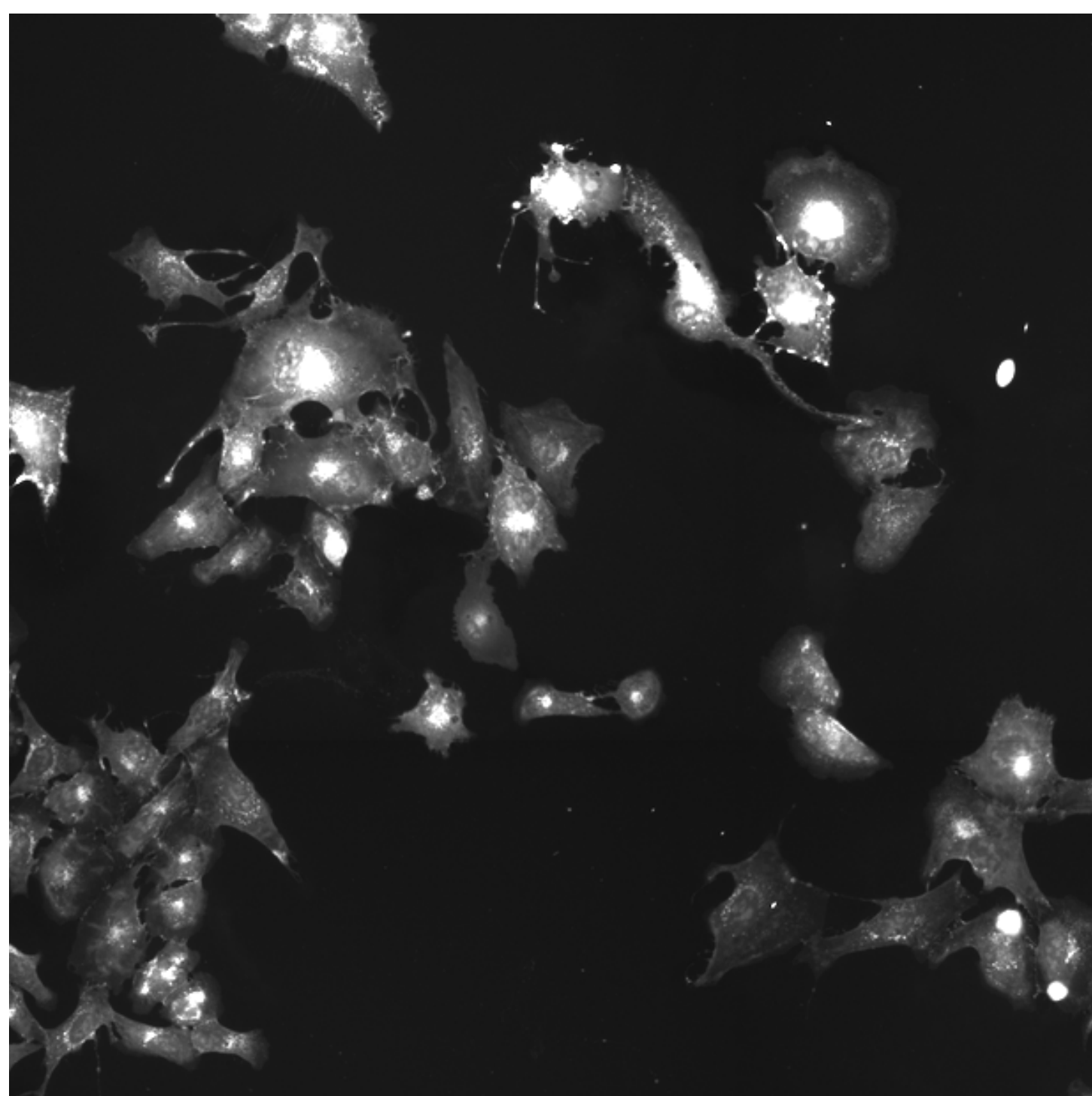
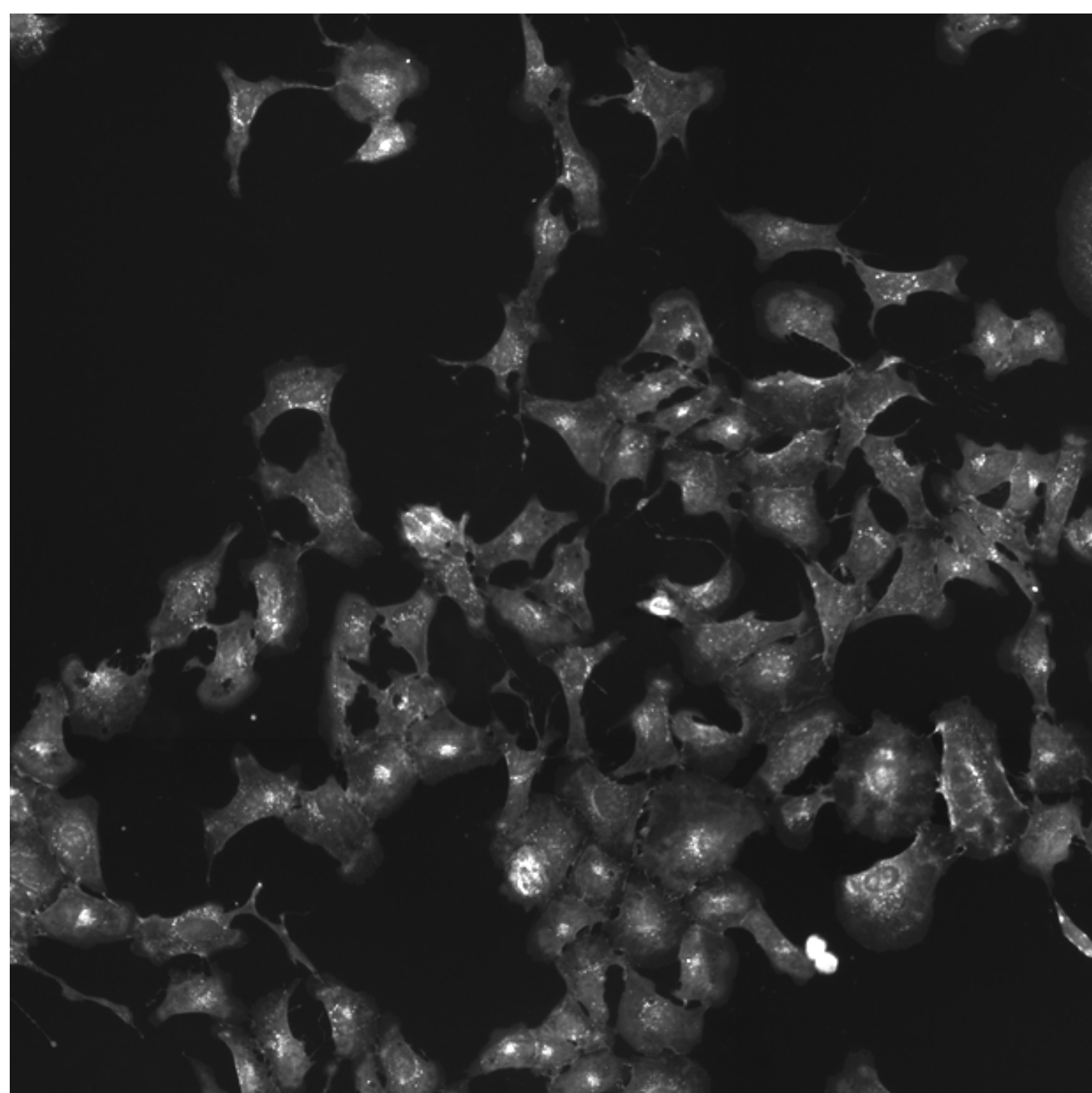
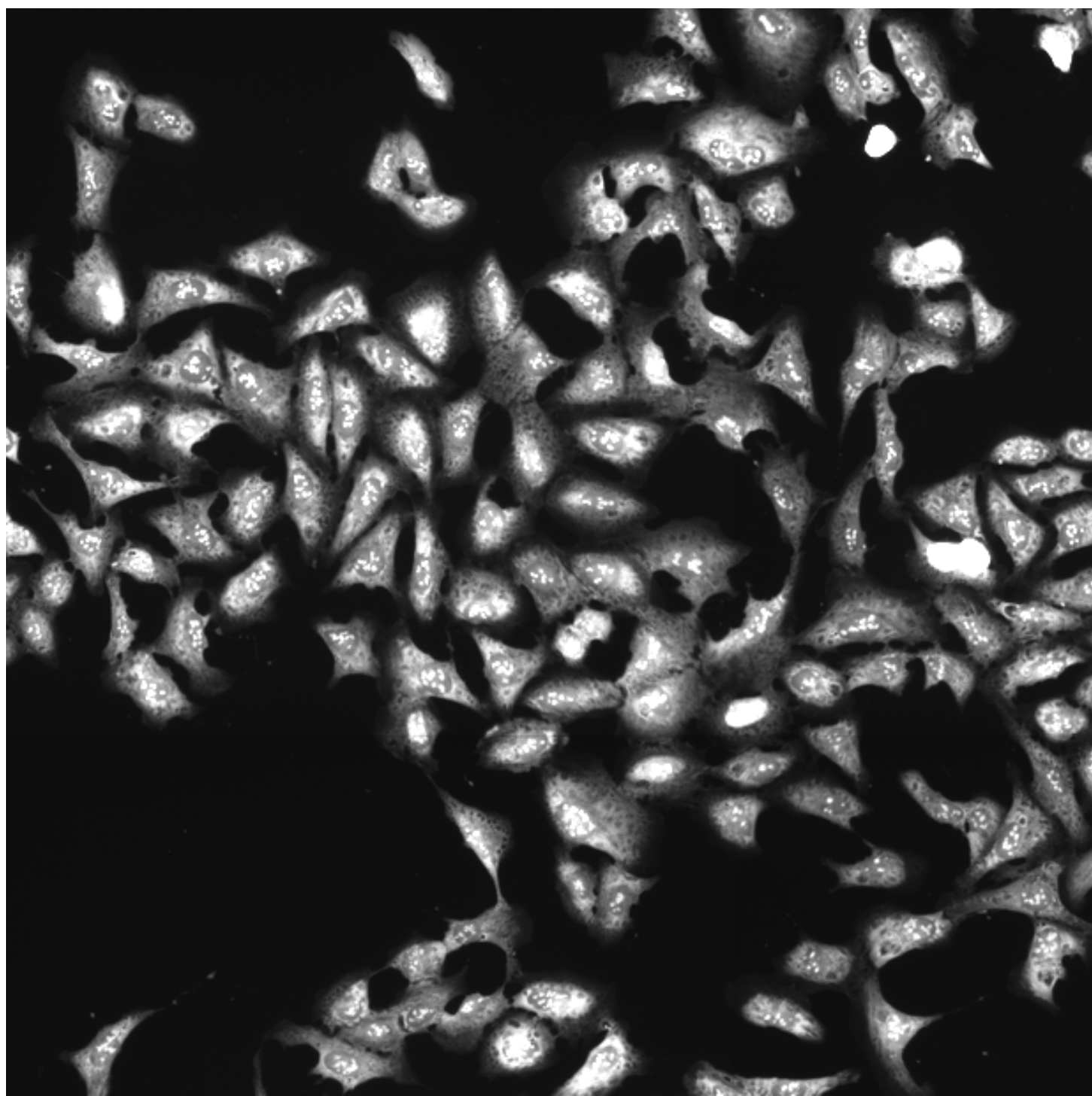
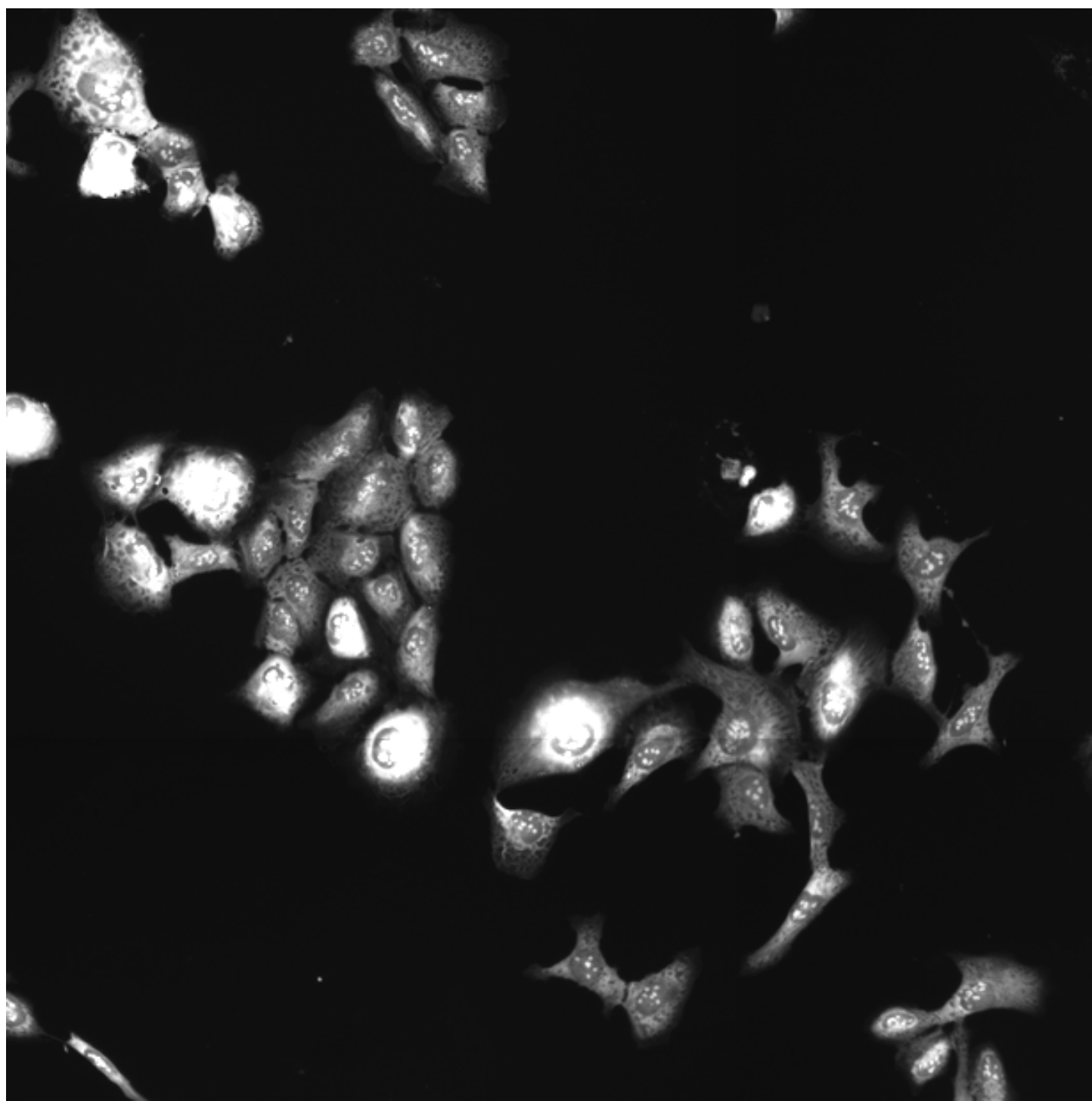
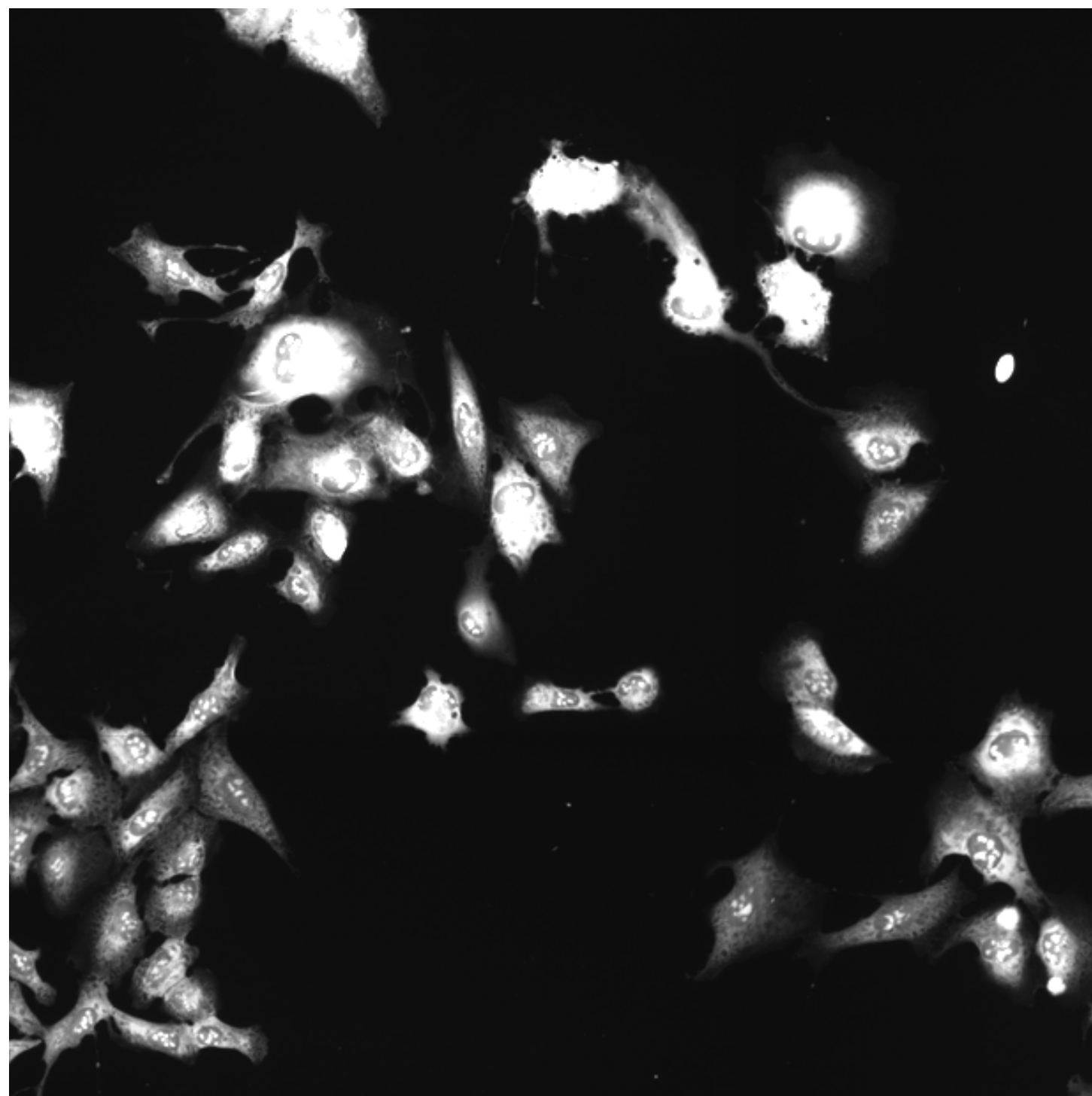
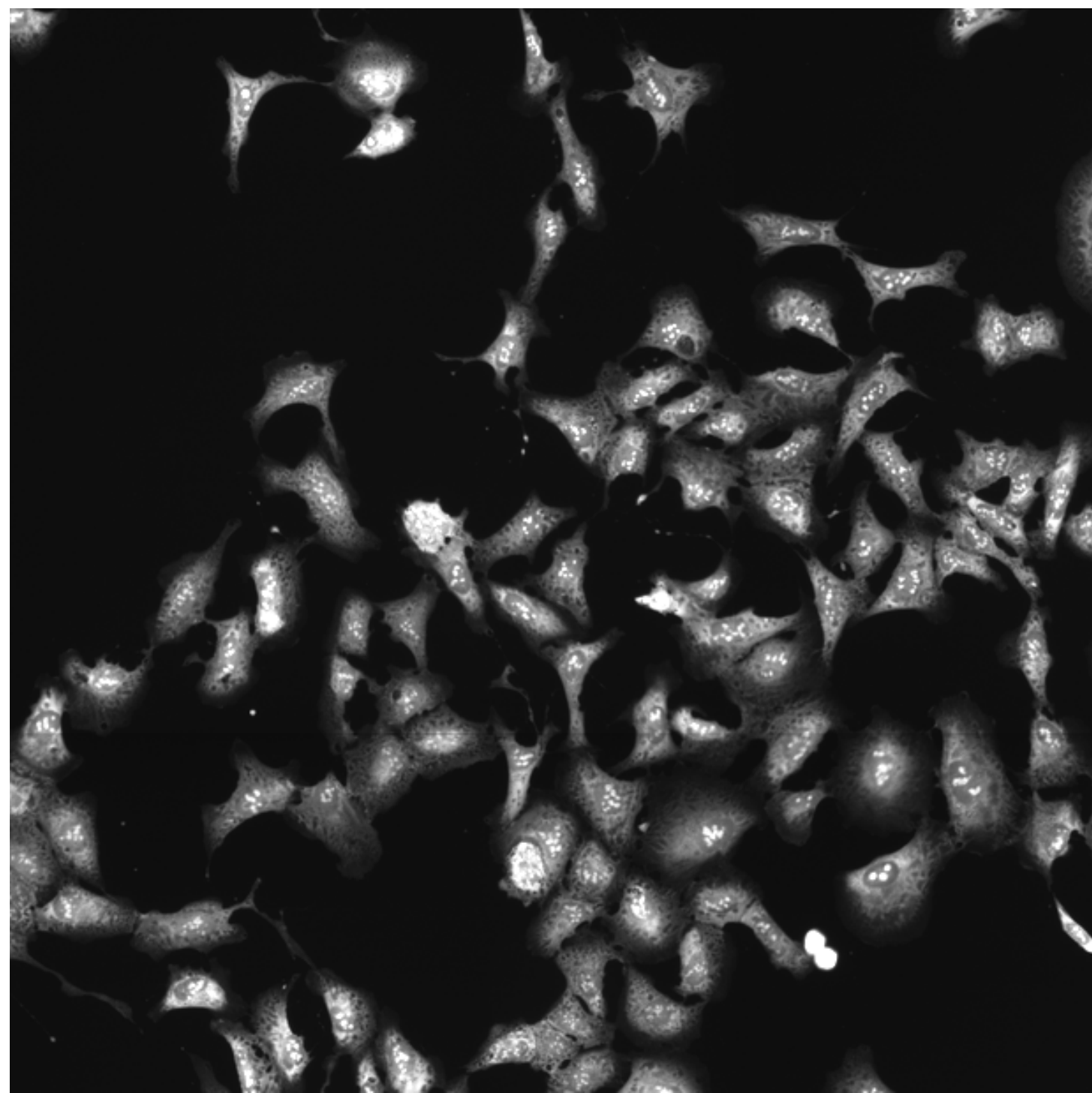


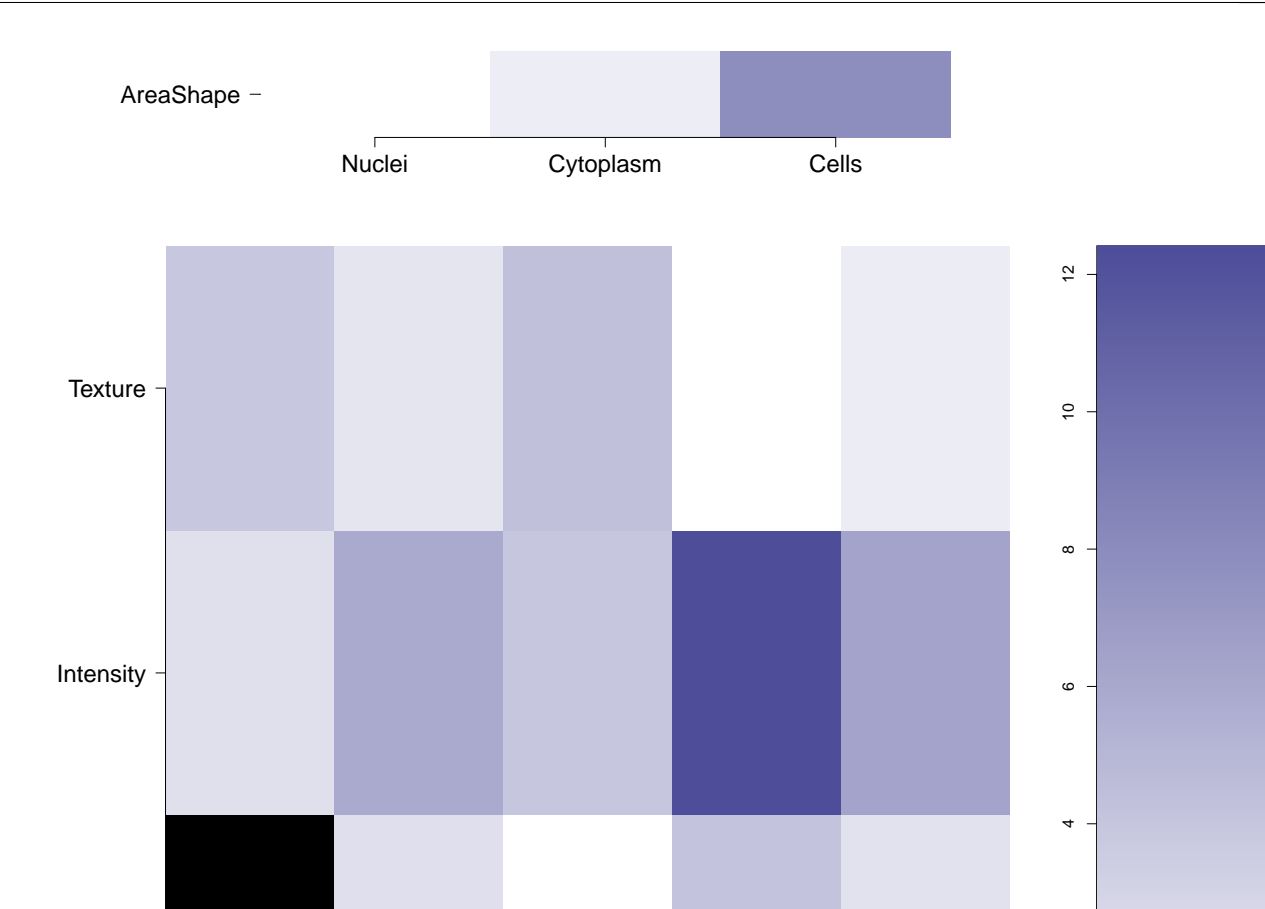
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MAP3K2\_WT.1

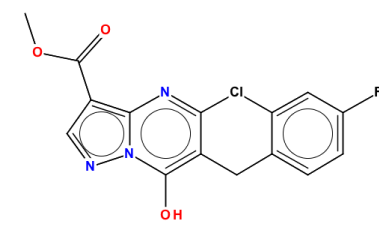
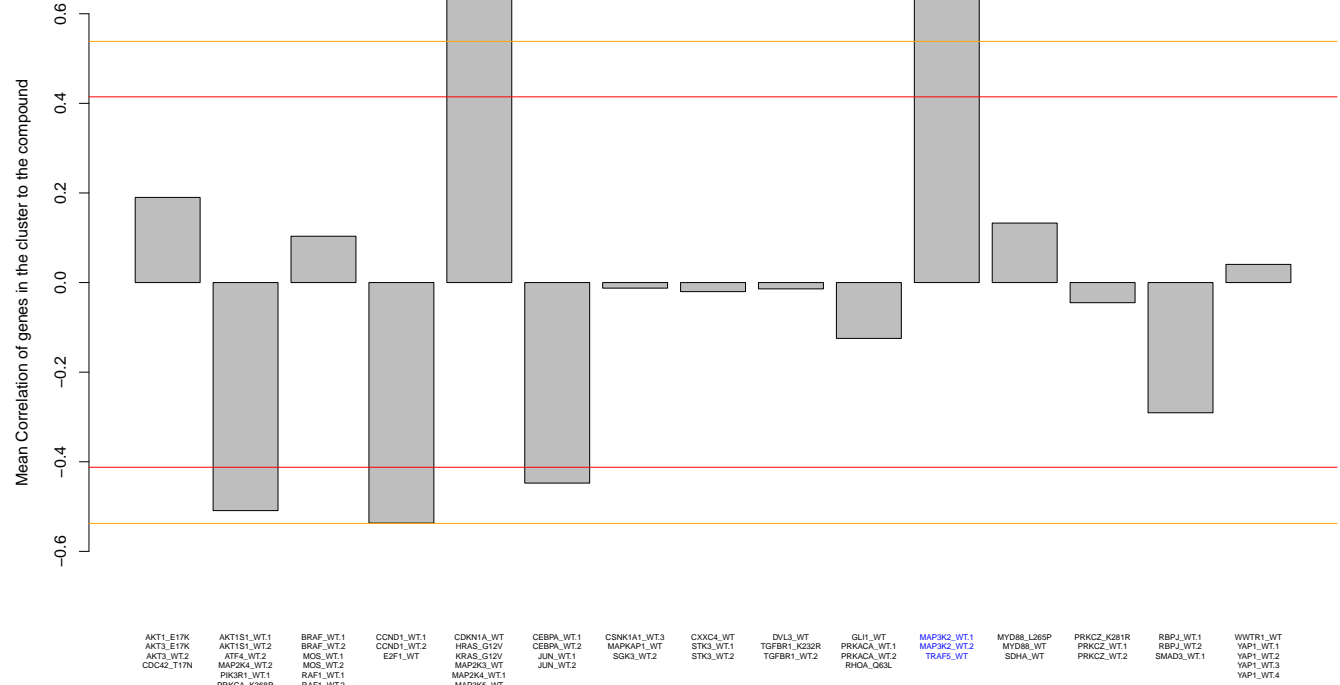
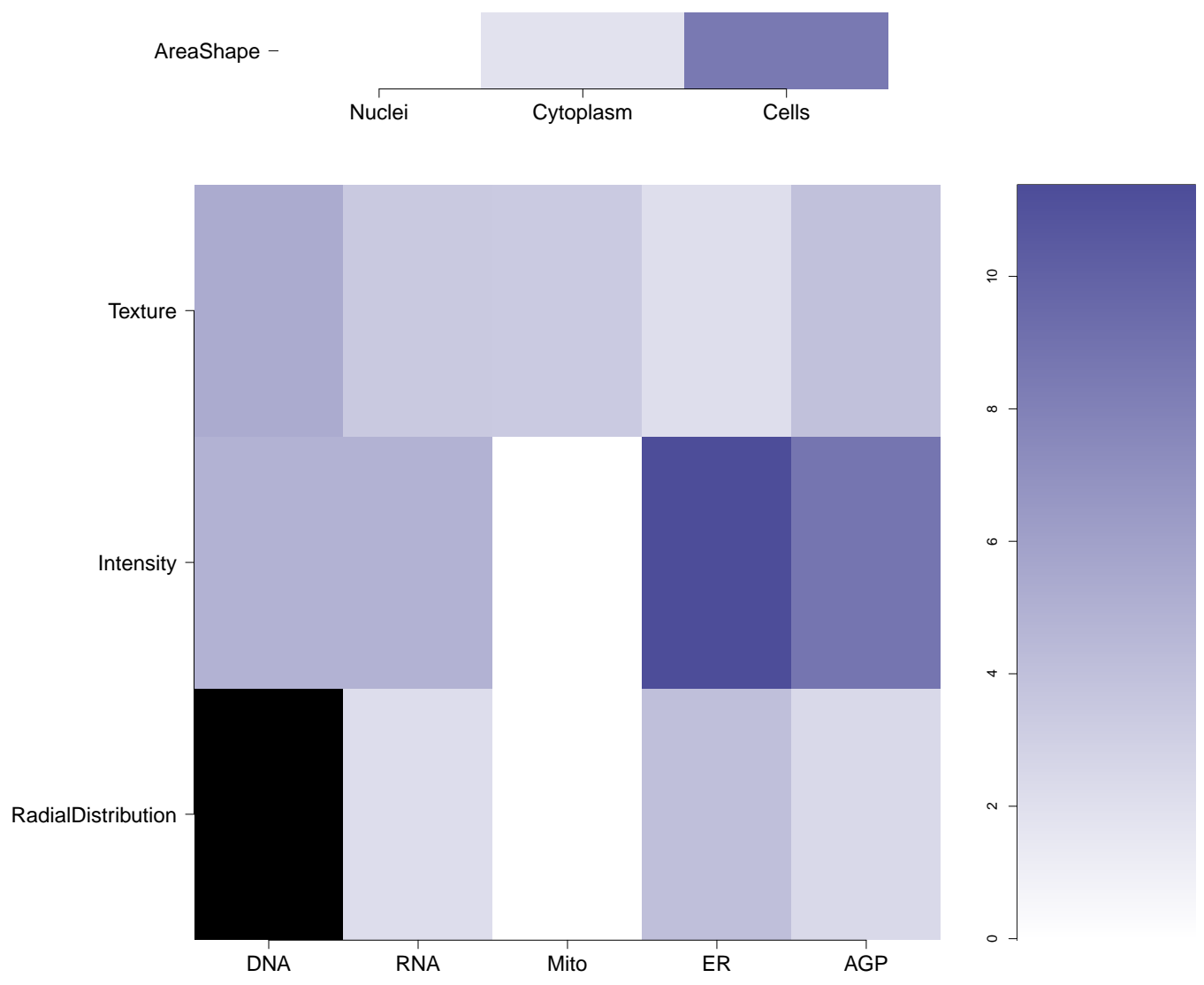
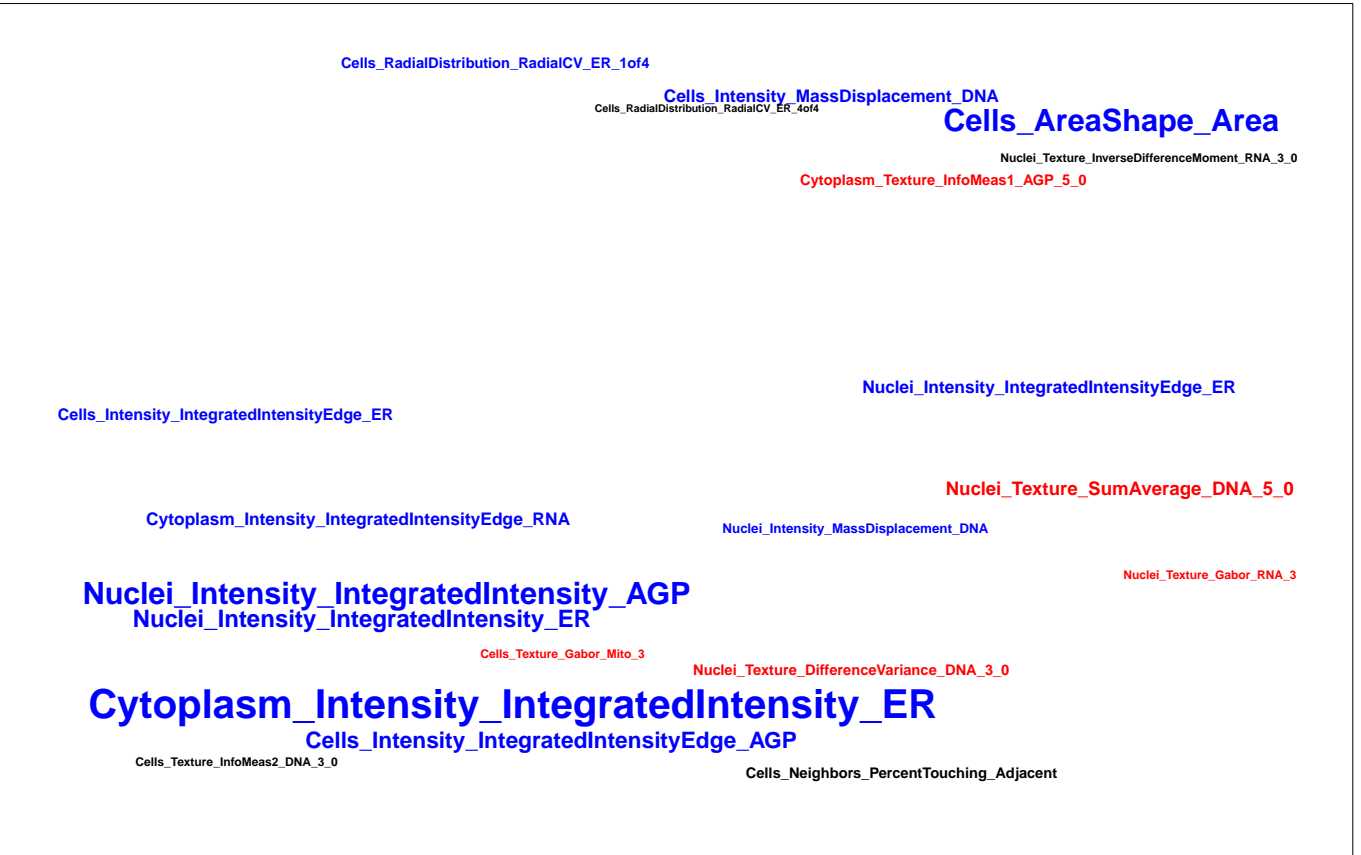
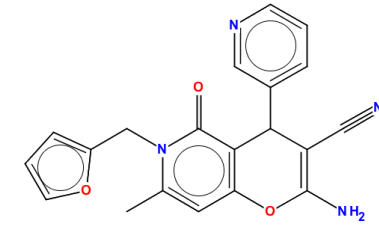
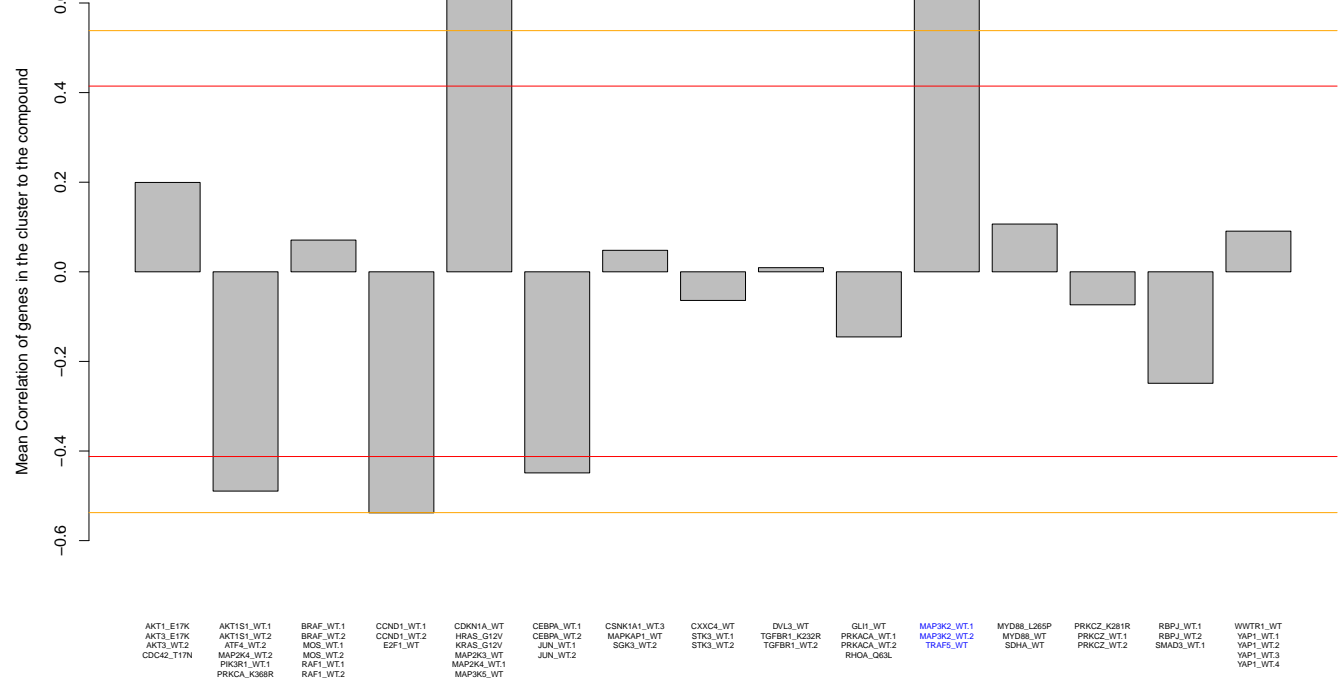
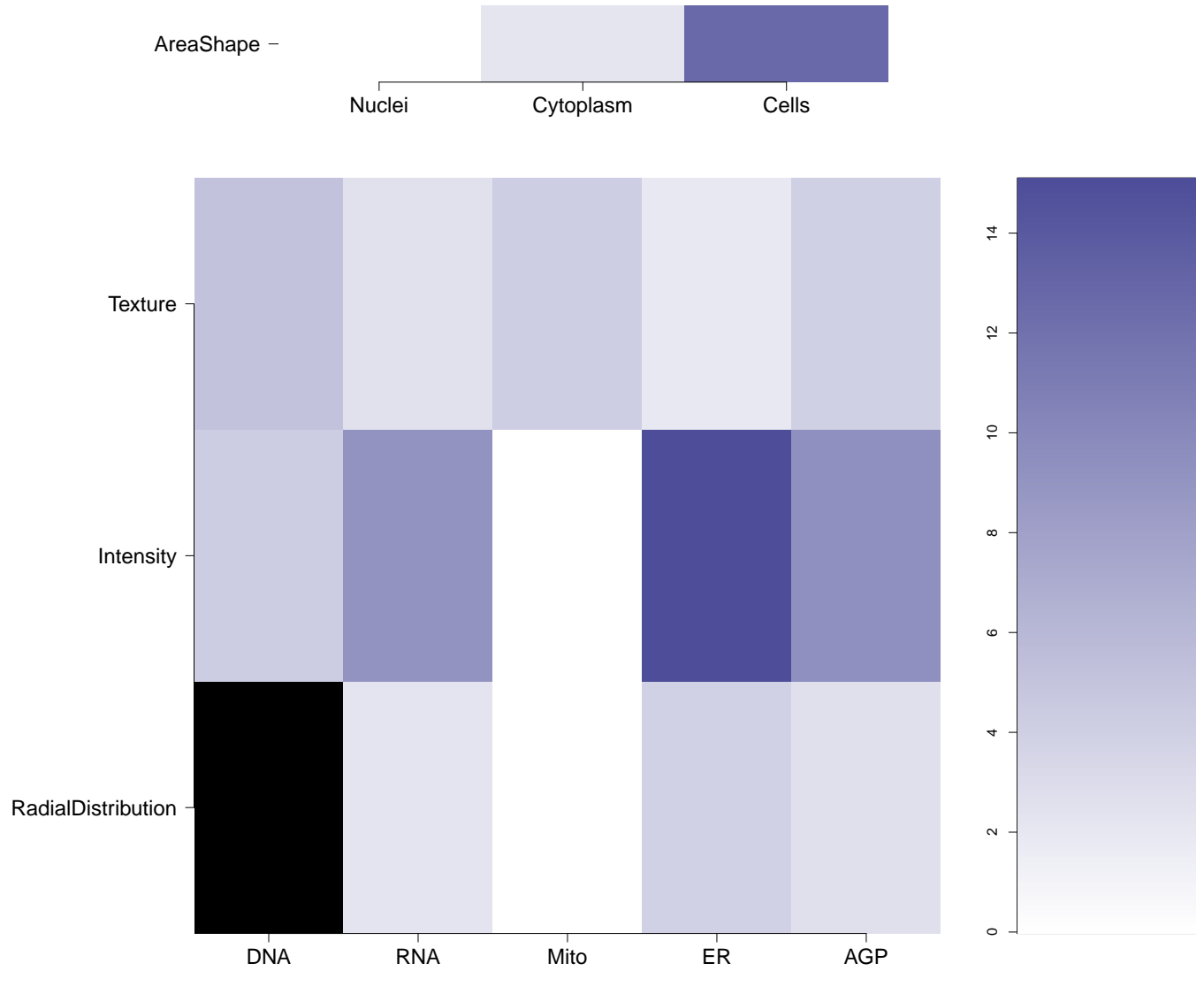
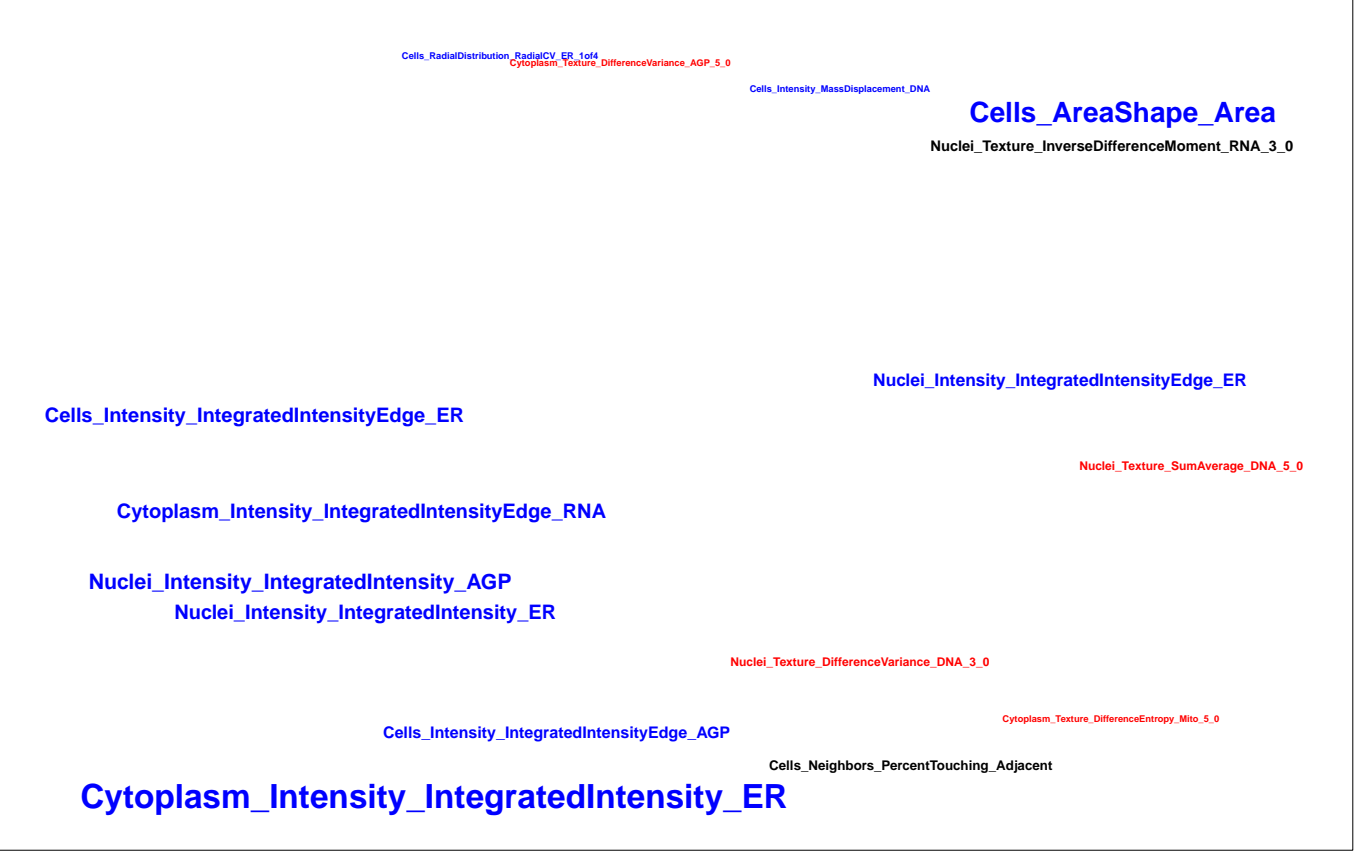
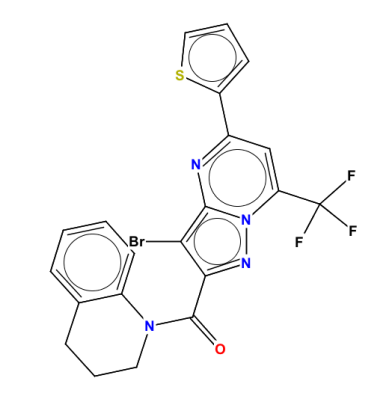
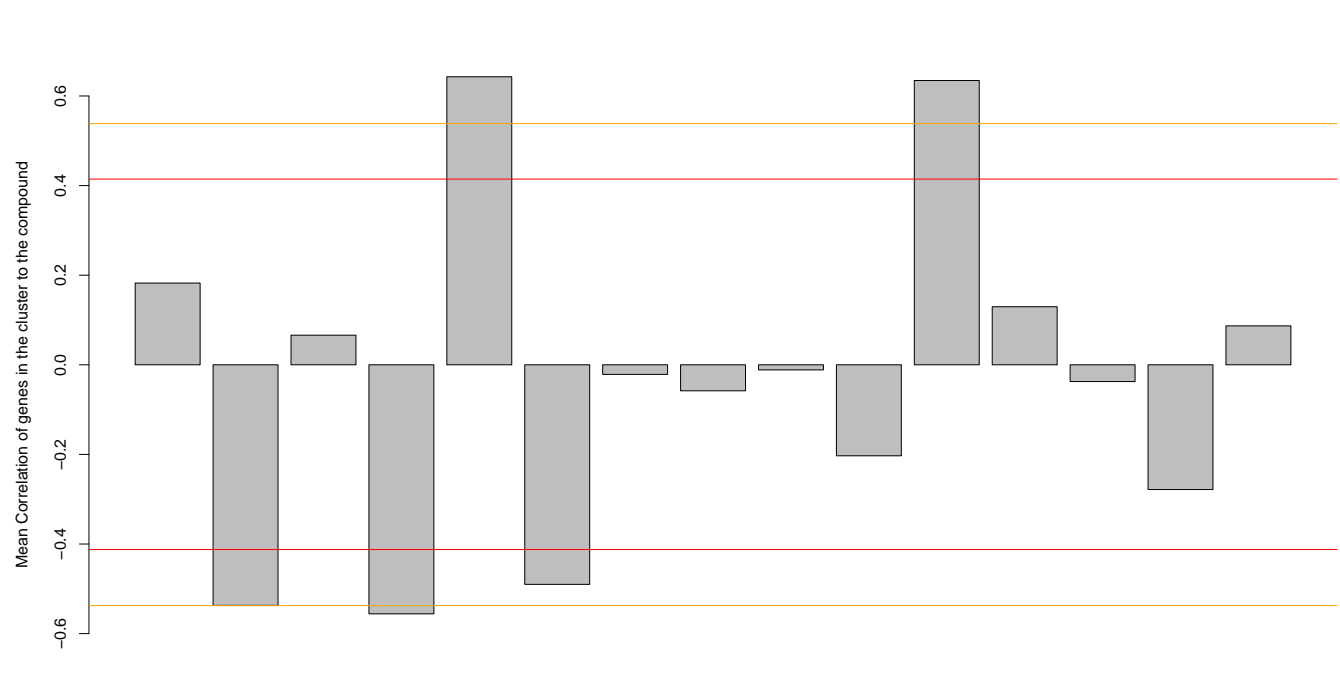
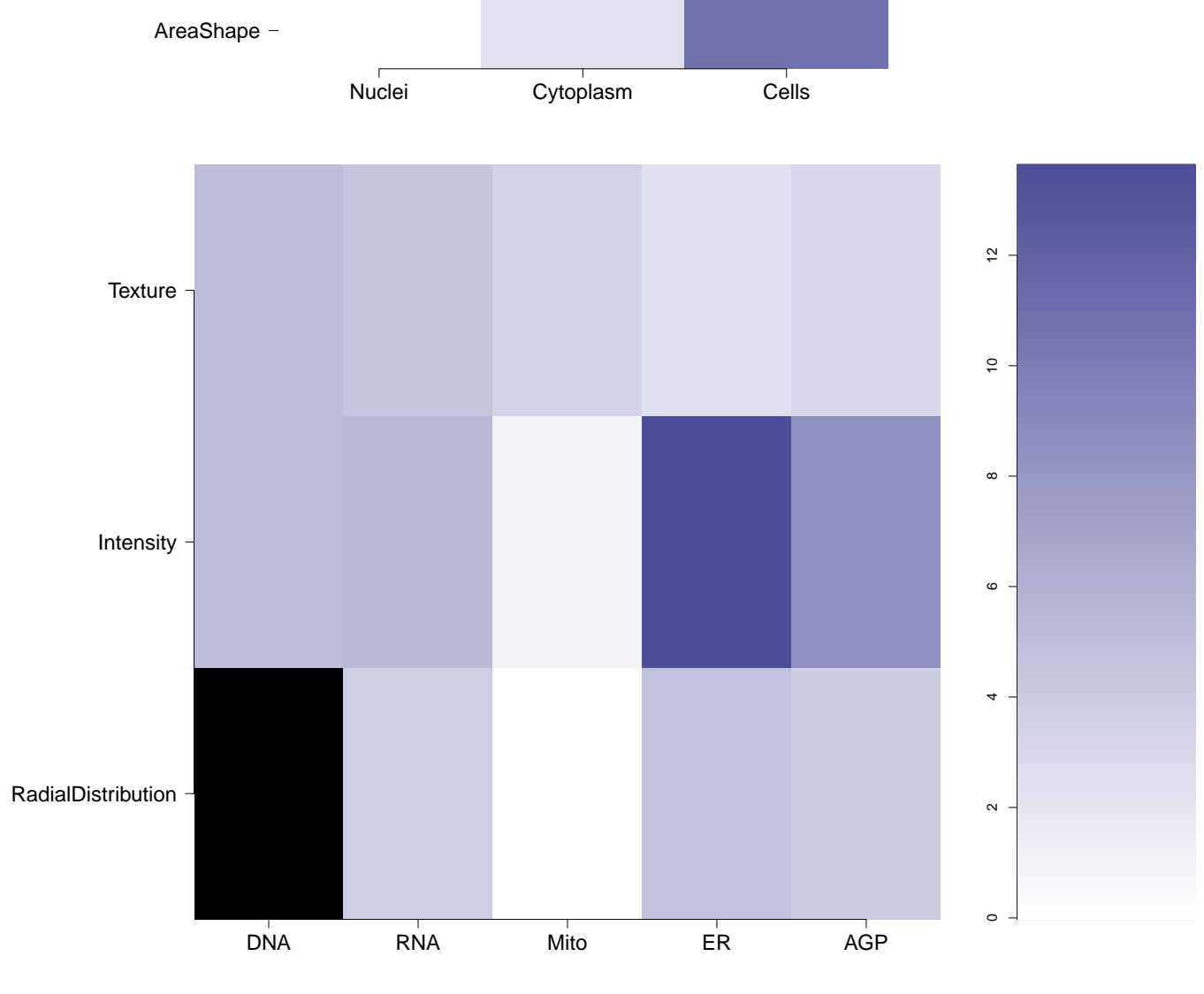
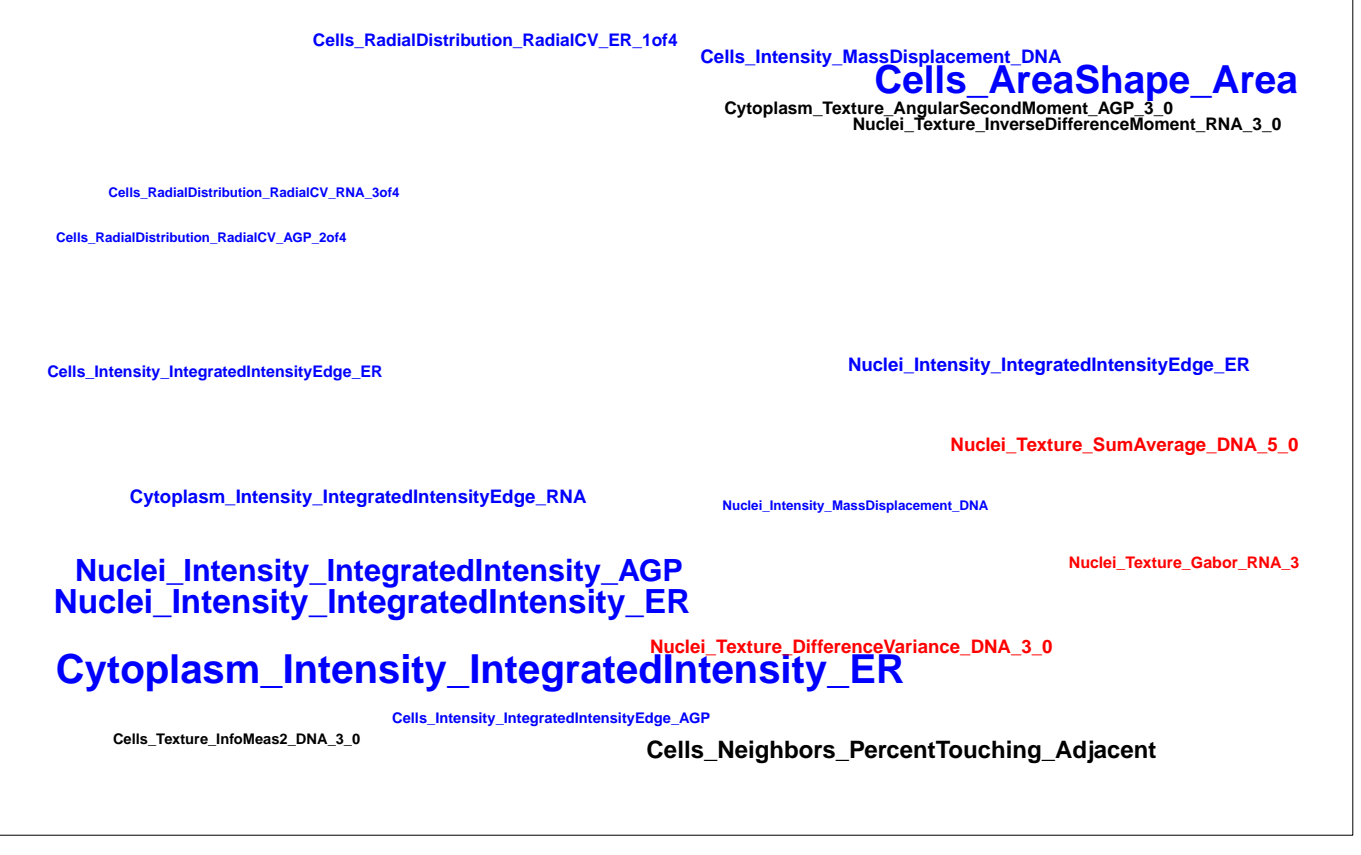
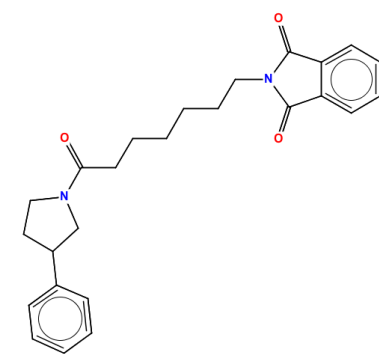
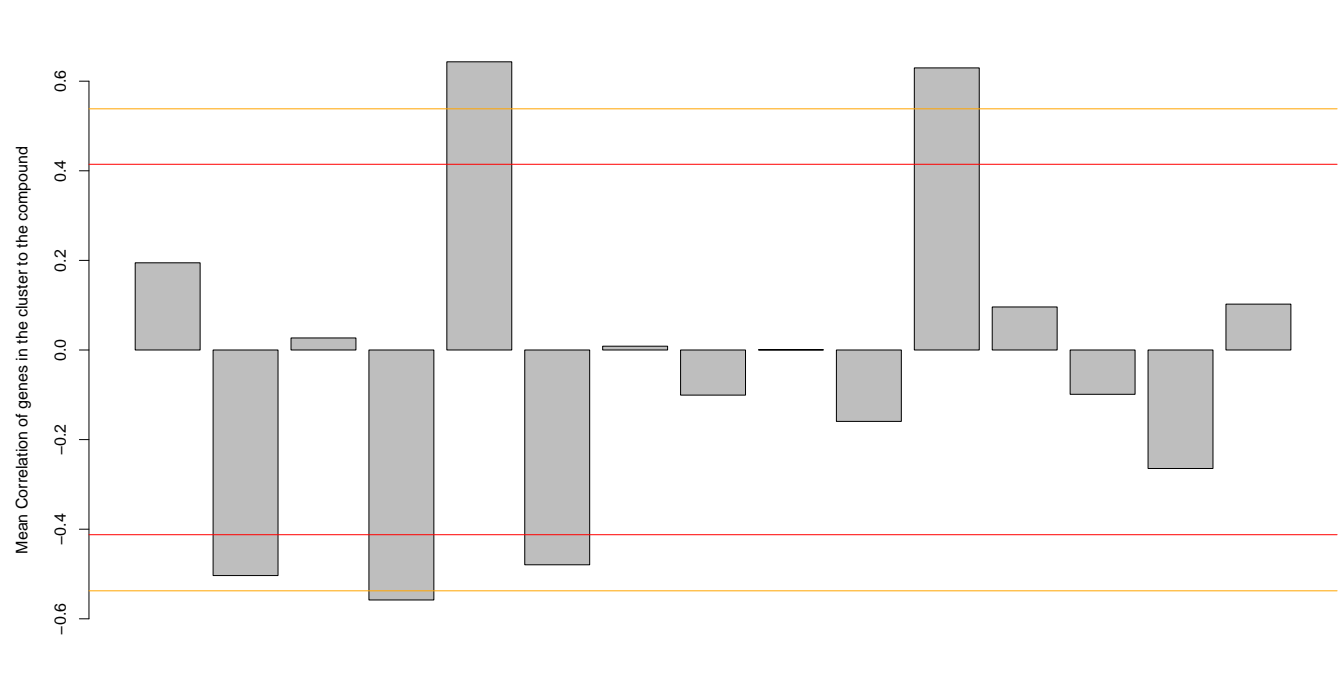
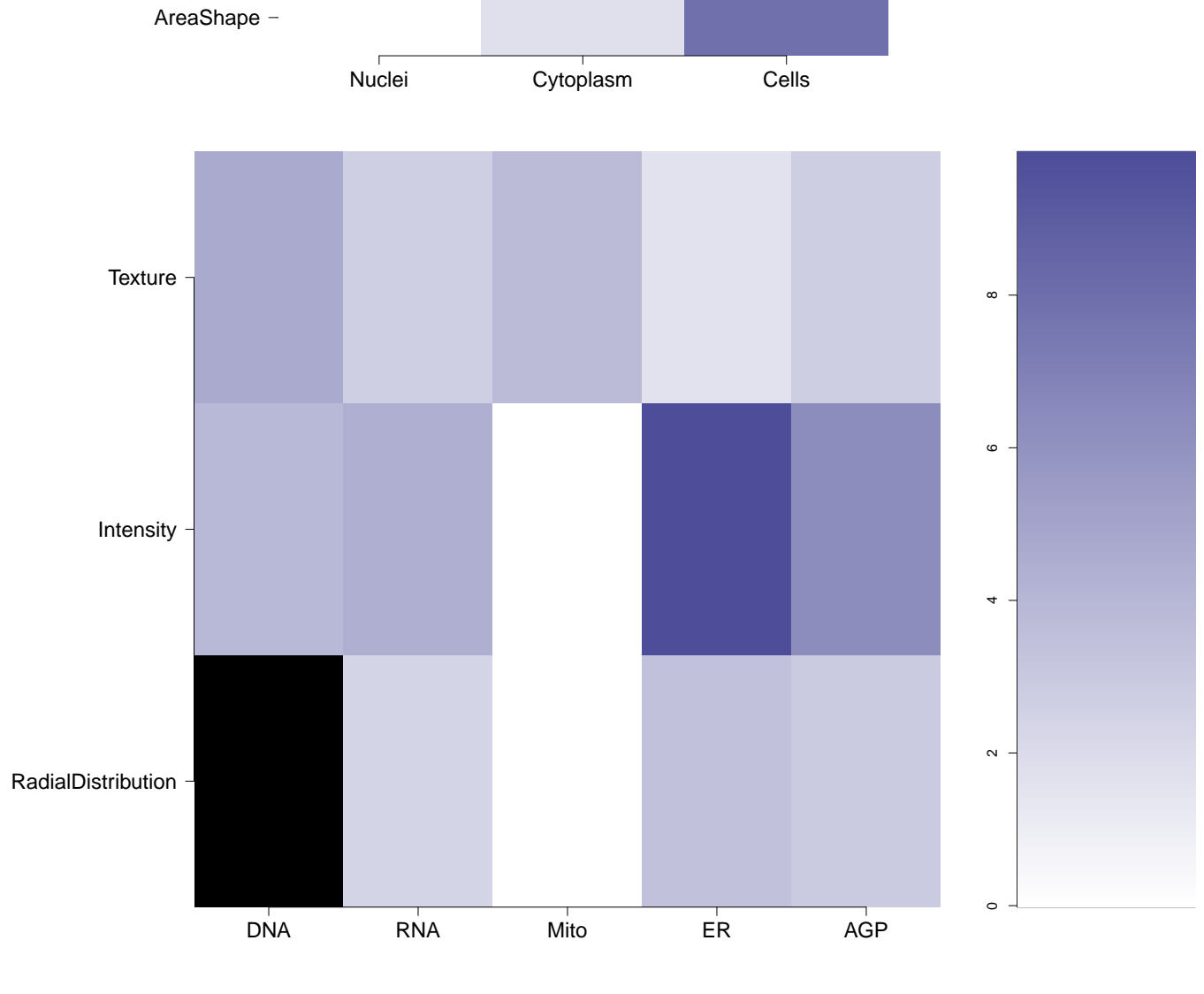
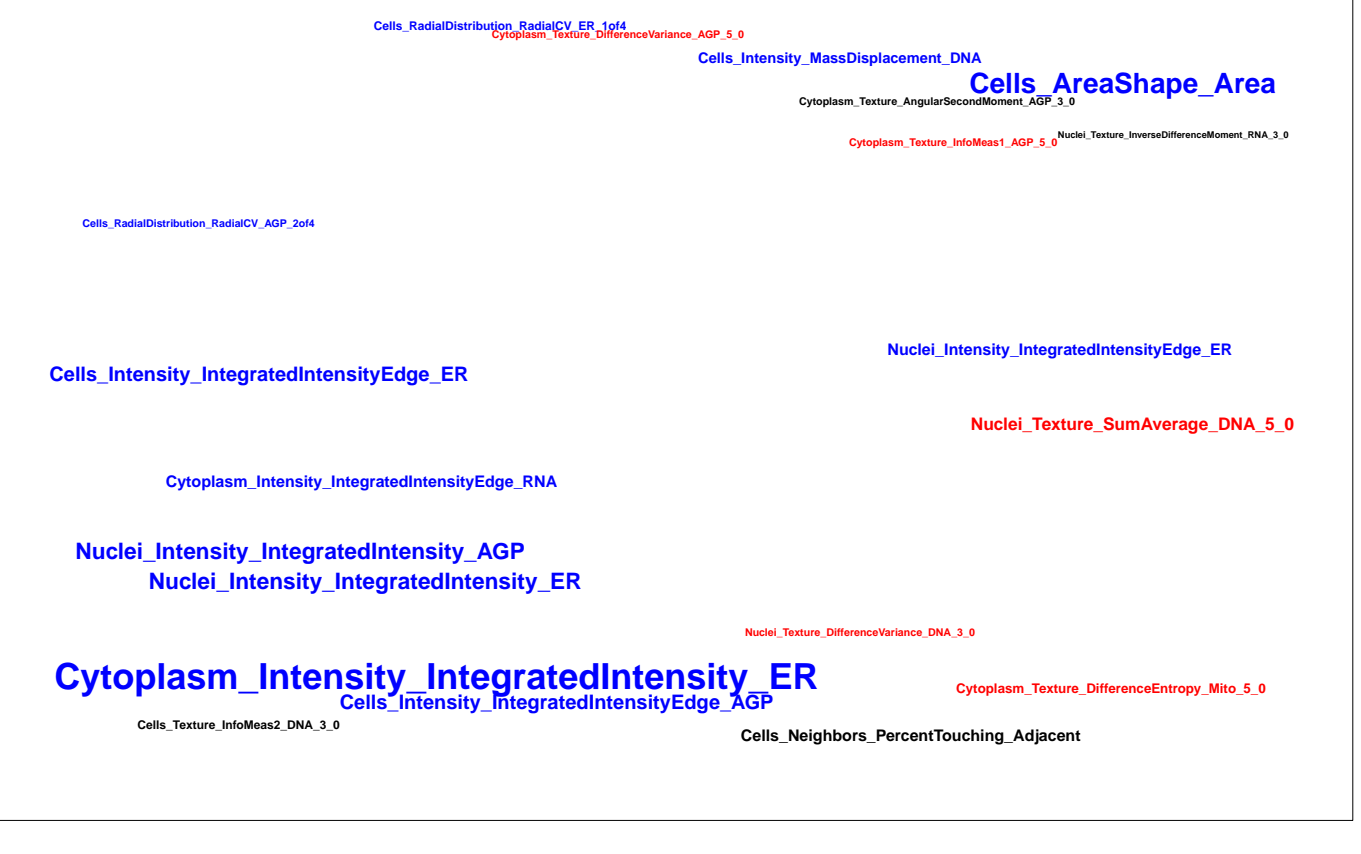
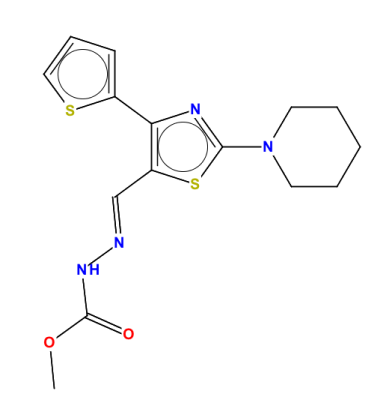
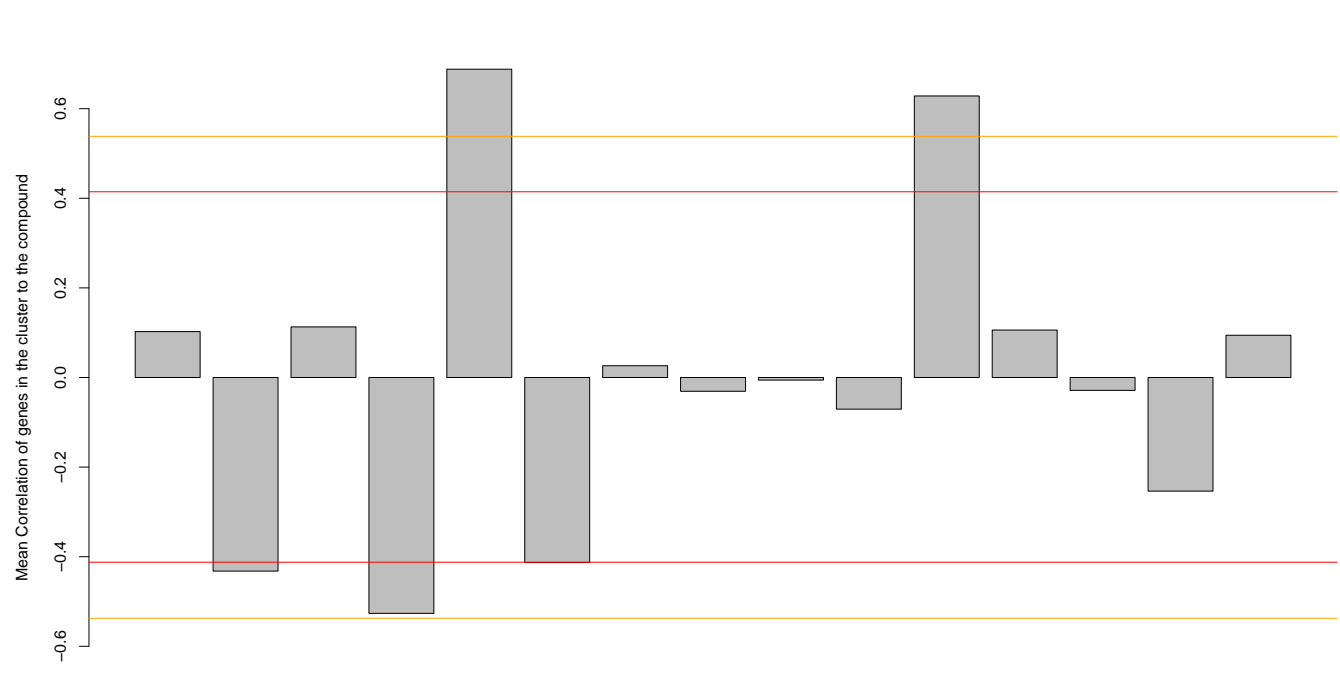
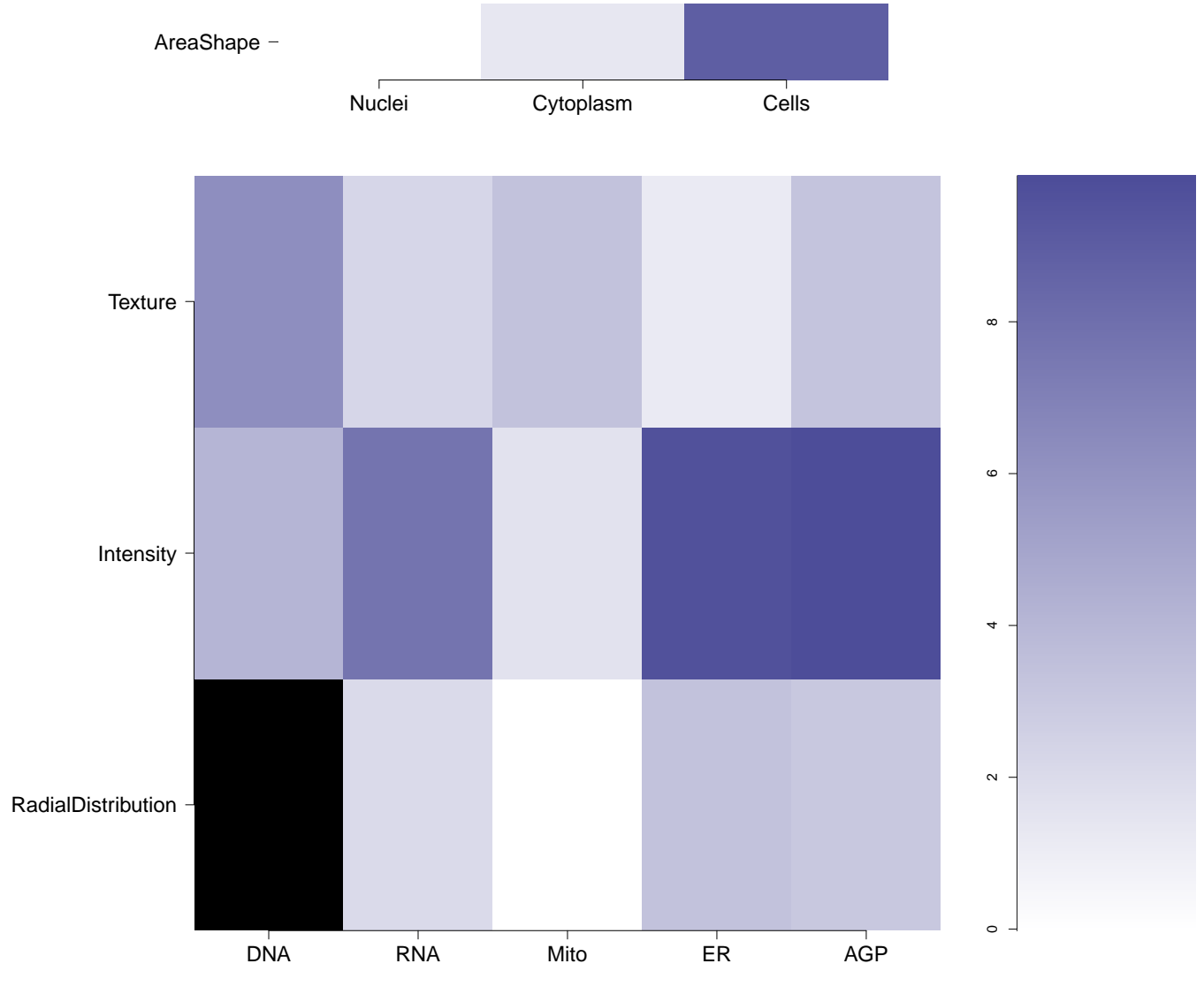

MAP3K2\_WT.2

TRAF5\_WT



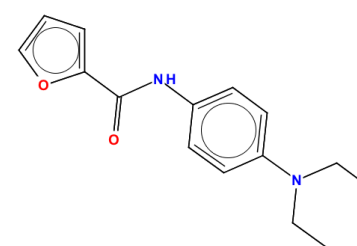
<div>Compound IDs and common names (where available); blue/red colored box means the matching compound is positively/negatively correlated with the cluster</div>	<div>Chemical structure</div>	<div>Mean pairwise replicates correlation of the compound signature (95th DMSO replicate correlation is 0.52)</div>	<div>Mean <math>\pm</math> standard deviation correlation between compound and each gene in cluster; Tables contain data for individual genes</div>	<div>Mean compound rank when scored against genes in cluster using L1000 profiling <math>\pm</math> standard deviation; Tables contain data for individual genes</div>	<div>How similar is the compound signature to the gene clusters in this experiment? (Yellow and red lines correspond to top/bottom 1st and 5th percentile DMSO correlation to all the genes)</div>	<div>Common distinguishing feature categories in the compound and genes in the cluster relative to the untreated samples</div>	<div>Distinguishing individual features for the compound relative to untreated samples. Black means a mismatch; i.e. active (= high z-score in magnitude) in the compound, and either inactive (= small z-score in magnitude) or oppositely active in the gene cluster</div>	<div>Number of PubChem assays in which the compound was tested; assays in which the compound was active are itemized</div>								
<div>BRD-A50921700-001-05-5 ST50843211 AC1MIGIXY MLS001035763 HMS2980J20 STK436533 SMR000666319 PubChem CID : 2954221</div>	<div></div>	<div>NA (in 1 replicates)</div>	<div><table><thead><tr><th>Treatment</th><th>Score</th></tr></thead><tbody><tr><td>MAP8K.WT.1</td><td>0.65</td></tr><tr><td>MAP8K.WT.2</td><td>0.65</td></tr><tr><td>TRAF3.WT</td><td>0.76</td></tr></tbody></table></div>	Treatment	Score	MAP8K.WT.1	0.65	MAP8K.WT.2	0.65	TRAF3.WT	0.76	<div>NA</div>	<div></div>	<div></div>	<div></div>	<div>Total number of assays tested in: 491. Active in the following assays:<ul style="list-style-type: none"><li>• hHTS Luminescent assay for identification of activators of human intestinal alkaline phosphatase (AID 2524)</li><li>• qHTS for inhibitors of ROR gamma transcriptional activity (AID 2551)</li></ul></div>
Treatment	Score															
MAP8K.WT.1	0.65															
MAP8K.WT.2	0.65															
TRAF3.WT	0.76															



BRD-K78412459-001-07-0 MLS000095975 SMR000031523 AC1MMEHN BDBM64930 HMS1510113 HMS2441M20 PubChem CID : 3237493		0.89 (in 3 replicates)	<div> <div> <div>Treatment</div> <div>Score</div> </div> <div> <div>MAPK2.WT1</div> <div>0.00</div> </div> <div> <div>MAPK2.WT2</div> <div>0.07</div> </div> <div> <div>TRAF5.WT</div> <div>0.09</div> </div> </div>	NA				<p>Total number of assays tested in: 789. Active in the following assays:</p> <ul style="list-style-type: none"> <li>CYP2C9 Assay (AID 777)</li> <li>HCS for Compounds that Up-Regulate Insulin Promoter Activity in MIN6 Cells (AID 1625)</li> <li>qHTS Multiplex Assay to Identify Dual Action Probes in a Cell Model of Huntington: Aggregate Formation (GFP) (AID 1688)</li> <li>Fluorescence Cell-Based Primary HTS of Calbicans growth in the presence of Fluconazole and compound (AID 1979)</li> <li>Fluorescence Cell-Based Secondary Assay to Identify Inhibitors of Resistant C. albicans Growth in the Presence of Fluconazole (AID 2423)</li> <li>Fluorescence Cell-Based Retest of C. albicans Growth in the Presence of Fluconazole (AID 2467)</li> <li>Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 96 hour incubation (AID 504834)</li> </ul>
BRD-A77566727-001-05-6 SMR000048526 AC1LDHJD MLS000084442 MLS002584781 HMS2405B07 STK788882 ST50129984 PubChem CID : 667105		0.87 (in 4 replicates)	<div> <div> <div>Treatment</div> <div>Score</div> </div> <div> <div>MAPK2.WT1</div> <div>0.09</div> </div> <div> <div>MAPK2.WT2</div> <div>0.03</div> </div> <div> <div>TRAF5.WT</div> <div>0.08</div> </div> </div>	NA				<p>Total number of assays tested in: 775. Active in the following assays:</p> <ul style="list-style-type: none"> <li>CYP2C9 Assay (AID 777)</li> <li>qHTS Assay for Inhibitors of Aldehyde Dehydrogenase 1 (ALDH1A1) (AID 1030)</li> <li>nHTS fluorescence polarization assay for the identification of translation initiation inhibitors (eIF4H) (AID 2012)</li> <li>nHTS fluorescence polarization assay for the identification of translation initiation inhibitors (PABP) (AID 2014)</li> <li>Fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of myeloid cell leukemia sequence 1 (MCL1) interactions with BIM-BI3 peptide. (AID 2057)</li> <li>Primary biochemical high throughput screening assay to identify inhibitors of BCL2-related protein, long isoform (BCLXL). (AID 2129)</li> <li>Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 96 hour incubation (AID 504834)</li> <li>Full deck counterscreen for antagonists of the human M1 muscarinic receptor (CHRM1): Fluorescence-based cell-based high throughput screening assay to identify nonselective inhibitors and assay artifacts using the parental CHOIK1 cell line (AID 602290)</li> <li>Luminescence-based biochemical primary high throughput screening assay to identify inhibitors of the interaction of the lipase co-activator protein, abhydrolase domain containing 5 (ABHD5) with perilipin-5 (MLDP; PLIN5) (AID 602281)</li> <li>Fluorescence-based cell-based primary high throughput screening assay to identify positive allosteric modulators (PAMs) of the human cholinergic receptor, muscarinic 4 (CHRM4) (AID 624126)</li> <li>Counterscreen for inhibitors of the interaction of the lipase co-activator protein, abhydrolase domain containing 5 (ABHD5) with perilipin-5 (MLDP; PLIN5): Luminescence-based biochemical high throughput assay to identify inhibitors of Hepatocyte nuclear factor 4 (HNF4) dimerization (AID 651674)</li> </ul>
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BRD-A80723361-001-06-7 MLS000120963 SMR000118340 BAS 03775057 AC1MK3FZ BDBM62892 HMS2349A13 STK840835 PubChem CID : 3148600		0.92 (in 4 replicates)	<div> <div> <div>Treatment</div> <div>Score</div> </div> <div> <div>MAPK2.WT1</div> <div>0.08</div> </div> <div> <div>MAPK2.WT2</div> <div>0.02</div> </div> <div> <div>TRAF5.WT</div> <div>0.08</div> </div> </div> <div> <div> <div>Treatment</div> <div>Score</div> </div> <div> <div>MAPK2.WT1</div> <div>0.700</div> </div> <div> <div>MAPK2.WT2</div> <div>0.800</div> </div> <div> <div>TRAF5.WT</div> <div>0.226</div> </div> </div>	0.579 ± 0.309				<p>Total number of assays tested in: 698. Active in the following assays:</p> <ul style="list-style-type: none"> <li>nHTS for Calpain Inhibitors (AID 1236)</li> <li>Dose Response Confirmation for Calpain Inhibitors (AID 1420)</li> <li>Luminescence Cell-Based Primary HTS to Identify Inhibitors of Heat Shock Factor 1 (HSF1). (AID 2098)</li> <li>Counterscreen for PME1 inhibitors: fluorescence polarization-based primary biochemical high throughput screening assay to identify inhibitors of lysophospholipase 1 (LYPLA1). (AID 2174)</li> <li>Counterscreen for PME1 inhibitors: fluorescence polarization-based primary biochemical high throughput confirmation assay to identify inhibitors of lysophospholipase 2 (LYPLA2). (AID 2177)</li> <li>Counterscreen for PME1 inhibitors: fluorescence polarization-based biochemical high throughput confirmation assay to identify inhibitors of lysophospholipase 2 (LYPLA2). (AID 2232)</li> <li>Counterscreen for PME1 inhibitors: fluorescence polarization-based biochemical high throughput confirmation assay for inhibitors of lysophospholipase 1 (LYPLA1). (AID 2253)</li> <li>Inhibitors of Cav3 T-type Calcium Channels: Primary Screen (AID 449739)</li> <li>High Throughput Screening for Cocaine Antagonists: Primary Screen (AID 449768)</li> <li>Primary cell-based screen for identification of compounds that inhibit the Choline Transporter (CHT) (AID 488975)</li> <li>Inhibitors of T-Type Calcium Channel (AID 489005)</li> <li>Inhibitors of T-Type Calcium Channels (AID 489021)</li> <li>Antagonist of Human D 1 Dopamine Receptor: qHTS (AID 504052)</li> <li>Confirmed inhibitors of the Cav3 T-type Calcium Channel (AID 1053190)</li> </ul>
BRD-K40926874-001-06-3 T6051781 AC1OBTHD MLS000516321 ZINC12727563 SMR000372882 PubChem CID : 6902822		0.90 (in 3 replicates)	<div> <div> <div>Treatment</div> <div>Score</div> </div> <div> <div>MAPK2.WT1</div> <div>0.07</div> </div> <div> <div>MAPK2.WT2</div> <div>0.00</div> </div> <div> <div>TRAF5.WT</div> <div>0.09</div> </div> </div>	NA				<p>Total number of assays tested in: 636. Active in the following assays:</p> <ul style="list-style-type: none"> <li>qHTS Assay for Inhibitors of Aldehyde Dehydrogenase 1 (ALDH1A1) (AID 1030)</li> <li>qHTS Assay for Inhibitors of Bacillus subtilis Sfp phosphopantetheinyl transferase (PPTase) (AID 1490)</li> <li>VP16 counterscreen qHTS for inhibitors of ROR gamma transcriptional activity (AID 2546)</li> <li>qHTS for inhibitors of ROR gamma transcriptional activity (AID 2551)</li> <li>nHTS identification of small molecule inhibitors of tim10-1 yeast via a luminescent assay (AID 463190)</li> <li>nHTS identification of small molecule inhibitors of tim23-1 yeast via a luminescent assay (AID 463212)</li> <li>Single concentration confirmation of small molecule inhibitors of tim0-1 yeast via a luminescent assay (AID 463213)</li> <li>Single concentration confirmation of small molecule inhibitors of tim23-1 yeast via a luminescent assay (AID 463218)</li> <li>HTS-Luminescent assay for inhibitors of ALR by detection of hydrogen peroxide production Measured in Biochemical System Using Plate Reader - 2036-02-Inhibitor.SinglePoint.HTS (AID 485317)</li> <li>qHTS Assay for Inhibitors of Histone Lysine Methyltransferase G9a (AID 504332)</li> </ul>



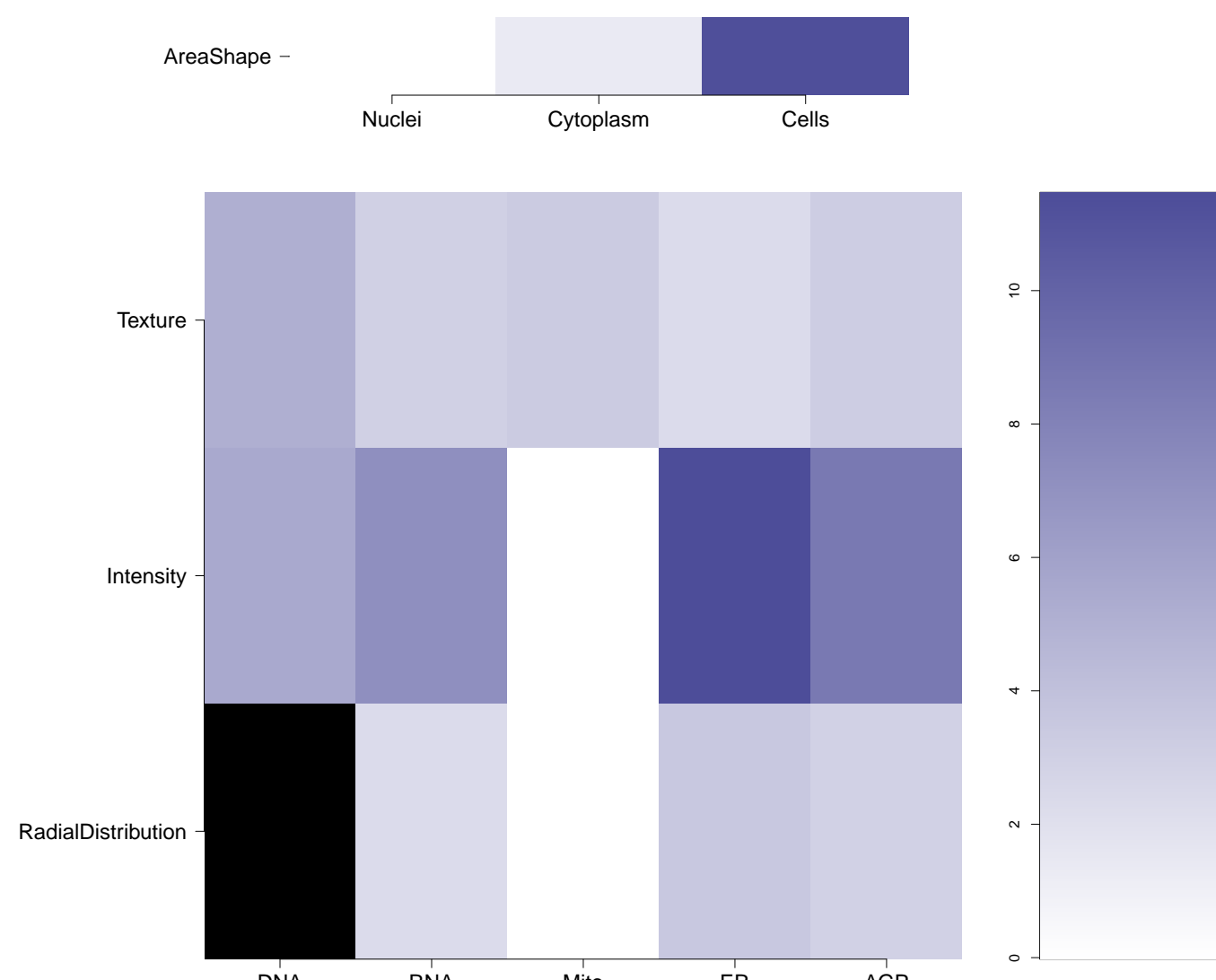
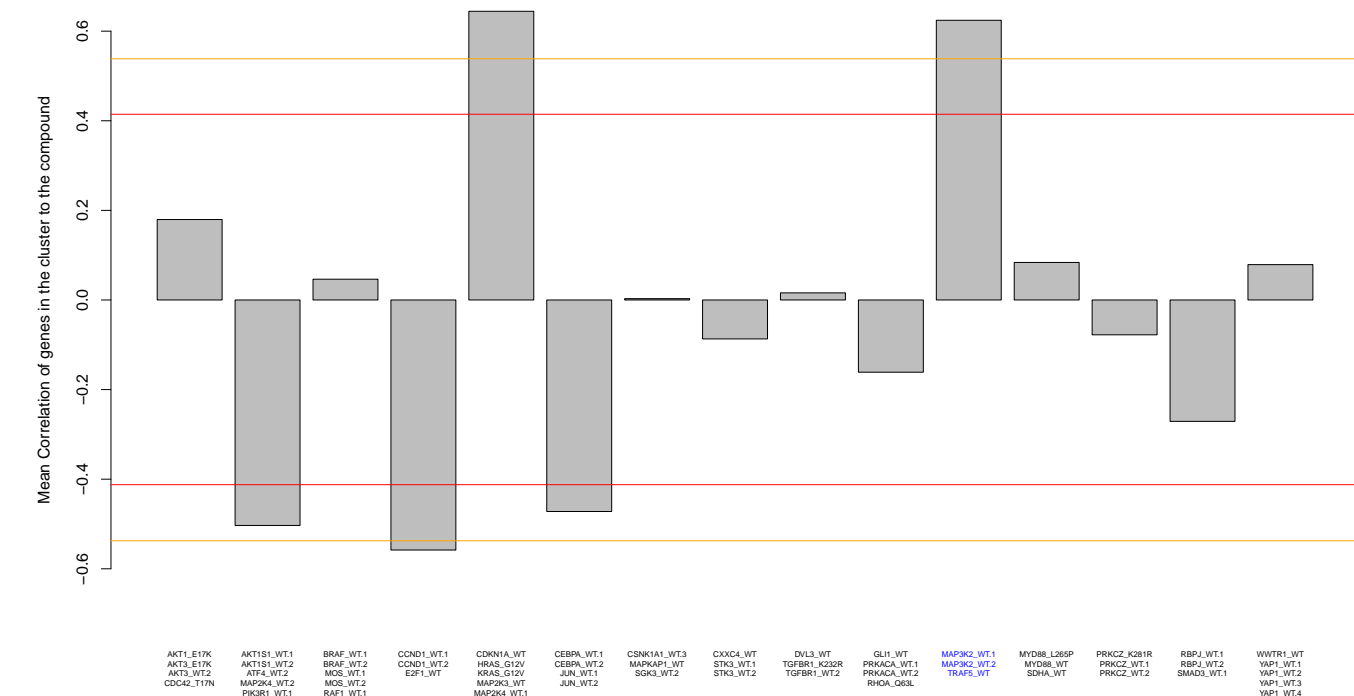
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0.92 (in 3 replicates)

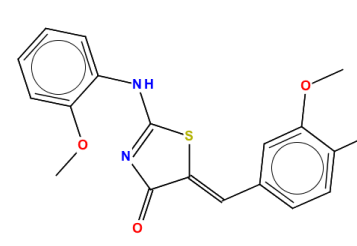
0.62 ± 0.05  
Treatment | Score  
MAPK2.WT1 | 0.68  
MAPK2.WT2 | 0.02  
TRAF6.WT | 0.07

NA



- Total number of assays tested in: 766. Active in the following assays:
- qHTS Assay for Inhibitors of Firefly Luciferase (AID 411)
  - Allosteric Modulators of D1 Receptors: Primary Screen (AID 641)
  - qHTS Screen for Compounds that Selectively Target Cancer Cells with p53 Mutations: Cytotoxicity of p53ts Cells at the Nonpermissive Temperature (AID 902)
  - qHTS Screen for Compounds that Selectively Target Cancer Cells with p53 Mutations: Cytotoxicity of p53ts Cells at the Permissive Temperature (AID 924)
  - Counter Screen for Luciferase-based Primary Inhibition Assays (AID 1006)
  - High Throughput Screen to Identify Compounds that increase expression of NF-kB in Human Neuronal Cells - Primary Screen (AID 1239)
  - Name: High Throughput Screen to Identify Compounds that increase expression of NF-kB in Human Neuronal Cells - Dose Response (AID 1241)
  - Primary screen for compounds that activate Alzheimer's amyloid precursor (AID 1276)
  - uHTS for the identification of compounds that potentiate TRAIL-induced apoptosis of cancer cells (AID 1443)
  - Identification of compounds which are cytotoxic to PPC-1 cells. (AID 1447)
  - qHTS Assay for Enhancers of SMN2 Splice Variant Expression (AID 1458)
  - uHTS absorbance assay for the identification of compounds that inhibit PHOSPHOI (AID 1565)
  - Identification of SV40 T antigen inhibitors: A route to novel anti-viral reagents (AID 1903)
  - Cycloheximide Counter screen for Small Molecule Inhibitors of Shiga Toxin (AID 2314)
  - A qHTS for Small Molecule Inhibitors of Shiga Toxin (AID 2315)
  - A biochemical assay using the ADP-Hunter methodology, purified TAG, and ATP to identify compounds that inhibit the ATPase activity of Tag - Counter Screen (AID 2501)
  - qHTS Assay for NPC1 Promoter Activators (AID 485313)
  - qHTS Assay for Inhibitors of Histone Lysine Methyltransferase G9a (AID 504332)
  - qHTS screen for small molecules that induce genotoxicity in human embryonic kidney (HEK293T) cells expressing luciferase-tagged ELG1 (AID 504466)
  - qHTS profiling assay for firefly luciferase inhibitor/activator using purified enzyme and Km concentrations of substrates (counterscreen for miR-21 project) (AID 588342)
  - uHTS identification of Caspase-8 TRAIL sensitizers in a luminescence assay (AID 624354)
  - Counterscreen of compound fluorescence effects on High-throughput multiplex microsphere screening for inhibitors of toxin protease (AID 624483)
  - Single concentration confirmation of Caspase-8 TRAIL sensitizer hits in a luminescence panel assay (AID 651596)
  - Luminescence-based cell-based primary high throughput screening assay for inhibitors of the orphan nuclear receptor subfamily 0, group B, member 1 (DAX1; NR0B1): repression of SF-1 (NR5A1) activated StAR promoter by full-length DAX-1 (AID 652010)
  - Luminescence-based cell-based primary high throughput screening assay to identify agonists of the DAF-12 from the parasite H. glycines (hgDAF-12). (AID 687014)
  - High Throughput Screen to Identify Inhibitors Targeting HIV-1 Vif-dependent Degradation of Human APOBEC3G: A time-resolved fluorescence resonance energy transfer (TR-FRET) assay for HIV-1 Vif-APOBEC3G interaction (AID 1117319)

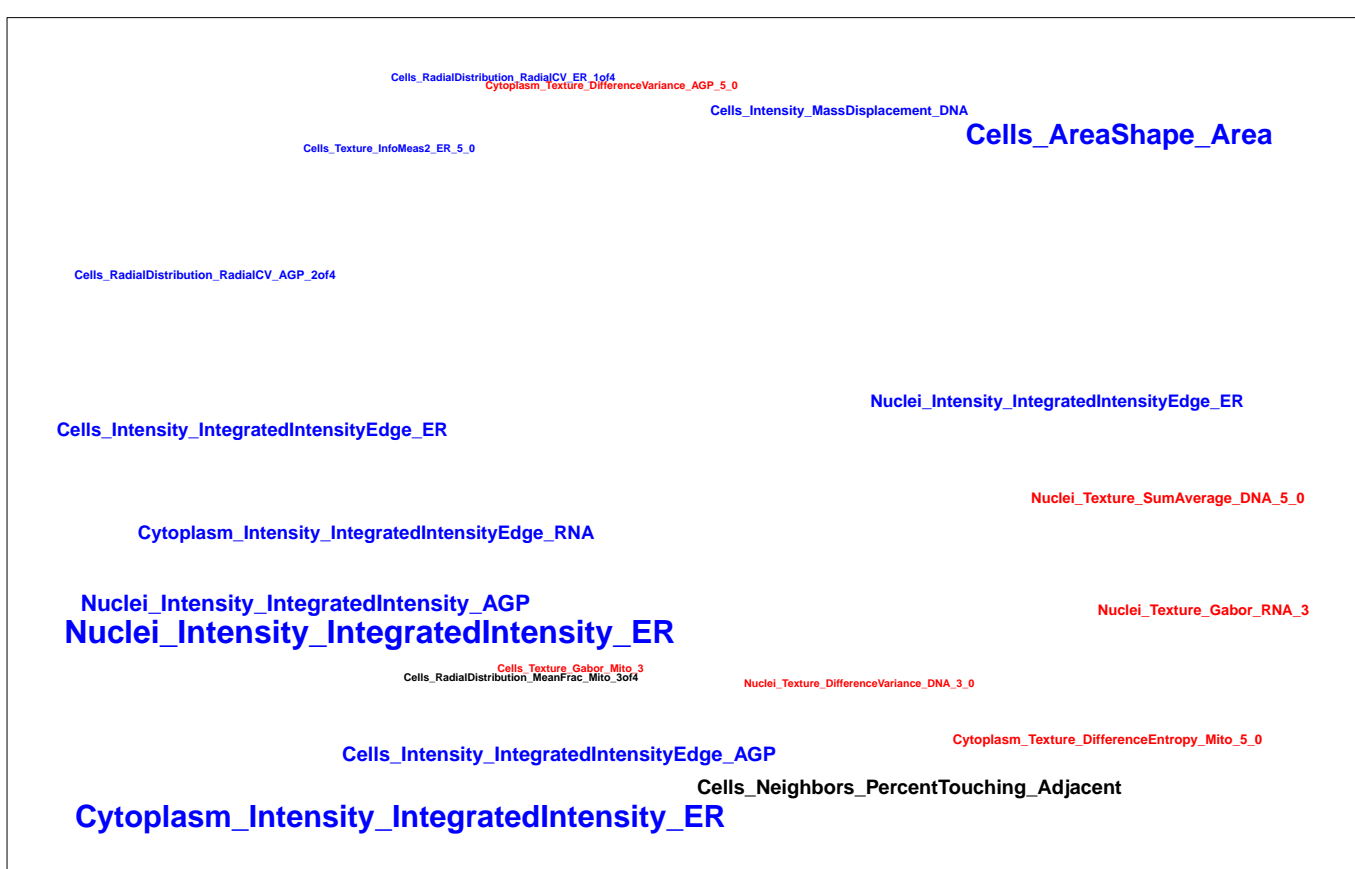
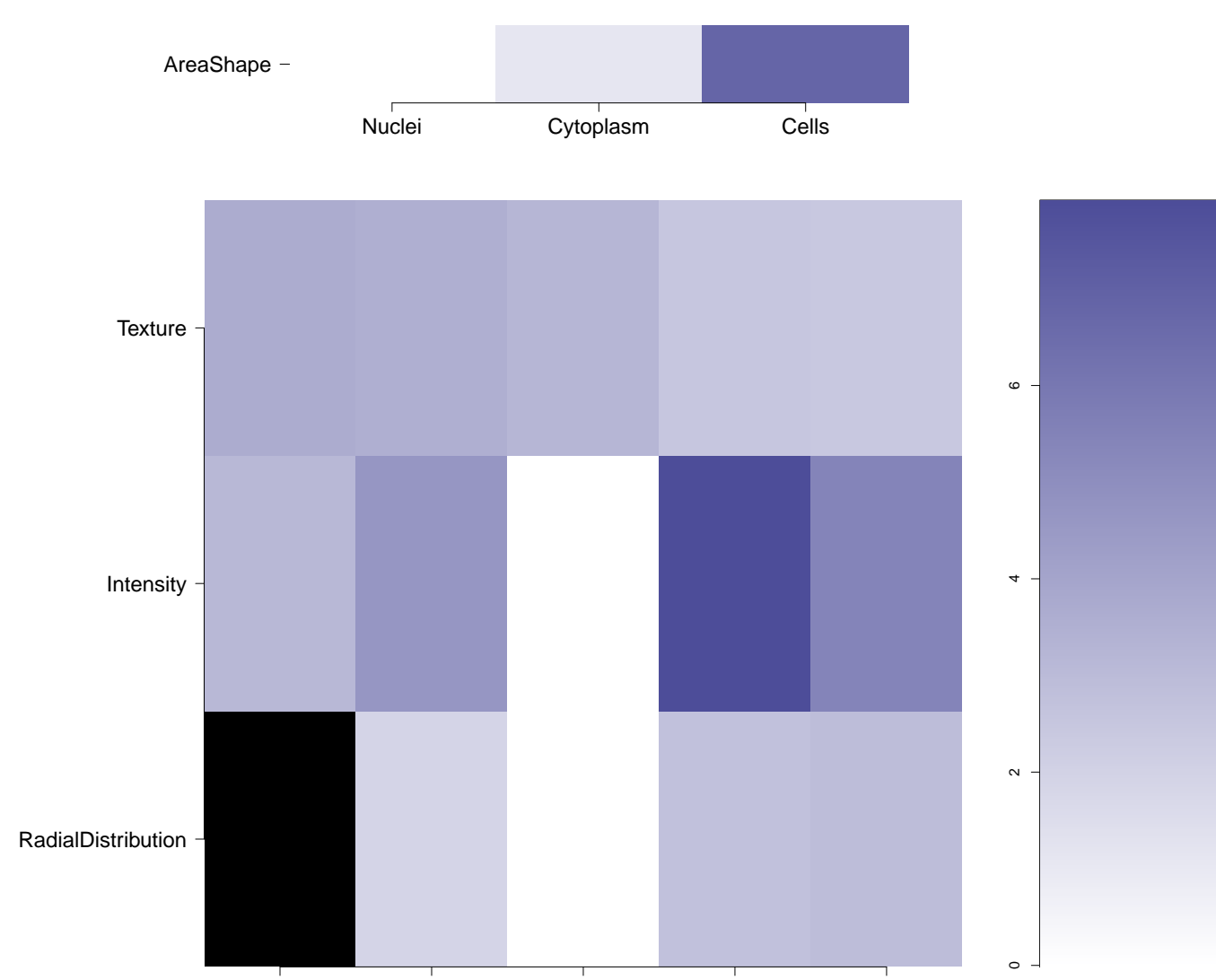
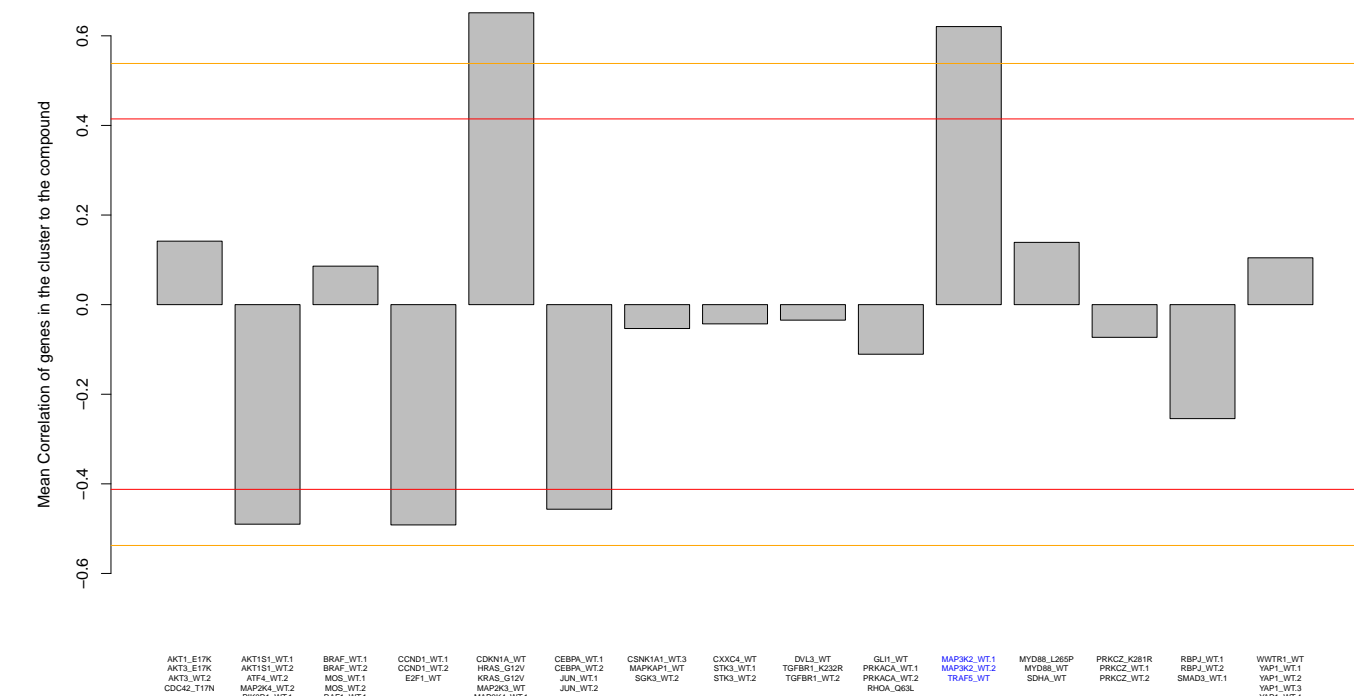
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BDBM67642  
HMS2817L13  
ML280  
ZINC4974015  
BAS 01966230  
PubChem CID : 5765514



0.85 (in 4 replicates)

0.62 ± 0.04  
Treatment | Score  
MAPK2.WT1 | 0.07  
MAPK2.WT2 | 0.03  
TRAF6.WT | 0.06

NA

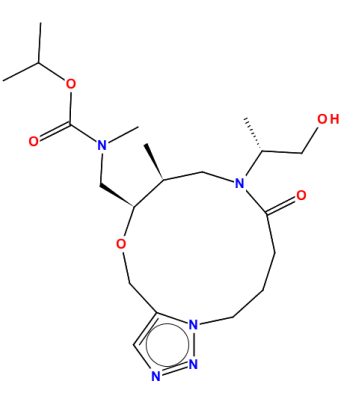
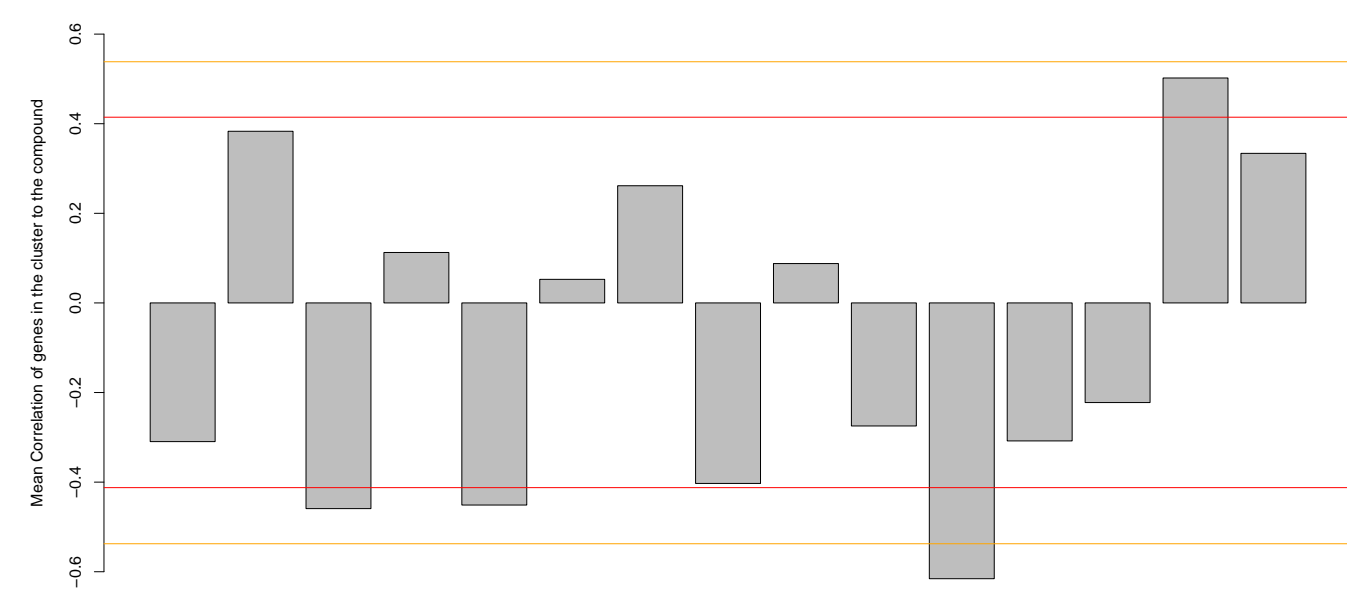
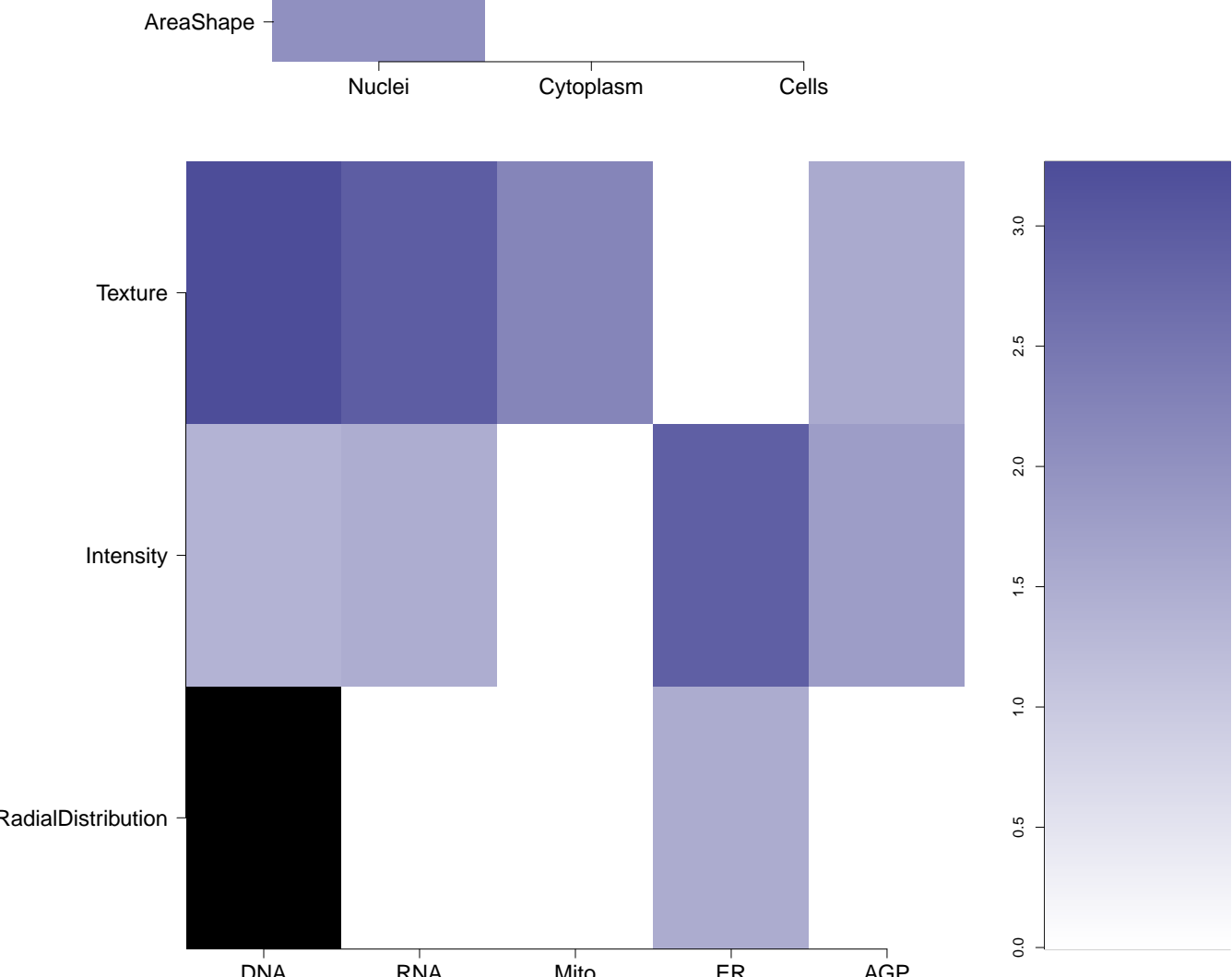
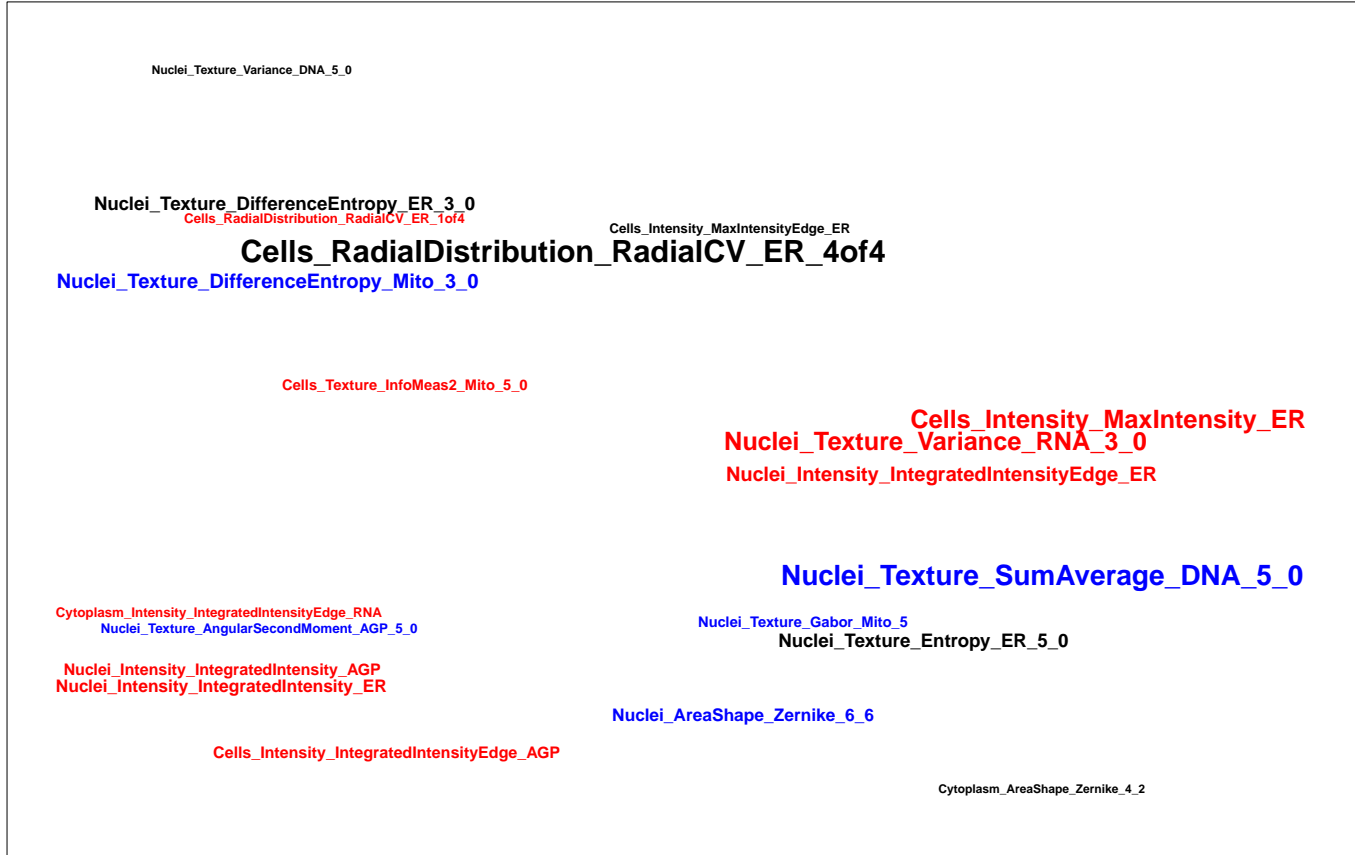
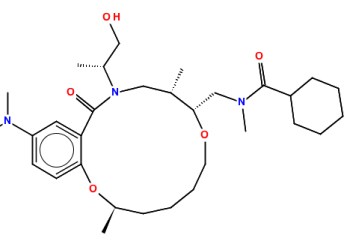
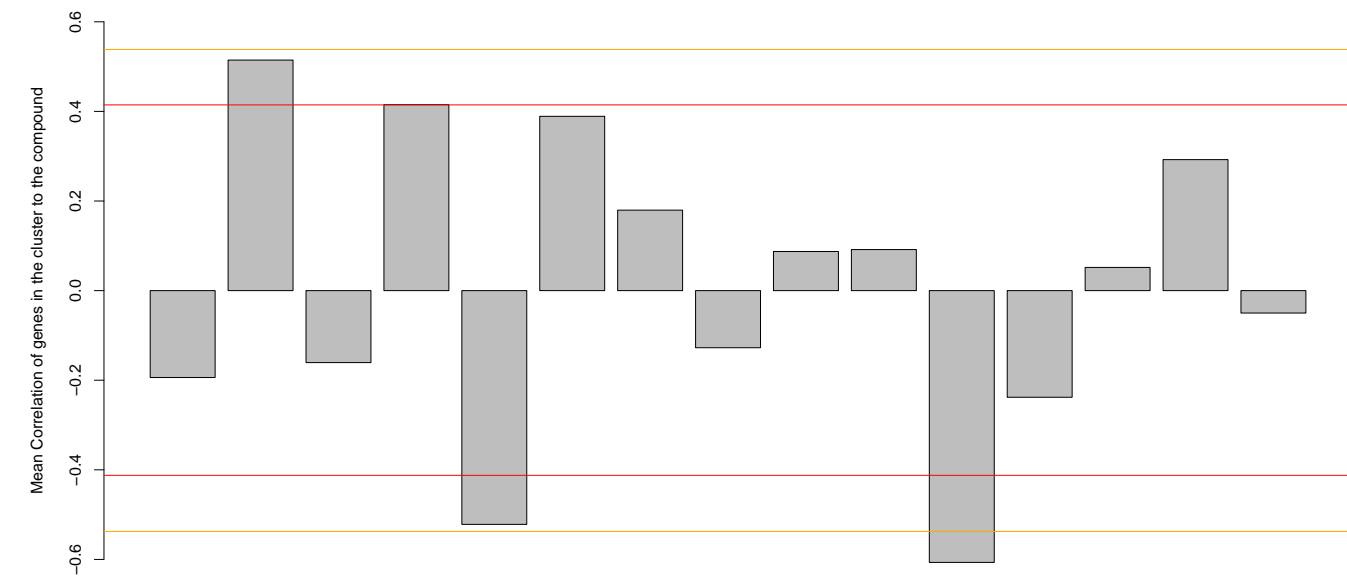
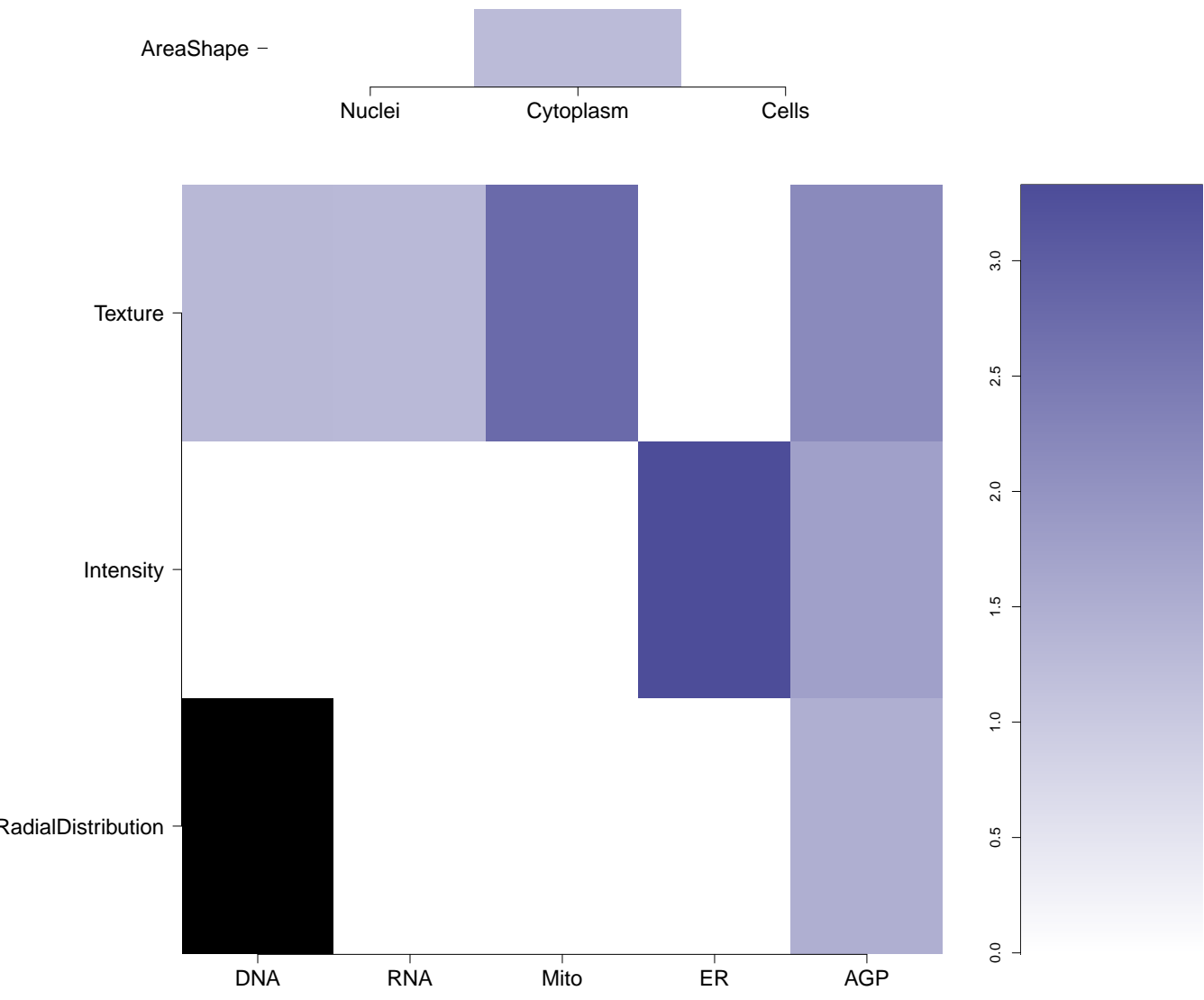
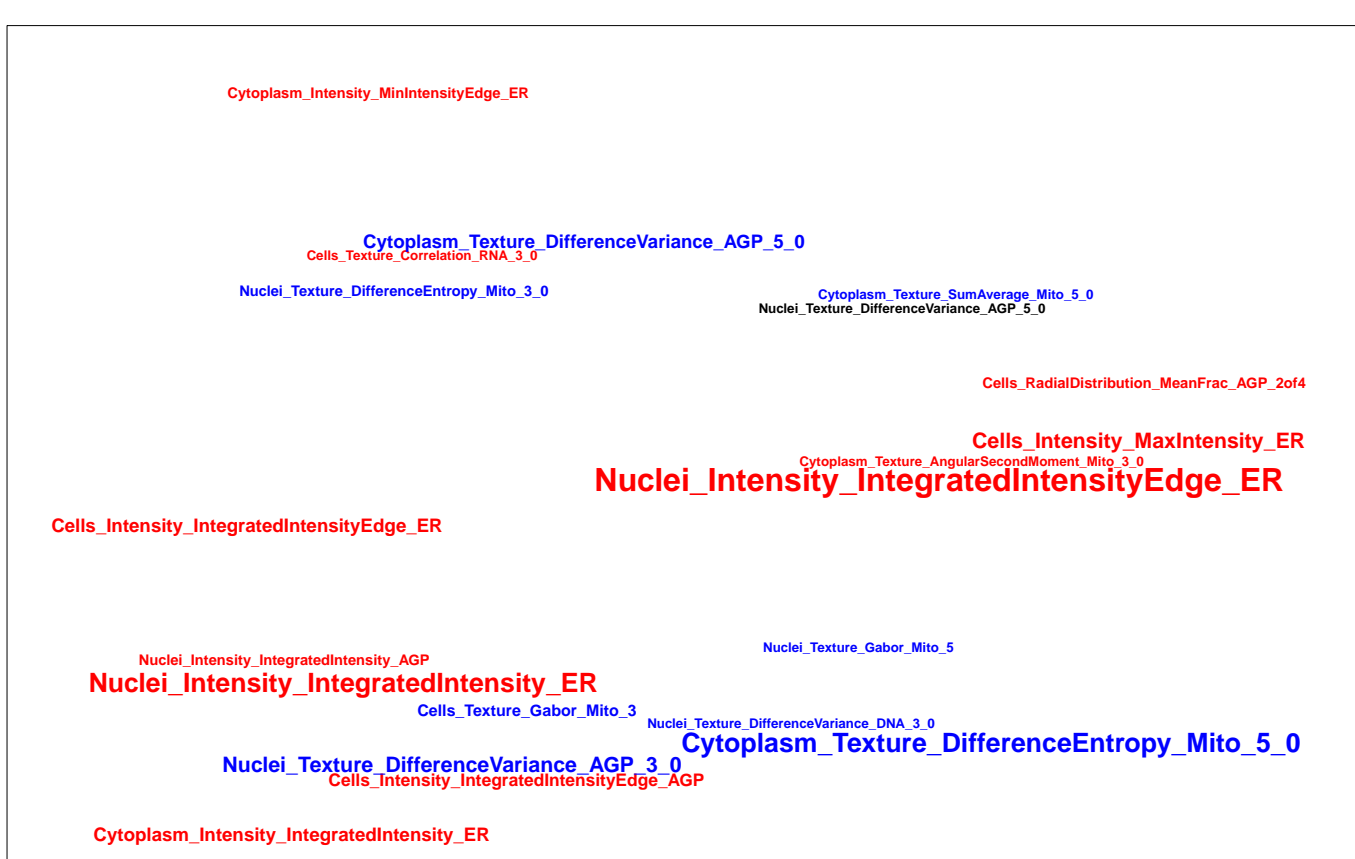
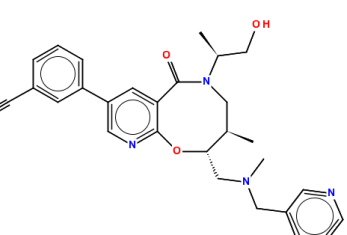
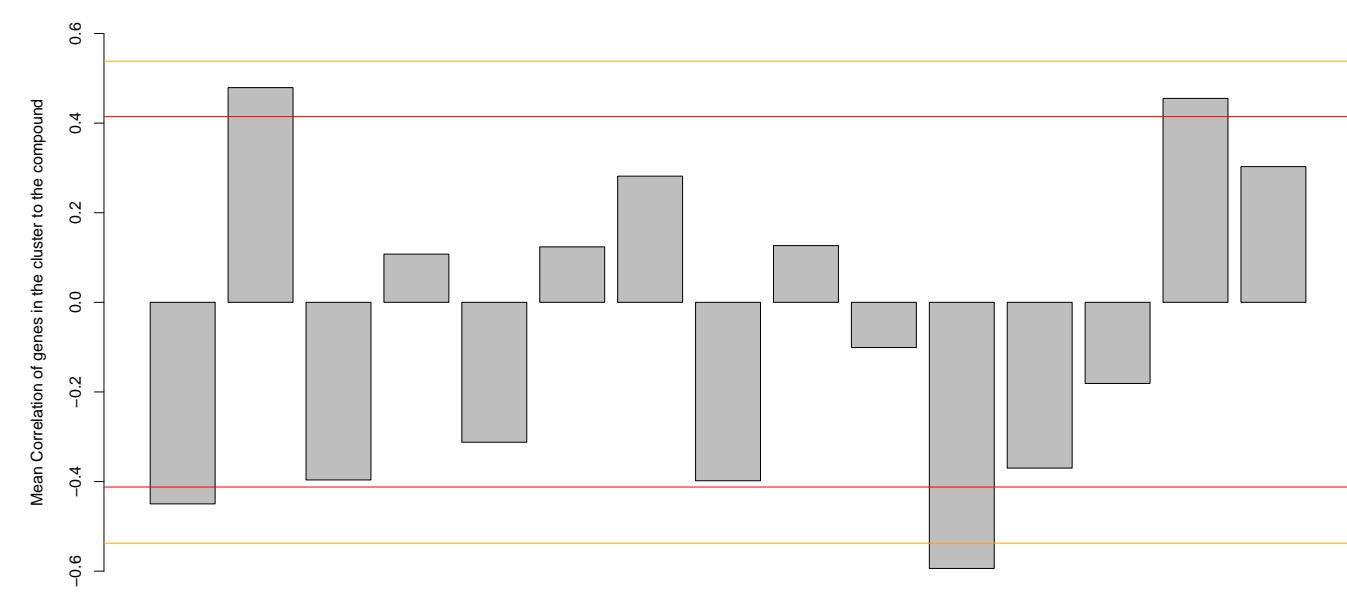
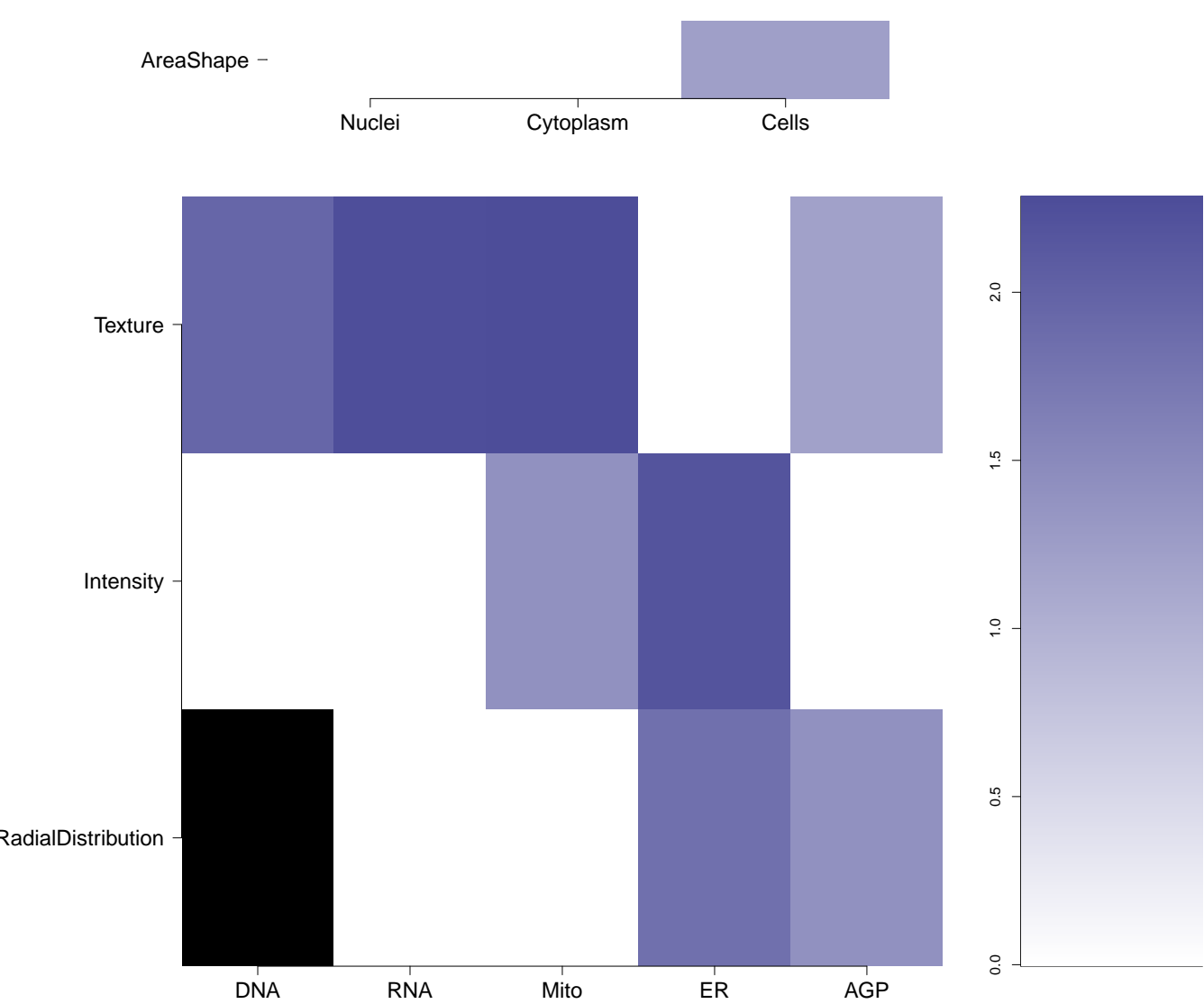
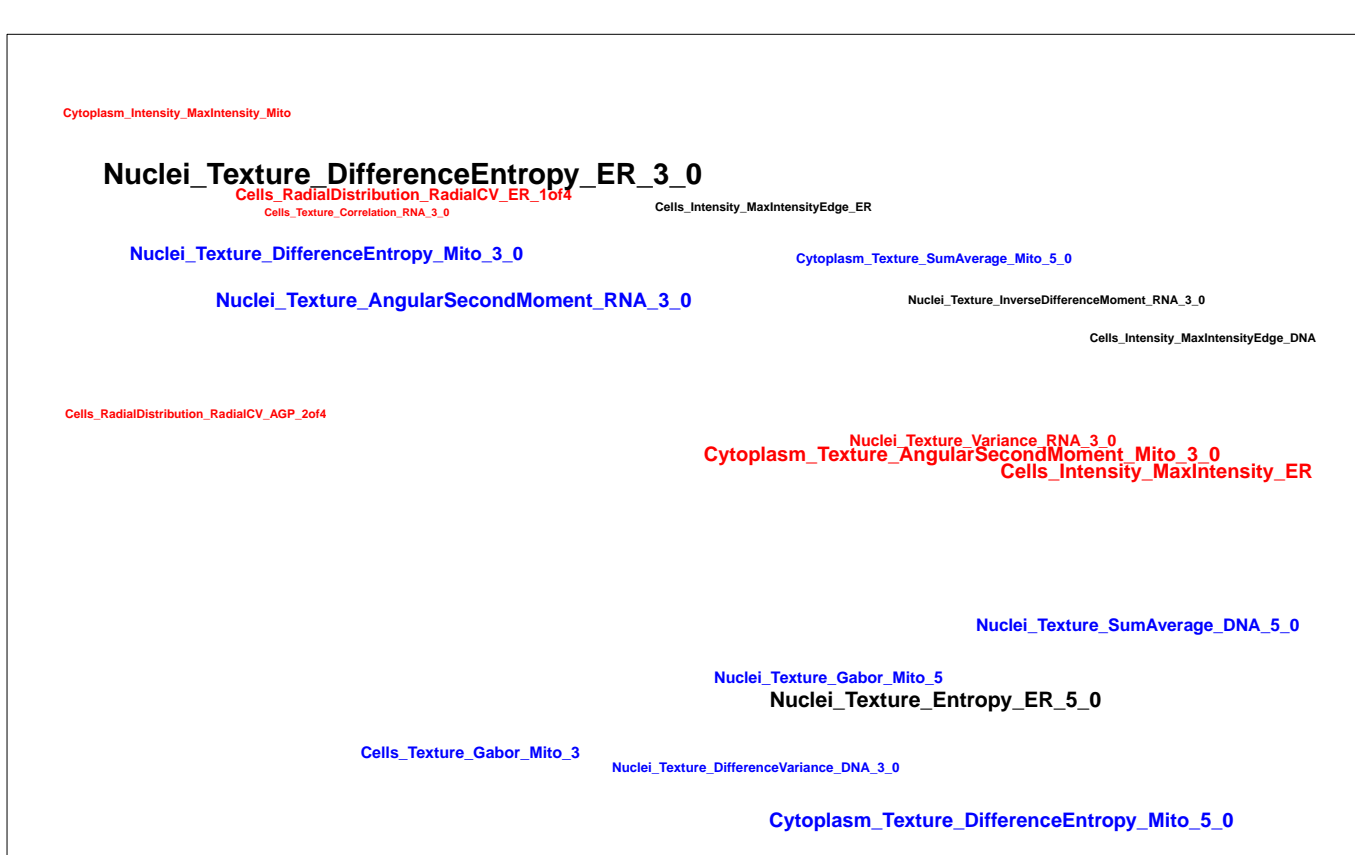
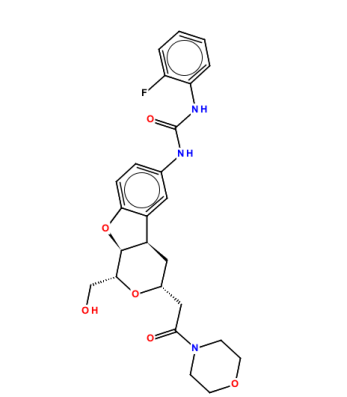
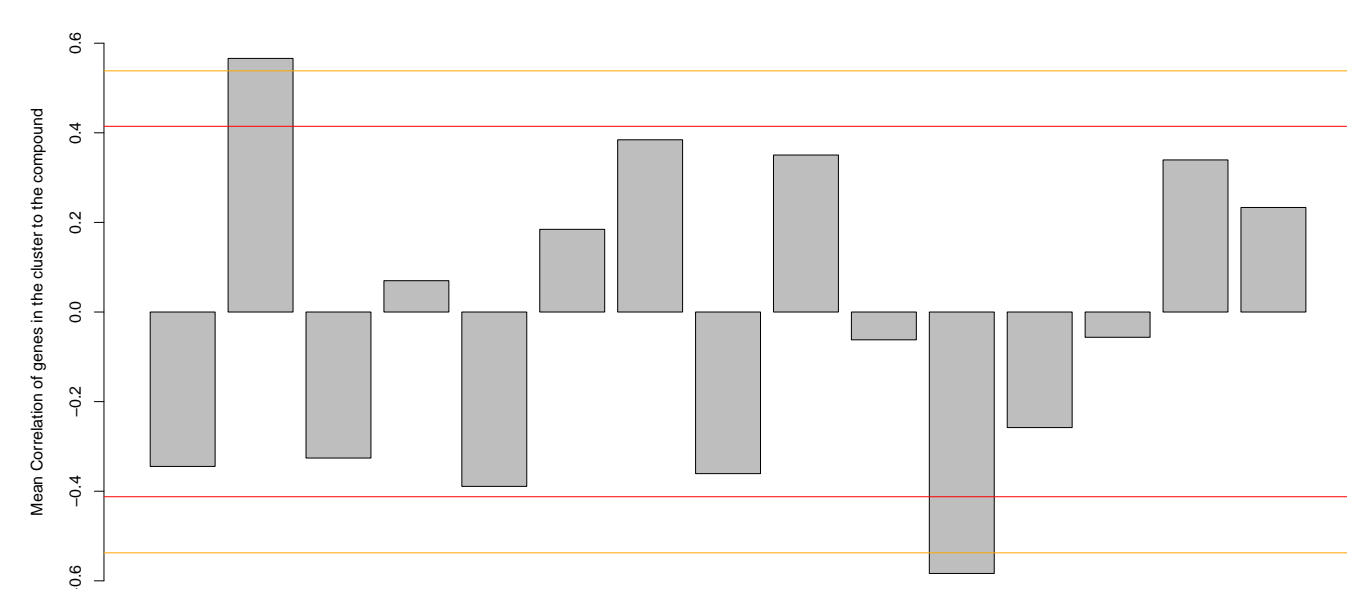
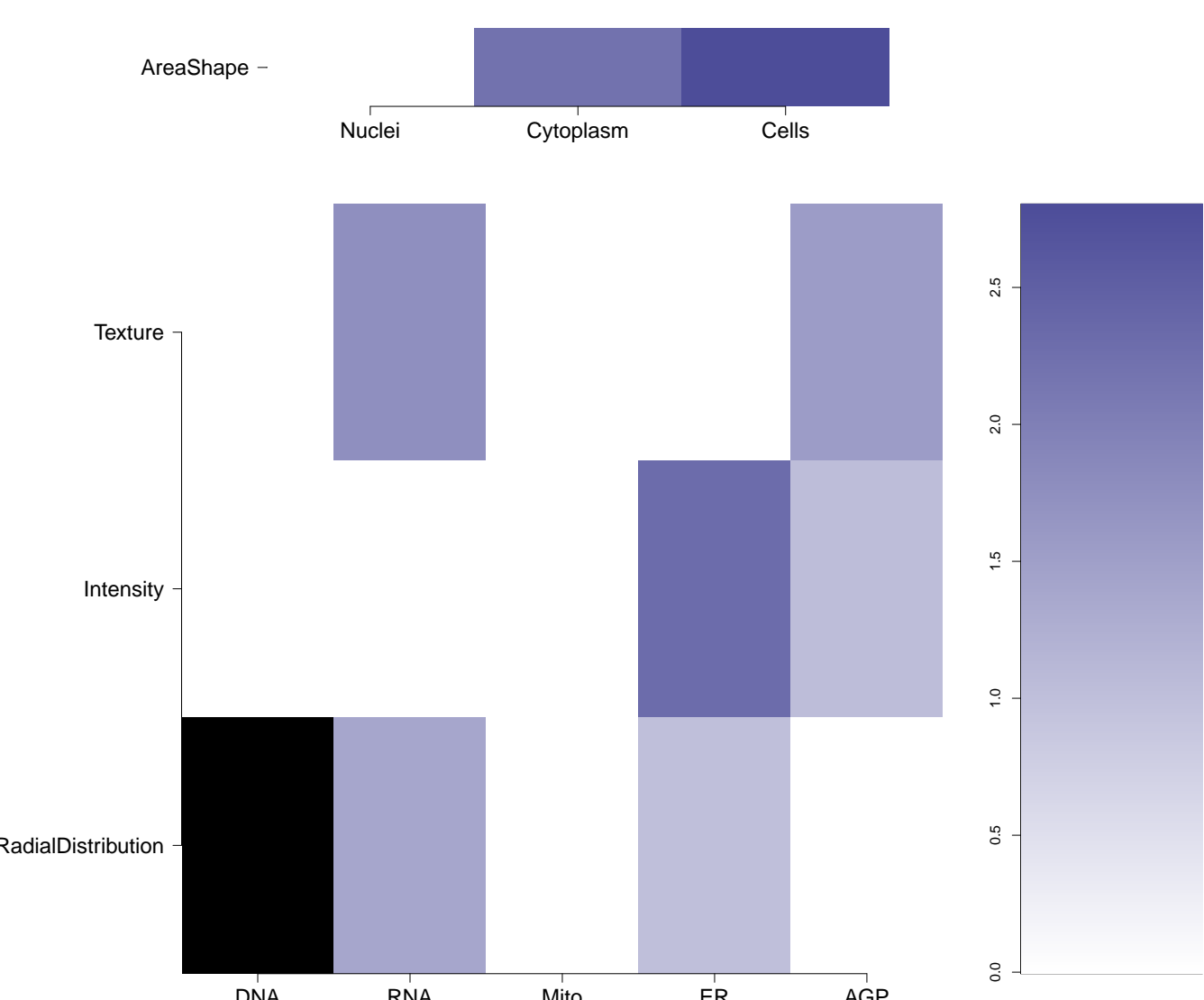
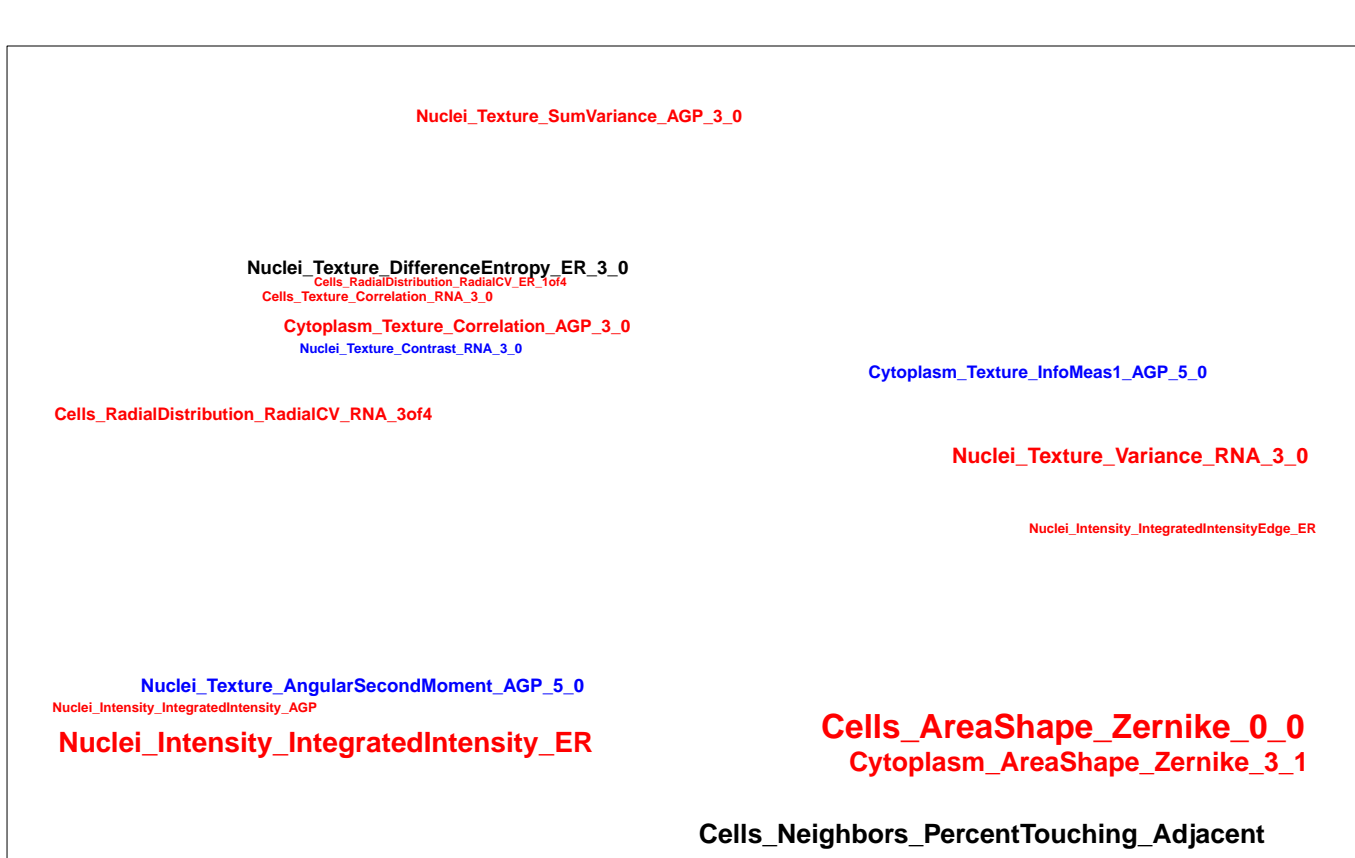
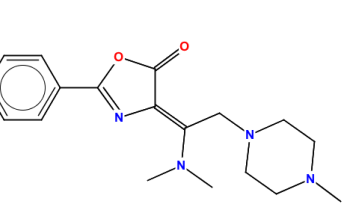
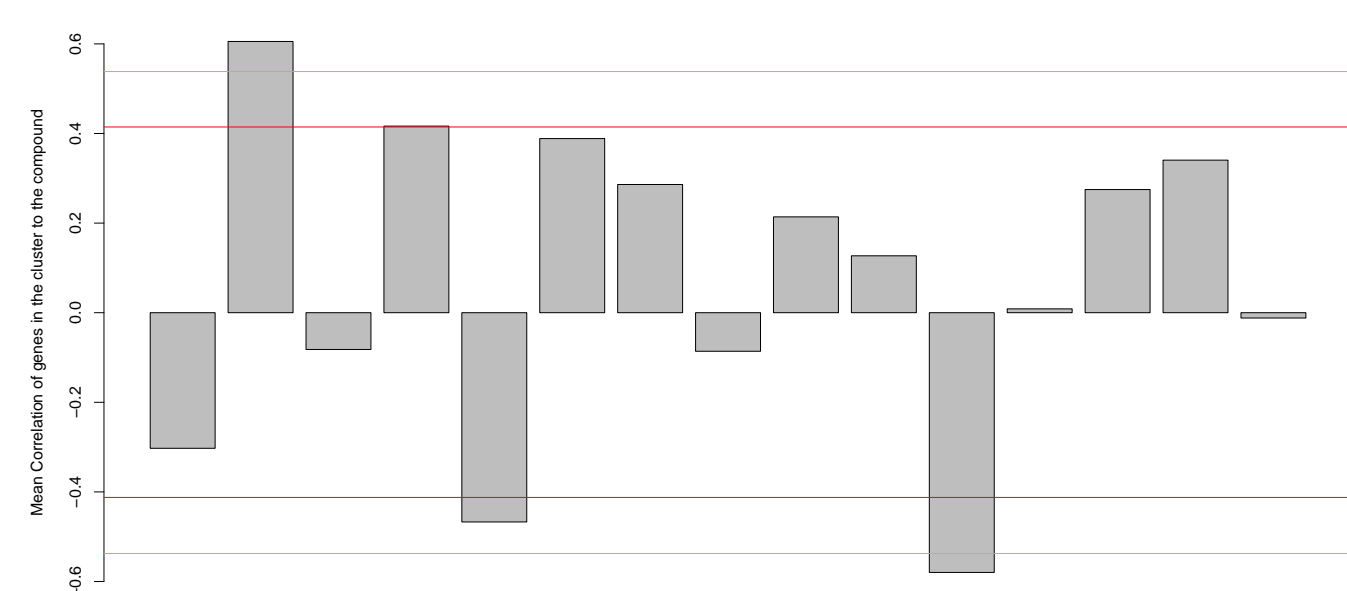
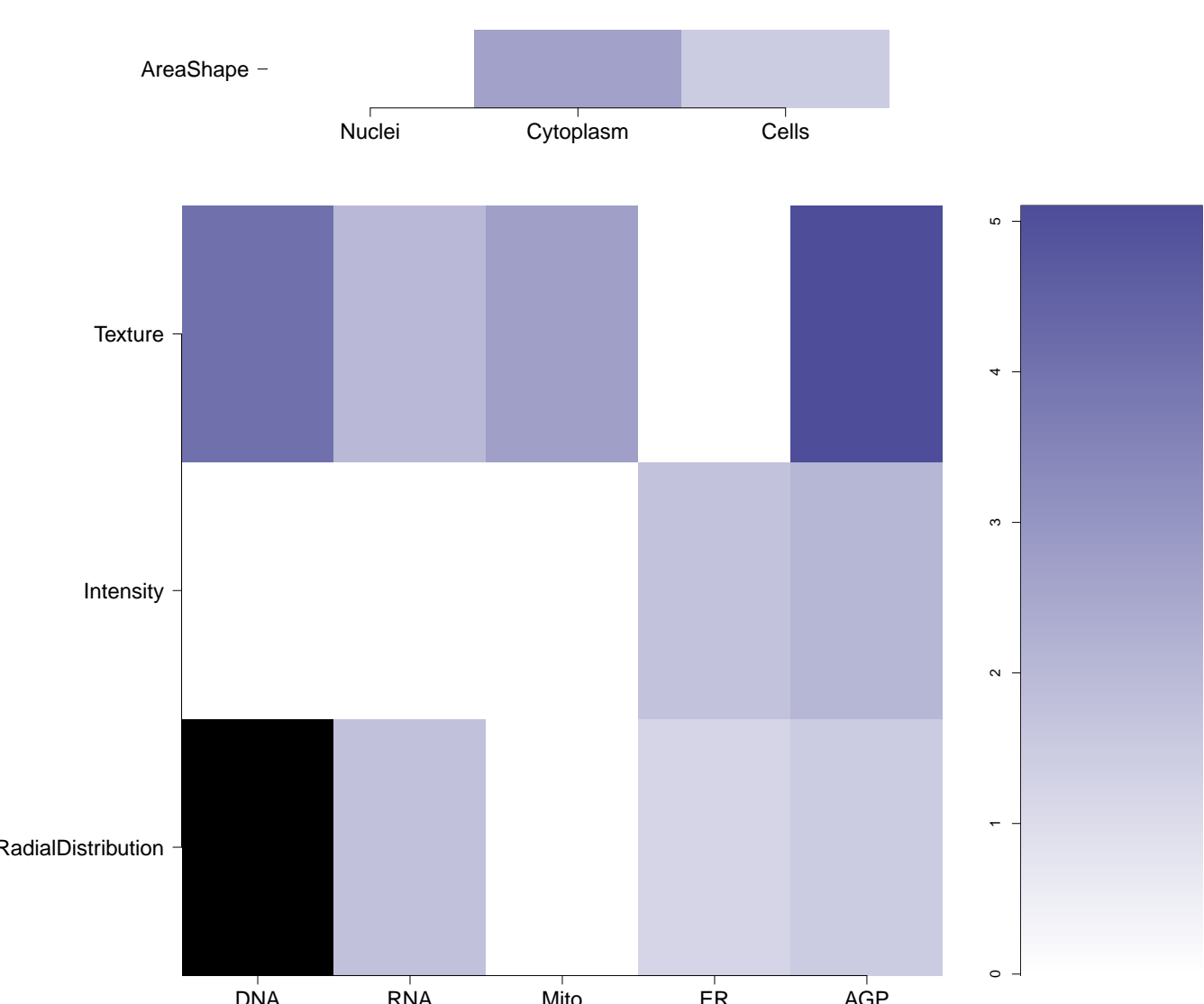
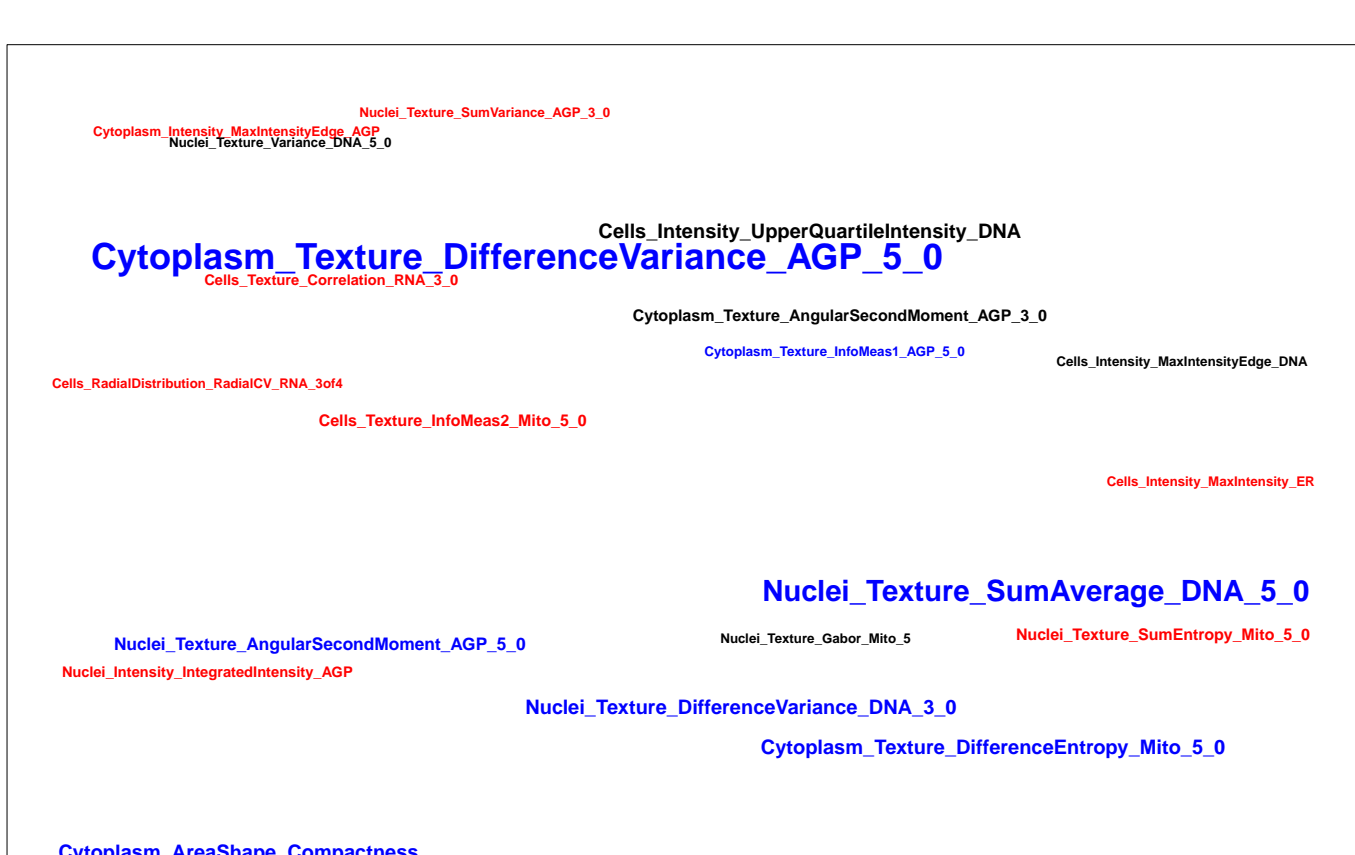


- Total number of assays tested in: 518. Active in the following assays:
- Cycloheximide Counter screen for Small Molecule Inhibitors of Shiga Toxin (AID 2314)
  - Luminescence Cell-Free Homogenous Primary HTS to Identify Inhibitors of Serine/Threonine Kinase 33 Activity (AID 2661)
  - Luminescence Cell-Free Homogenous Dose Retest to Identify Inhibitors of Serine/Threonine Kinase 33 Activity (AID 2821)
  - Phenotypic HTS multiplex for antifungal efflux pump inhibitors (AID 485275)
  - HTS-Luminescent assay for inhibitors of ALR by detection of hydrogen peroxide production Measured in Biochemical System Using Plate Reader - 2036-02-Inhibitor.SinglePoint.HTS (AID 485317)
  - Primary cell-based screen for identification of compounds that inhibit the Choline Transporter (CHT) (AID 488975)
  - Dyrk1 A HTS Measured in Biochemical System Using Plate Reader - 2124-01-Inhibitor.SinglePoint.HTS.Activity (AID 504441)
  - MLPCN Dyrk1A Kinase Measured in Biochemical System Using Plate Reader - 2124-01-Inhibitor.Dose.CherryPick.Activity (AID 588345)
  - HTS Assay for Peg3 Promoter Inhibitors (AID 588405)
  - STK-33 Kinase Inhibition Measured in Biochemical System Using Plate Reader - 2052-02-Inhibitor.Dose.DryPowder.Activity.Set2 (AID 588480)
  - uHTS identification of inhibitors of Rpn11 in a Fluorescent Polarization assay (AID 588493)
  - STK-33 Kinase Inhibition Measured in Biochemical System Using Plate Reader - 2052-02-Inhibitor.Dose.DryPowder.Activity (AID 588632)
  - Counter screen for activity against Aurora B, in dose Measured in Biochemical System Using Scintillation - 2052-06-Inhibitor.Dose.DryPowder.Activity.Set2 (AID 588756)
  - uHTS identification of cystic fibrosis induced NFkB Inhibitors in a fluorescence assay (AID 588860)
  - Single concentration confirmation of uHTS inhibitor hits from RPN11 in a Fluorescence Polarization assay (AID 602318)
  - Single concentration validation of uHTS RPN11 inhibitor hits using a Thrombin Fluorescence Polarization assay (AID 602333)
  - Single concentration confirmation of uHTS hits for Peg3 Promoter Inhibitors via a luciferase reporter assay (AID 602417)
  - A quantitative high throughput screen for small molecules that induce DNA re-replication in MCF 10a normal breast cells. (AID 624296)
  - A quantitative high throughput screen for small molecules that induce DNA re-replication in SW480 colon adenocarcinoma cells. (AID 624297)
  - Discovery of small molecule inhibitors of the oncogenic and cytokinetic protein MgcRacGAP - HeLa Cytotoxicity (AID 624300)
  - Discovery of small molecule inhibitors of the oncogenic and cytokinetic protein MgcRacGAP - Primary and Confirmatory Screens (AID 624330)
  - Discovery of small molecule inhibitors of the oncogenic and cytokinetic protein MgcRacGAP - Counter Screen Coupled Enzyme (AID 624351)
  - HTS for PAX8 inhibitors using PAX8 luciferase reporter gene assay in RMG-1 cells Measured in Cell-Based System Using Plate Reader - 7054-01-Inhibitor.SinglePoint.HTS.Activity (AID 652154)
  - qHTS for induction of synthetic lethality in tumor cells producing 2HG: qHTS for the HT-1080-NT fibrosarcoma cell line (AID 686870)
  - qHTS for induction of synthetic lethality in tumor cells producing 2HG: qHTS for the HT-1080-IDB1KD cell line (AID 686971)
  - qHTS for Inhibitors of Inflammation Signaling: IL-1-beta AlphaLISA Primary Screen (AID 743279)
  - Confirmed inhibitors of Serine Threonine Kinase 33, STK33 (AID 743321)







BRD-K04648846-001-02-1 MLS003129529 SMR001833975 PubChem CID : 44505579		0.74 (in 3 replicates)	$-0.62 \pm 0.03$ Treatment Score MAPK2.WT.1 -0.62 MAPK2.WT.2 -0.65 TRAP5.WT -0.58 $0.262 \pm 0.128$ Treatment Score MAPK2.WT.1 0.178 MAPK2.WT.2 0.280 TRAP5.WT 0.400				Total number of assays tested in: 222.
BRD-K60430317-001-01-7 PubChem CID : 44490267		0.67 (in 4 replicates)	$-0.61 \pm 0.05$ Treatment Score MAPK2.WT.1 -0.58 MAPK2.WT.2 -0.66 TRAP5.WT -0.58 $0.367 \pm 0.311$ Treatment Score MAPK2.WT.1 0.280 MAPK2.WT.2 0.102 TRAP5.WT 0.700				Total number of assays tested in: 54.
BRD-K60656884-001-01-0 PubChem CID : 54618107		0.76 (in 4 replicates)	$-0.59 \pm 0.06$ Treatment Score MAPK2.WT.1 -0.60 MAPK2.WT.2 -0.65 TRAP5.WT -0.53 $0.513 \pm 0.340$ Treatment Score MAPK2.WT.1 0.387 MAPK2.WT.2 0.500 TRAP5.WT 0.400				Total number of assays tested in: 36.
BRD-K08668362-001-01-1 PubChem CID : 54646090		NA (in 1 replicates)	$-0.58 \pm 0.05$ Treatment Score MAPK2.WT.1 -0.56 MAPK2.WT.2 -0.64 TRAP5.WT -0.55 $0.455 \pm 0.475$ Treatment Score MAPK2.WT.1 0.280 MAPK2.WT.2 0.090 TRAP5.WT 0.080				Total number of assays tested in: 41.
BRD-K64231918-001-05-9 MS-3063 AC1NXO4W HMS244N09 ZINC20445571 SMR000180808 PubChem CID : 5786980		NA (in 1 replicates)	$-0.58 \pm 0.03$ Treatment Score MAPK2.WT.1 -0.55 MAPK2.WT.2 -0.58 TRAP5.WT -0.61 NA				Total number of assays tested in: 660. Active in the following assays: <ul style="list-style-type: none"><li>Primary cell-based high-throughput screening assay for identification of compounds that allostERICALLY potentiate transient receptor potential cation channel C4 (TRPC4) (AID 2227)</li><li>HTS-Luminescent assay for inhibitors of ALR by detection of hydrogen peroxide production Measured in Biochemical System Using Plate Reader - 2036-02.Inhibitor SinglePoint.HTS (AID 485317)</li><li>Absorbance-based biochemical primary high throughput screening assay to identify inhibitors of Methionine sulfoxide reductase A (MsrA) (AID 651718)</li></ul>