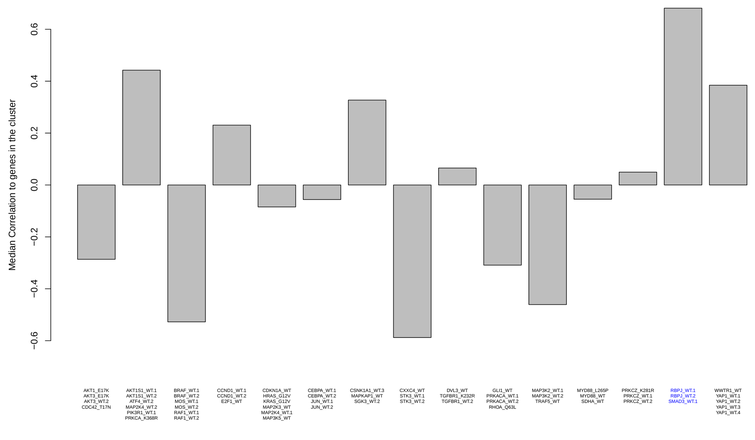
CONFIDENTIAL, contact the Imaging Platform to collaborate on the findings herein

How similar is this cluster to the other clusters?



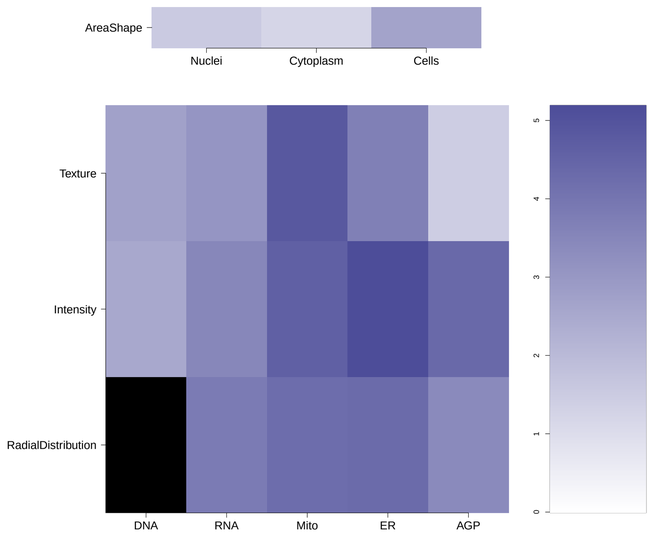
Top 5 genes negatively correlated to the cluster

	Expert Annotation			
Treatment	Pathway	Regulation Type	Mean Correlation	Standard Deviation
RAF1_WT.2	Canonical MAPK	Activator	-0.62	0.06
CXXC4_WT	WNT	Inhibitor	-0.60	0.01
STK3_WT.1	Canonical Hippo	Activator	-0.60	0.09
MAP3K2_WT.1	Canonical MAPK	Activator	-0.58	0.16
PIK3CB_WT.2	Canonical PI3K/AKT	Activator	-0.55	0.13

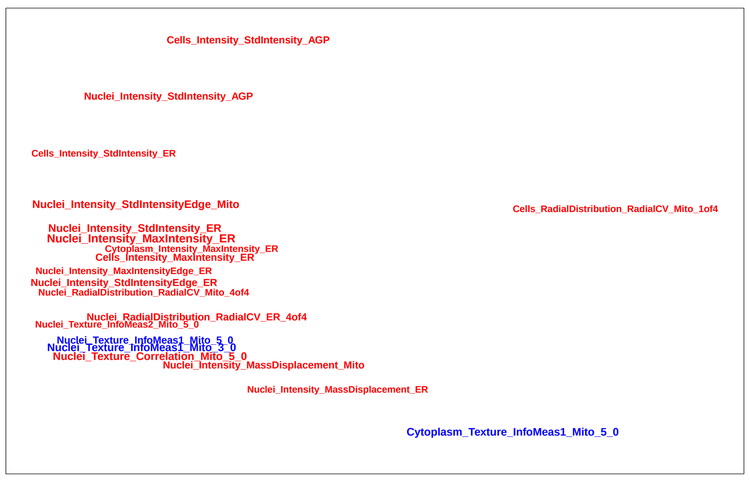
Genes in the cluster along with the pathways as annotated by experts

	Expert Annotation	
Treatment	Pathway	Regulation Type
SMAD3_WT.1	Canonical SMAD	Activator
RBPJ_WT.1	NOTCH	Activator
RBPJ_WT.2	NOTCH	Activator

What groups of morphological features are distinguishing in the cluster relative to the untreated samples? (maximum of absolute m-score for the features belonging to the same category; m-score defined as median of a feature z-score across genes in the cluster) Black means no feature is available in the category



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.



How strongly are genes within the cluster correlated?

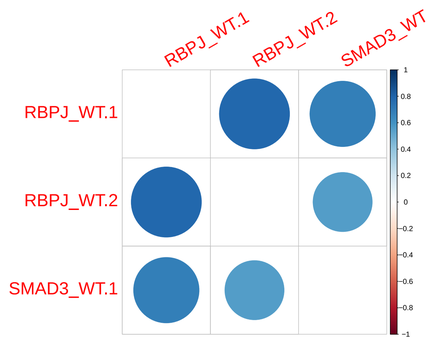
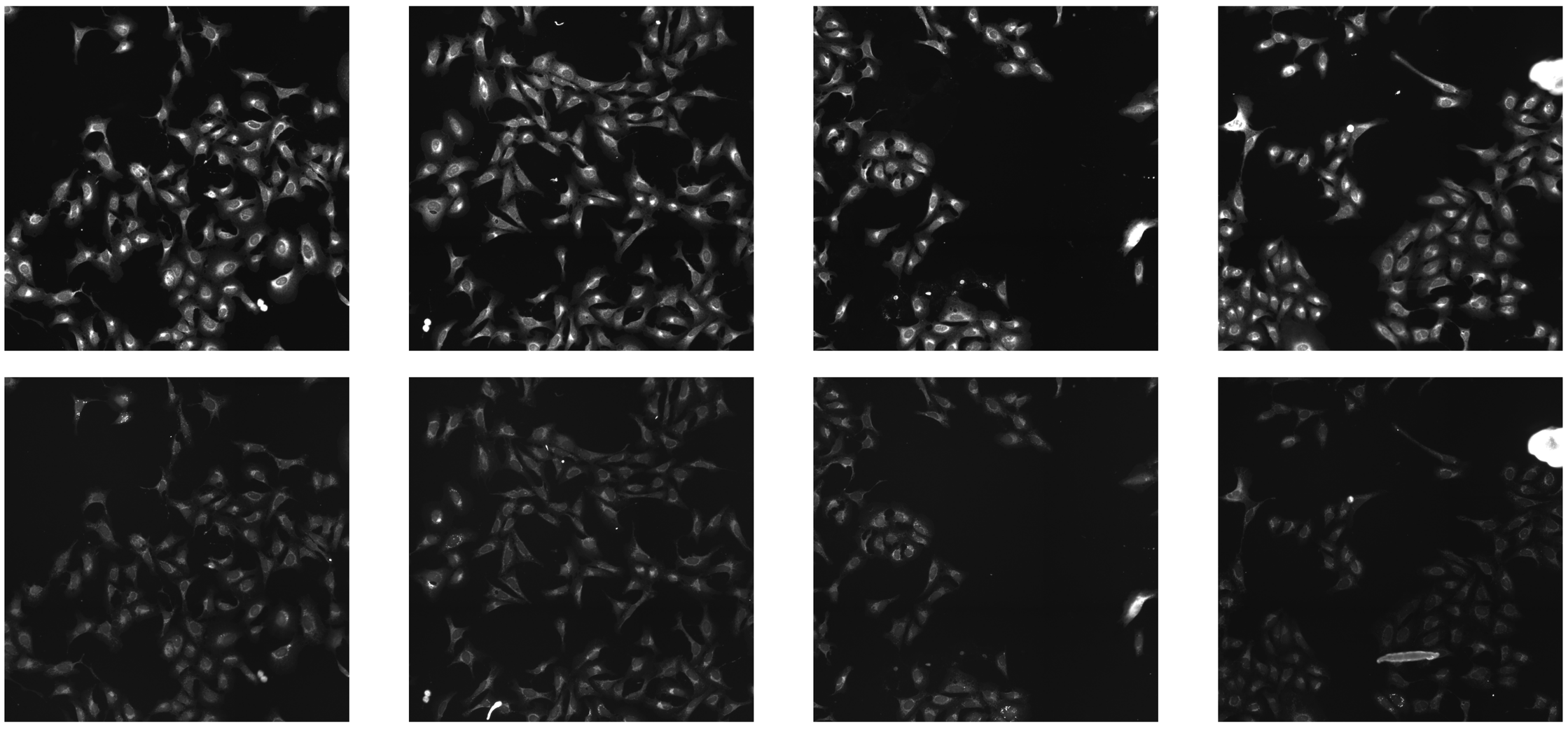
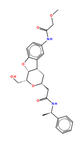
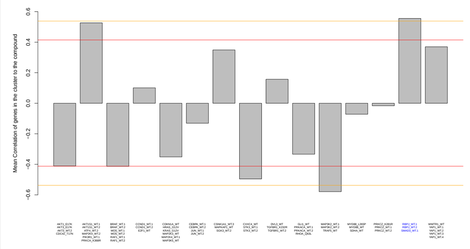
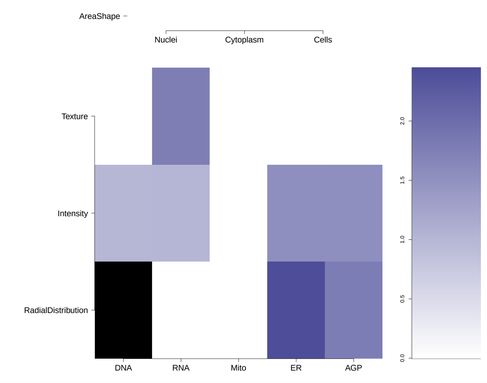
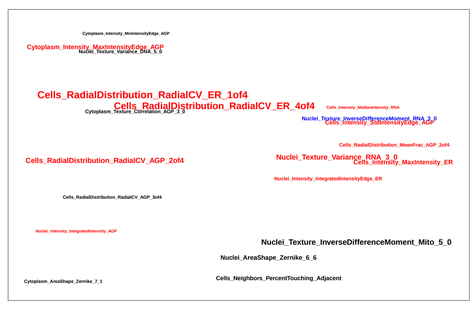
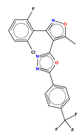
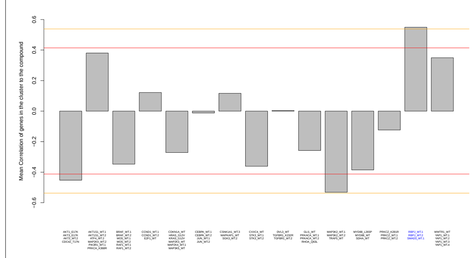
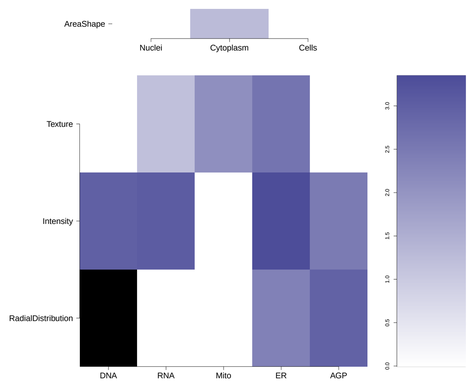
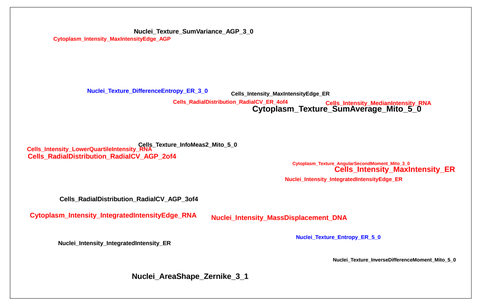
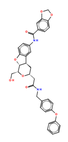
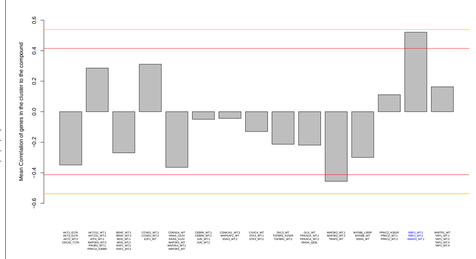
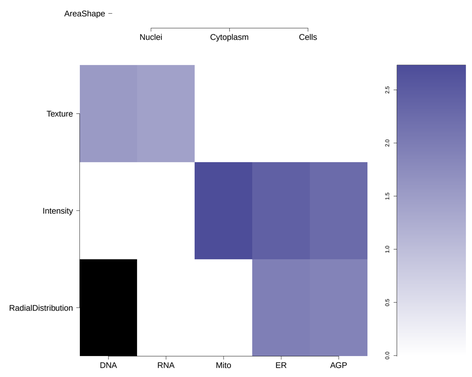
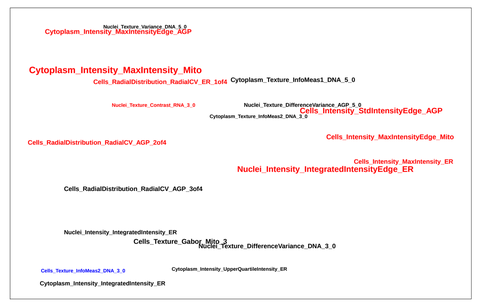
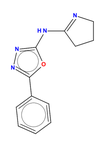
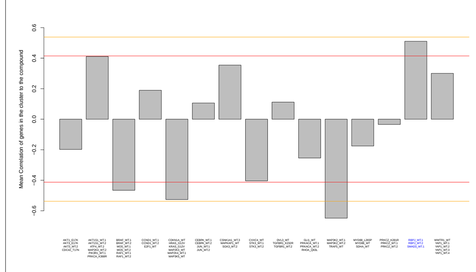
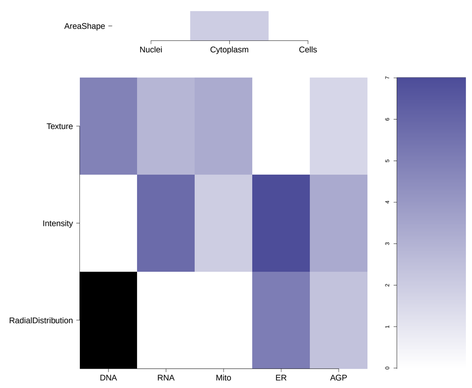
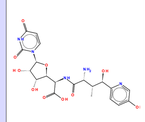
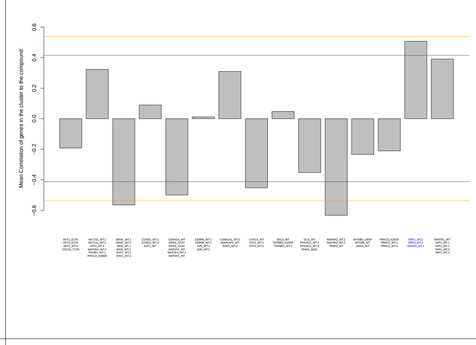
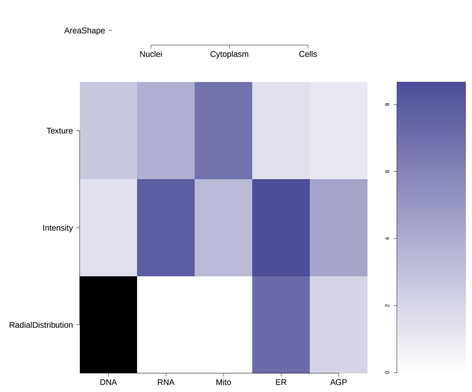
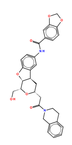
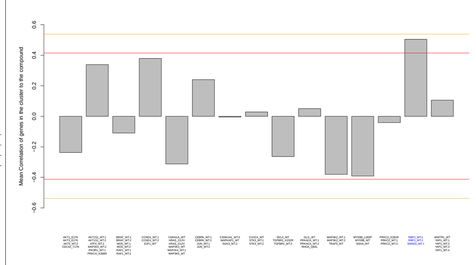
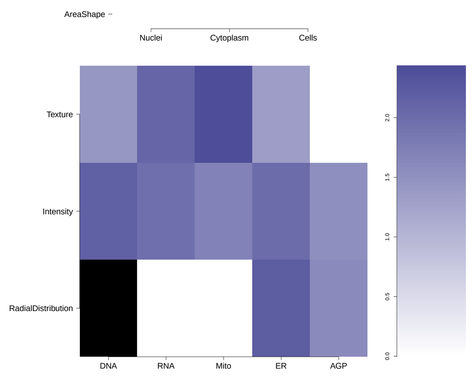
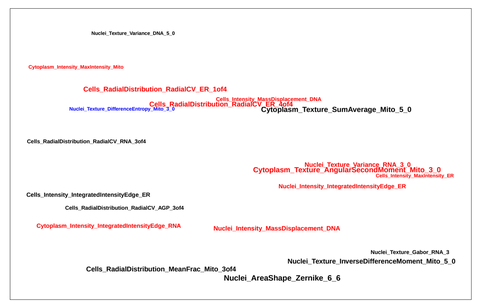
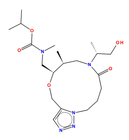
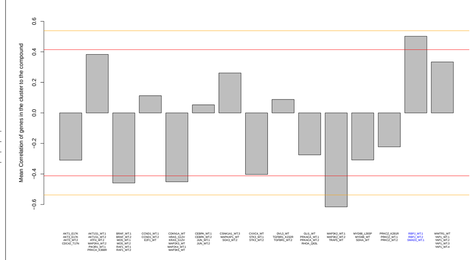
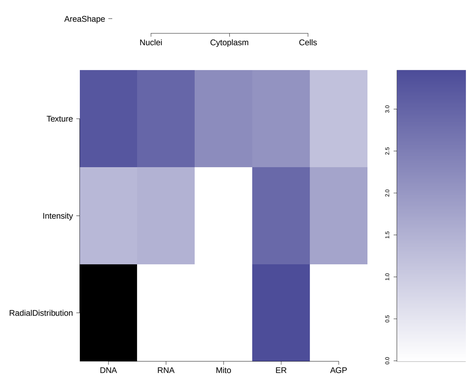
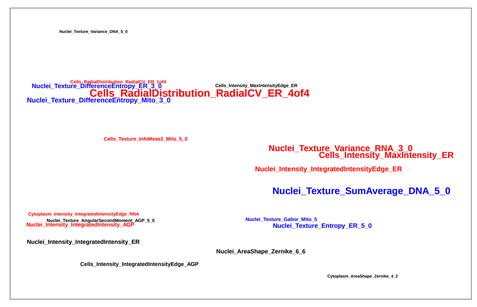
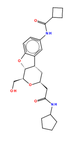
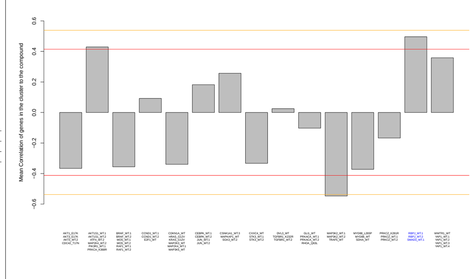
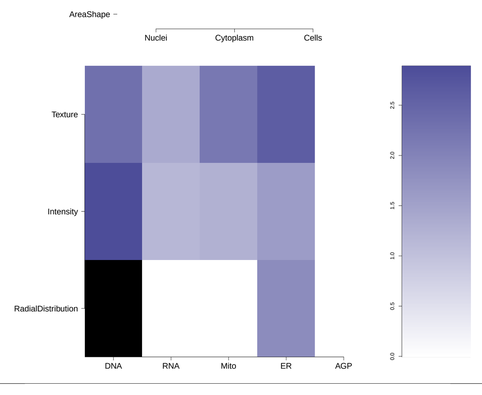
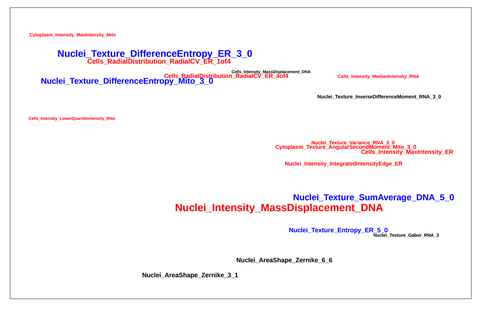
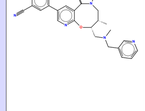
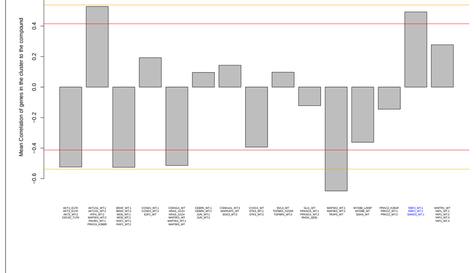
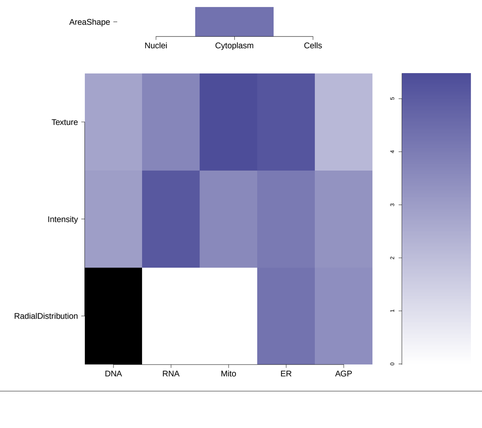
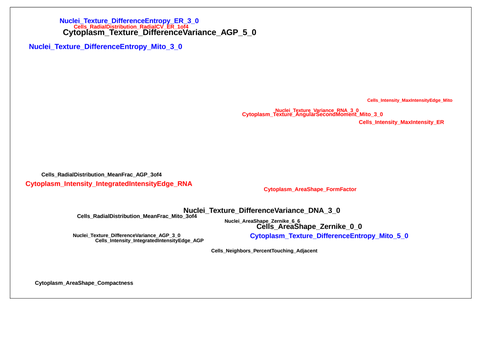
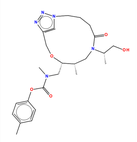
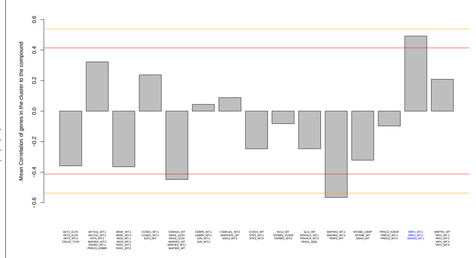
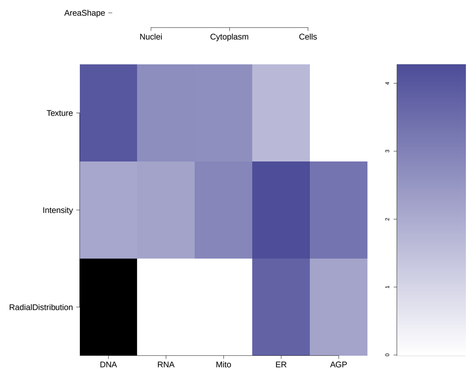
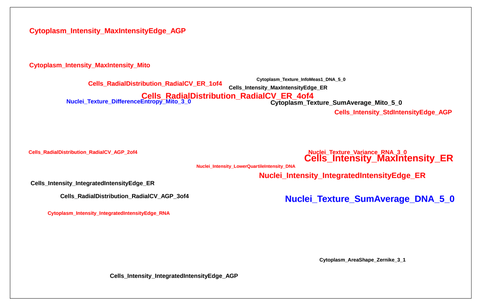
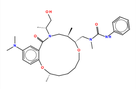
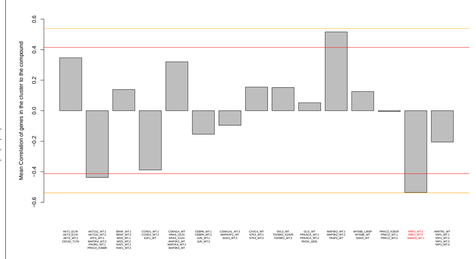
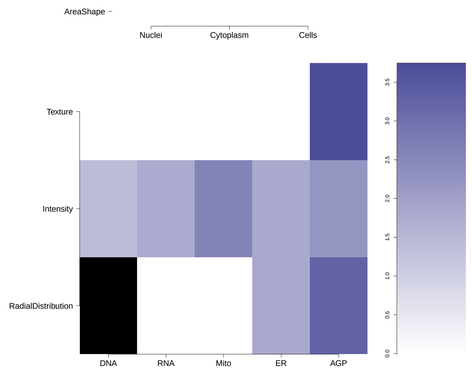
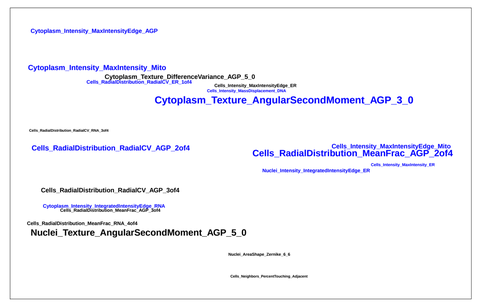
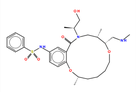
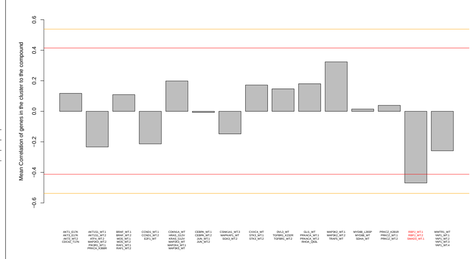
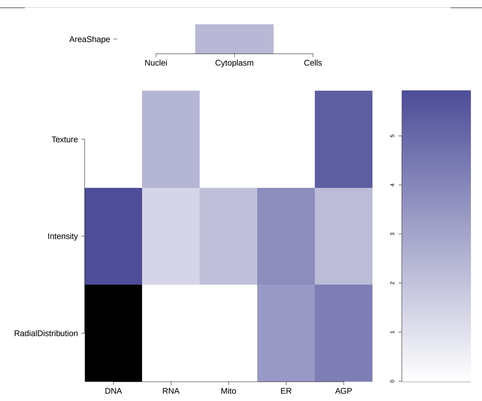
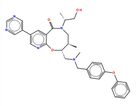
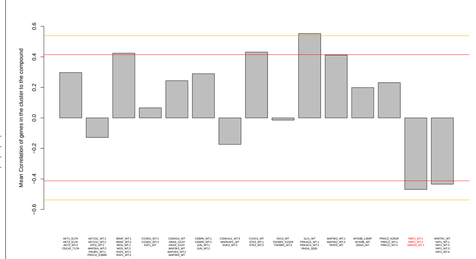
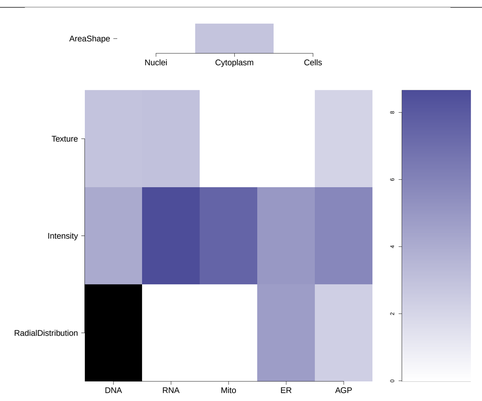
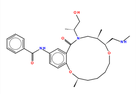
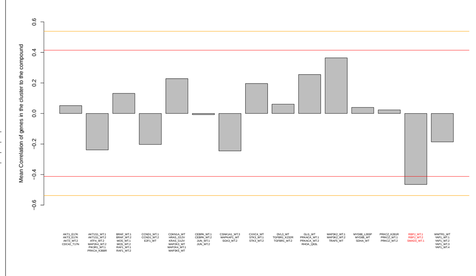
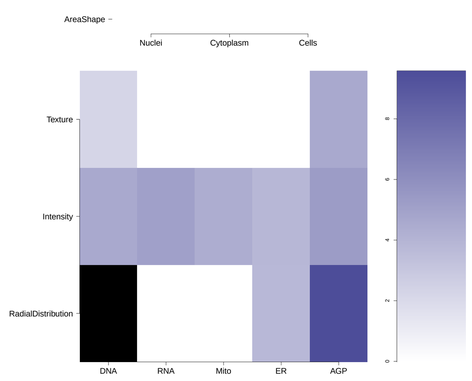
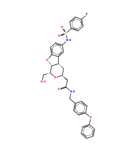
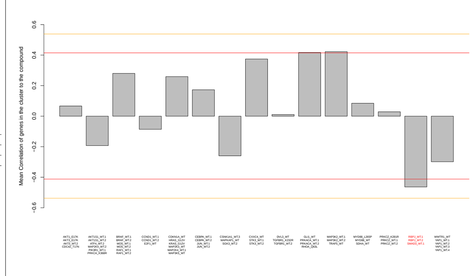
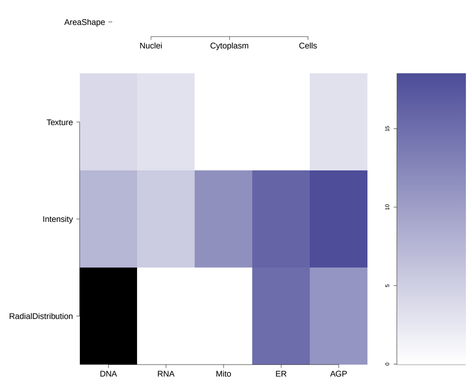
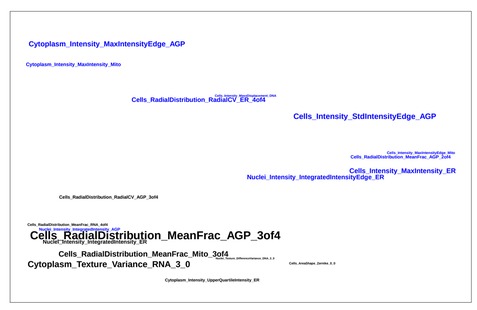
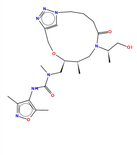
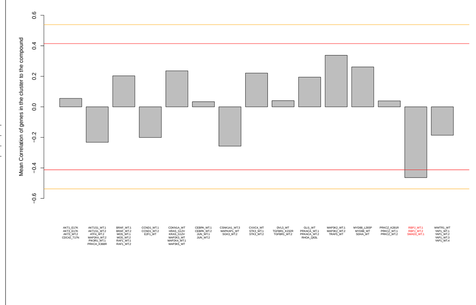
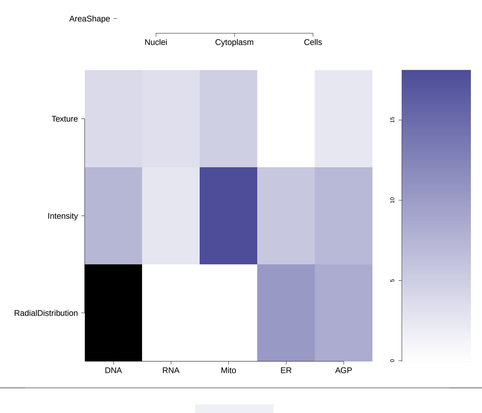
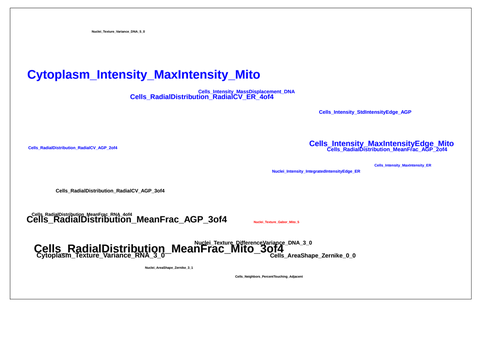
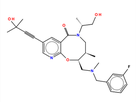
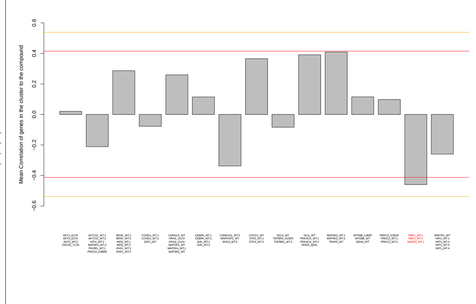
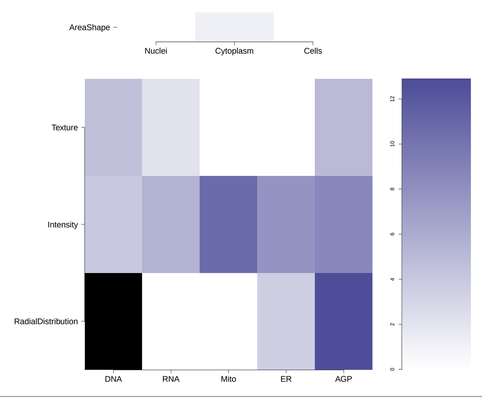
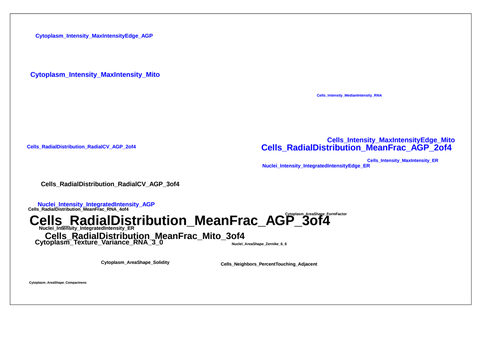


Plate : 41744 - Genes in the Cluster (Channels are sorted based on their dominance in the grid plot)

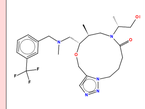


Compound IDs and common names (where available); blue/red colored box means the matching compound is positively/negatively correlated with the cluster	Chemical structure	Mean pairwise replicates correlation of the compound signature (95th DMSO replicate correlation is 0.52)	Mean ± standard deviation correlation between compound and each gene in cluster; Tables contain data for individual genes	Mean compound rank when scored against genes in cluster using L1000 profiling ± standard deviation; Tables contain data for individual genes	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)	Common distinguishing feature categories in the compound and genes in the cluster relative to the untreated samples	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	Number of PubChem assays in which the compound was tested; assays in which the compound was active are itemized
BRD-K62943397-001-01-0 PubChem CID : 54646065		NA (in 1 replicates)	0.56 ± 0.08 Treatment | Score RBPJ_WT.1 | 0.62 RBPJ_WT.2 | 0.57 SMAD3_WT.1 | 0.47	0.729 ± 0.042 Treatment | Score RBPJ_WT.1 | 0.730 RBPJ_WT.2 | 0.770 SMAD3_WT.1 | 0.686				Total number of assays tested in: 39.

BRD-K04968712-001-05-7 MLS000858711 SMR000458790 AC1MDPY6 BDBM45738 HMS2811A04 ZINC1034543 ZINC01034543 PubChem CID : 2814981		NA (in 1 replicates)	0.55 ± 0.03 Treatment / Score RBPJ.WT.1 / 0.58 RBPJ.WT.2 / 0.55 SMAD3.WT.1 / 0.52	NA				Total number of assays tested in: 545. Active in the following assays: • Factor XIIa 1536 HTS (AID 800) • Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 48 hour incubation (AID 504832) • Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 96 hour incubation (AID 504834) • Confirmation screen for delayed death inhibitors of the malarial parasite plastid, 96 hour incubation (AID 504848) • Confirmation screen for delayed death inhibitors of the malarial parasite plastid, 48 hour incubation (AID 504850) • qHTS for induction of synthetic lethality in tumor cells producing 2HG: qHTS for the HT-1080-IDH1KD cell line (AID 686971)
BRD-K52184420-001-01-4 PubChem CID : 54645920		NA (in 1 replicates)	0.52 ± 0.13 Treatment / Score RBPJ.WT.1 / 0.51 RBPJ.WT.2 / 0.40 SMAD3.WT.1 / 0.66	0.148 ± 0.102 Treatment / Score RBPJ.WT.1 / 0.031 RBPJ.WT.2 / 0.218 SMAD3.WT.1 / 0.196				Total number of assays tested in: 44. Active in the following assays: • Inhibition of T.cruzi proliferation in culture Measured in Cell-Based System Using Plate Reader - 2138-01_Inhibitor_SinglePoint_HTS_Activity (AID 624255) • Inhibition of T.cruzi proliferation in culture Measured in Cell-Based System Using Plate Reader - 2138-01_Inhibitor_SinglePoint_CherryPick_Activity (AID 651739) • NIH/3T3 (mouse embryonic fibroblast) toxicity Measured in Cell-Based System Using Plate Reader - 2138-02_Inhibitor_SinglePoint_CherryPick_Activity_Set2 (AID 651744)
BRD-K15827540-001-05-0 T5250099 AC1M2QX1 MLS001010624 HMS1774C11 HMS2718E22 ZINC12531006 SMR000352827 PubChem CID : 2123280		NA (in 1 replicates)	0.51 ± 0.07 Treatment / Score RBPJ.WT.1 / 0.59 RBPJ.WT.2 / 0.47 SMAD3.WT.1 / 0.47	NA				Total number of assays tested in: 643. Active in the following assays: • Primary cell-based high throughput screening assay to measure STAT3 inhibition (AID 862) • Counter Screen for Luciferase-based Primary Inhibition Assays (AID 1006) • qHTS Assay for Enhancers of SMN2 Splice Variant Expression (AID 1458) • qHTS Assay for Inhibitors of Leishmania Mexicana Pyruvate Kinase (LmPK) (AID 1721) • Luminescence-based primary biochemical high throughput screening assay to identify inhibitors of the Heat Shock Protein 90 (HSP90) (AID 1789) • qHTS for inhibitors of ROR gamma transcriptional activity (AID 2551) • qHTS Assay for Rab9 Promoter Activators (AID 485297) • qHTS screen for small molecules that induce genotoxicity in human embryonic kidney (HEK293T) cells expressing luciferase-tagged ELG1 (AID 504466) • qHTS for Inhibitors of binding or entry into cells for Lassa Virus (AID 540256) • qHTS profiling assay for firefly luciferase inhibitor/activator using purifed enzyme and Km concentrations of substrates (counterscreen for miR-21 project) (AID 588342) • 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) • qHTS for Inhibitors of PLK1-PDB (polo-like kinase 1 - polo-box domain): Primary Screen (AID 720504)
BRD-K76218980-001-11-3 nikkomycin z AC1NUQ0P MLS000028371 HMS2233C10 SMR000058642 PubChem CID : 5458181		NA (in 1 replicates)	0.51 ± 0.06 Treatment / Score RBPJ.WT.1 / 0.56 RBPJ.WT.2 / 0.51 SMAD3.WT.1 / 0.44	NA				Total number of assays tested in: 698. Active in the following assays: • qHTS Assay for Inhibitors of Bacillus subtilis Sfp phosphopantetheinyl transferase (PPTase) (AID 1490) • Fluorescence Cell-Based Secondary Assay to Identify Inhibitors of Resistant C. albicans Growth in the Presence of Fluconazole (AID 2423) • Fluorescence Cell-Based Retest of C. albicans Growth in the Presence of Fluconazole (AID 2467) • qHTS Assay for Inhibitors of Histone Lysine Methyltransferase G9a (AID 504332) • qHTS of TDP-43 Inhibitors (AID 652104)
BRD-K78761249-001-01-8 PubChem CID : 54645870		NA (in 1 replicates)	0.50 ± 0.06 Treatment / Score RBPJ.WT.1 / 0.47 RBPJ.WT.2 / 0.47 SMAD3.WT.1 / 0.57	0.561 ± 0.439 Treatment / Score RBPJ.WT.1 / 0.730 RBPJ.WT.2 / 0.891 SMAD3.WT.1 / 0.063				Total number of assays tested in: 42.
BRD-K04648846-001-02-1 MLS003129529 SMR001833975 PubChem CID : 44505579		0.74 (in 3 replicates)	0.50 ± 0.12 Treatment / Score RBPJ.WT.1 / 0.55 RBPJ.WT.2 / 0.59 SMAD3.WT.1 / 0.37	0.627 ± 0.445 Treatment / Score RBPJ.WT.1 / 0.810 RBPJ.WT.2 / 0.120 SMAD3.WT.1 / 0.951				Total number of assays tested in: 222.
BRD-K97101742-001-01-6 PubChem CID : 54645950		NA (in 1 replicates)	0.50 ± 0.20 Treatment / Score RBPJ.WT.1 / 0.57 RBPJ.WT.2 / 0.64 SMAD3.WT.1 / 0.27	0.548 ± 0.277 Treatment / Score RBPJ.WT.1 / 0.730 RBPJ.WT.2 / 0.229 SMAD3.WT.1 / 0.686				Total number of assays tested in: 40.
BRD-K48693155-001-01-2 PubCHem CID : 54618096		0.87 (in 4 replicates)	0.49 ± 0.14 Treatment / Score RBPJ.WT.1 / 0.64 RBPJ.WT.2 / 0.49 SMAD3.WT.1 / 0.35	NA				Total number of assays tested in: 37.

BRD-K26273696-001-01-5 PubChem CID : 44486963		0.59 (in 3 replicates)	0.49 ± 0.03 Treatment | Score RBPJ.WT.1 | 0.52 RBPJ.WT.2 | 0.47 SMAD3.WT.1 | 0.48	0.768 ± 0.038 Treatment | Score RBPJ.WT.1 | 0.730 RBPJ.WT.2 | 0.770 SMAD3.WT.1 | 0.805				Total number of assays tested in: 34.
BRD-K86946907-001-01-8 PubChem CID : 44494582		0.72 (in 4 replicates)	-0.54 ± 0.06 Treatment | Score RBPJ.WT.1 | -0.54 RBPJ.WT.2 | -0.47 SMAD3.WT.1 | -0.59	0.711 ± 0.382 Treatment | Score RBPJ.WT.1 | 0.270 RBPJ.WT.2 | 0.941 SMAD3.WT.1 | 0.922				Total number of assays tested in: 34. Active in the following assays: • MLPCN PGC1a Modulators Measured in Cell-Based System Using Plate Reader - 2139-01_Activator_SinglePoint_HTS_Activity (AID 651723) • MLPCN PGC1a Modulators Measured in Cell-Based System Using Plate Reader - 2139-01_Activator_Dose_CherryPick_Activity_Set6 (AID 720513)
BRD-K57969466-001-01-8 PubChem CID : 44489309		0.80 (in 4 replicates)	-0.47 ± 0.10 Treatment | Score RBPJ.WT.1 | -0.41 RBPJ.WT.2 | -0.41 SMAD3.WT.1 | -0.59	0.429 ± 0.311 Treatment | Score RBPJ.WT.1 | 0.270 RBPJ.WT.2 | 0.230 SMAD3.WT.1 | 0.788				Total number of assays tested in: 46.
BRD-K29290722-001-01-4 PubChem CID : 54618609		0.68 (in 4 replicates)	-0.47 ± 0.05 Treatment | Score RBPJ.WT.1 | -0.43 RBPJ.WT.2 | -0.45 SMAD3.WT.1 | -0.53	0.456 ± 0.353 Treatment | Score RBPJ.WT.1 | 0.857 RBPJ.WT.2 | 0.196 SMAD3.WT.1 | 0.314				Total number of assays tested in: 23. Active in the following assays: • Small molecule inhibitors of miR122 Measured in Cell-Based System Using Plate Reader - 2144-01_Activator_SinglePoint_HTS_Activity (AID 623901) • Small molecule inhibitors of miR122 Measured in Cell-Based System Using Plate Reader - 2144-01_Activator_Dose_CherryPick_Activity (AID 651956)
BRD-K90429860-001-01-4 PubChem CID : 54614935		0.91 (in 4 replicates)	-0.47 ± 0.08 Treatment | Score RBPJ.WT.1 | -0.43 RBPJ.WT.2 | -0.41 SMAD3.WT.1 | -0.56	0.169 ± 0.142 Treatment | Score RBPJ.WT.1 | 0.270 RBPJ.WT.2 | 0.230 SMAD3.WT.1 | 0.006				Total number of assays tested in: 19.
BRD-K19876534-001-01-0 PubChem CID : 54646516		0.96 (in 4 replicates)	-0.46 ± 0.04 Treatment | Score RBPJ.WT.1 | -0.45 RBPJ.WT.2 | -0.43 SMAD3.WT.1 | -0.51	0.460 ± 0.292 Treatment | Score RBPJ.WT.1 | 0.270 RBPJ.WT.2 | 0.796 SMAD3.WT.1 | 0.314				Total number of assays tested in: 44. Active in the following assays: • Small molecule inhibitors of miR122 Measured in Cell-Based System Using Plate Reader - 2144-01_Inhibitor_SinglePoint_HTS_Activity (AID 602342) • Inhibitors of Epstein-Barr LMP1 inducible NF-kappaB luciferase reporter Measured in Cell-Based System Using Plate Reader - 2122-05_Inhibitor_DryPowder_Activity_Set2 (AID 624369) • Inhibitors of Epstein-Barr LMP1 inducible NF-kappaB luciferase reporter Measured in Cell-Based System Using Plate Reader - 2122-01_Inhibitor_Dose_DryPowder_Activity_Set2 (AID 624376) • Luminescence Cell-Based Primary HTS to identify inhibitors of the oncoprotein EWS/Fli transcriptional activity Measured in Cell-Based System Using Plate Reader - 7014-01_Inhibitor_SinglePoint_HTS_Activity (AID 651661) • HTS for PAX8 inhibitors using PAX8 luciferase reporter gene assay in RMG-I cells Measured in Cell-Based System Using Plate Reader - 7054-01_Inhibitor_SinglePoint_HTS_Activity (AID 652154)
BRD-K08043024-001-01-7 PubChem CID : 44486366		0.89 (in 3 replicates)	-0.46 ± 0.02 Treatment | Score RBPJ.WT.1 | -0.46 RBPJ.WT.2 | -0.48 SMAD3.WT.1 | -0.45	0.139 ± 0.086 Treatment | Score RBPJ.WT.1 | 0.129 RBPJ.WT.2 | 0.230 SMAD3.WT.1 | 0.059				Total number of assays tested in: 37.
BRD-K12834930-001-01-6 PubChem CID : 54618605		0.91 (in 4 replicates)	-0.46 ± 0.01 Treatment | Score RBPJ.WT.1 | -0.44 RBPJ.WT.2 | -0.46 SMAD3.WT.1 | -0.47	0.458 ± 0.325 Treatment | Score RBPJ.WT.1 | 0.830 RBPJ.WT.2 | 0.230 SMAD3.WT.1 | 0.314				Total number of assays tested in: 23.

BRD-K51762600-001-02-8
MLS003129301
SMR001833747
PubChem CID : 44505038



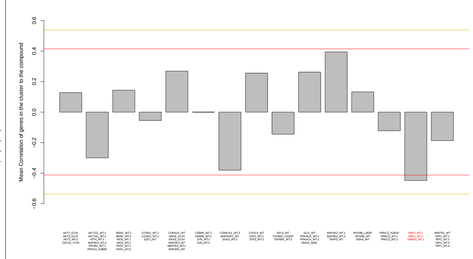
0.94 (in 3 replicates)

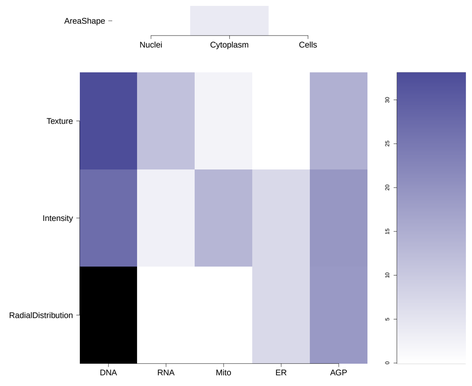
-0.45 ± 0.01

Treatment	Score
RBPJ.WT.1	-0.44
RBPJ.WT.2	-0.44
SMAD3.WT.1	-0.46

0.421 ± 0.296

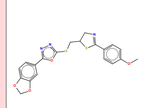
Treatment	Score
RBPJ.WT.1	0.270
RBPJ.WT.2	0.230
SMAD3.WT.1	0.762





Total number of assays tested in: 229.

BRD-A83852736-001-06-9
T5235042
SMR000063406
AC1MHBUZ
MLS000053977
MLS002635527
TCMDC-143594
HMS1727O03
HMS2385I15
PubChem CID : 2999476

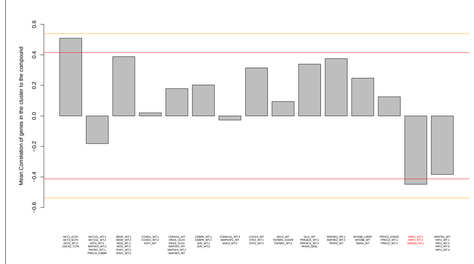


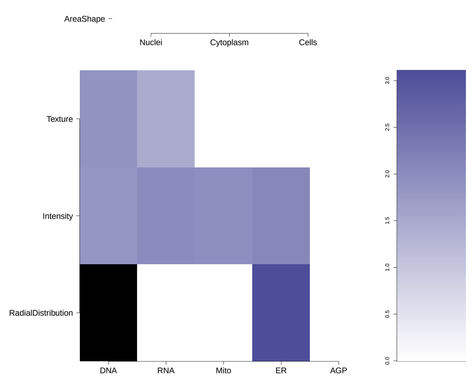
0.63 (in 2 replicates)

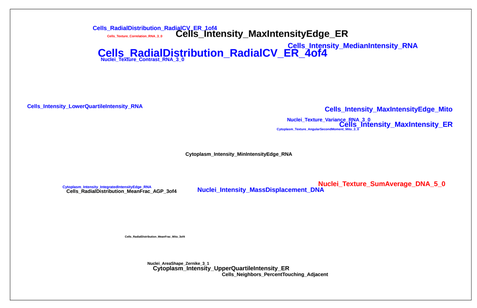
-0.45 ± 0.01

Treatment	Score
RBPJ.WT.1	-0.43
RBPJ.WT.2	-0.46
SMAD3.WT.1	-0.45

NA



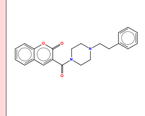




Total number of assays tested in: 805. Active in the following assays:

- Screening for Modulators of Post-Golgi Transport, Control Strain (AID 738)
- qHTS Assay for Inhibitors of HPGD (15-Hydroxyprostaglandin Dehydrogenase) (AID 894)
- Leishmania major promastigote HTS (AID 1063)
- Leishmania major promastigote HTS - primary screen repeat 1 uM (AID 1258)
- Counterscreen for inhibitors of Janus kinase 2 mutant JAK2V617F: Cell-based high throughput assay to identify inhibitors of parental Ba/F3 cell viability. (AID 1486)
- Luminescence Cell-Based/Microorganism Primary HTS to Identify Inhibitors of T.Cruzi Replication (AID 1885)
- Leishmania major promastigote EC50 determinations (AID 2008)
- Luminescence Cell-Based/Microorganism Dose Confirmation HTS to Identify Inhibitors of T.Cruzi Replication. (AID 2044)
- Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the orexin 1 receptor (OX1R; HCRTR1) (AID 434989)
- qHTS profiling assay for firefly luciferase inhibitor/activator using purifed enzyme and Km concentrations of substrates (counterscreen for miR-21 project) (AID 588342)
- Primary cell-based high-throughput screening for identification of compounds that inhibit/block calcium-activated chloride channels (TMEM16A) (AID 588511)
- uHTS identification of small molecule inhibitors of the mitochondrial permeability transition pore via an absorbance assay (AID 602449)
- qHTS for Antagonists of gsp, the Etiologic Mutation Responsible for Fibrous Dysplasia/McCune-Albright Syndrome: qHTS (AID 624288)
- Fluorescence-based cell-based primary high throughput screening assay to identify antagonists of the human trace amine associated receptor 1 (TAAR1) (AID 624466)
- Single concentration confirmation of uHTS inhibitor hits of the mitochondrial permeability transition pore via a fluorescent based assay (AID 624504)
- Trypanosoma brucei. Primary growth inhibition assay (AID 1159557)
- TcCYP51 enzymatic inhibition (AID 1159558)
- Trypanosoma cruzi. Primary growth inhibition assay (AID 1159559)
- Leishmania donovani. Primary growth inhibition assay (AID 1159560)
- Intra-macrophage L. donovani assay (AID 1159564)
- Trypanosoma cruzi intracellular imaging assay (AID 1159565)

BRD-K86231088-001-07-3
SMR000080398
MLS000065727
ST50868443
AC1LORJA
MLS002547888
BDBM74661
HMS2457N19
STK461645
ZINC55060307
T5713242
PubChem CID : 1245644

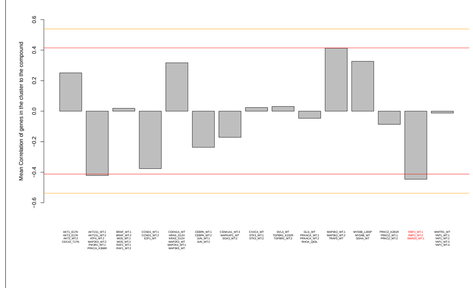


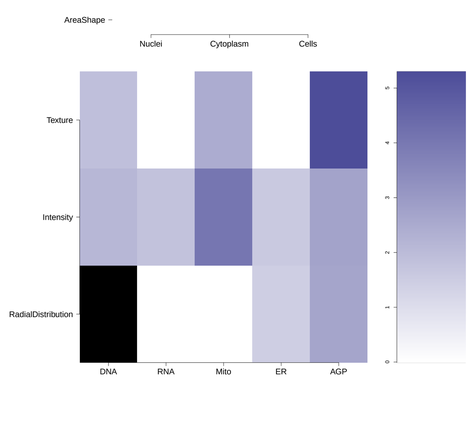
0.64 (in 4 replicates)

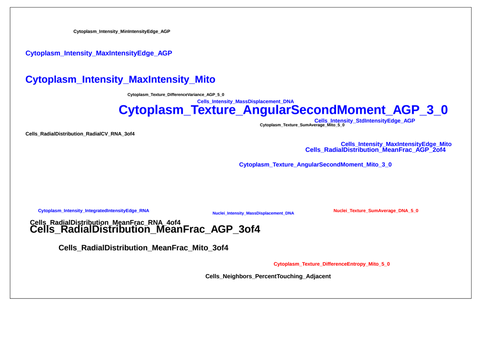
-0.45 ± 0.03

Treatment	Score
RBPJ.WT.1	-0.48
RBPJ.WT.2	-0.42
SMAD3.WT.1	-0.44

NA







Total number of assays tested in: 727. Active in the following assays:

- uHTS identification of compounds inhibiting the binding between the RUNX1 Runt domain and CBFb-SMMHC via a fluorescence resonance energy transfer (FRET) assay. (AID 1434)
- Identification of compounds inhibiting the binding between the RUNX1 Runt domain and CBFb-SMMHC via a time resolved fluorescence resonance energy transfer (TR-FRET) assay. (AID 1438)
- Fluorescence Cell-Free Homogeneous Primary HTS to Identify Inhibitors of the RanGTP-Importin-beta complex (AID 2216)
- Fluorescence Cell-Free Homogeneous Dose Retest to Identify Inhibitors of the RanGTP-Importin-beta complex (AID 2823)
- Fluorescence Cell-Free Homogeneous Counterscreen to Identify Inhibitors of the RanGTP-Importin-beta complex. (AID 435026)
- Primary qHTS for delayed death inhibitors of the malarial parasite plastid, 96 hour incubation (AID 504834)
- Primary cell-based high-throughput screening for identification of compounds that inhibit/block calcium-activated chloride channels (TMEM16A) (AID 588511)