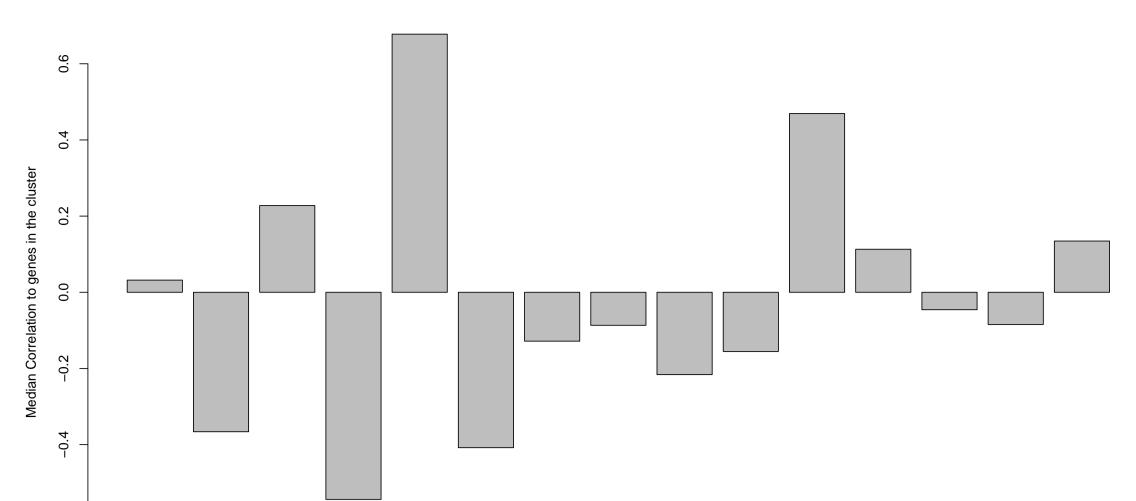
How similar is this cluster to the other clusters?

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

	Expert Annotation		
Treatment	Pathway	Regulation Type	
CDKN1A_WT	Canonical Cell Cycle	Inhibitor	
MAP3K5_WT	Canonical MAPK	Activator	
MAP2K4_WT.1	Canonical MAPK	Activator	
MAP2K3_WT	Canonical MAPK	Activator	
KRAS_G12V	RTK	Activator	
HRAS_G12V	RTK	Activator	



Top 5 genes	negatively	correlated	\mathbf{to}	the	cluster

		•	0	U		
Expert Annotation						
	Treatment	Pathway	Regulation Ty	pe Mean Correlation	Standard Deviation	
	E2F1_WT	Canonical Cell Cycle	Activator	-0.59	0.09	
	CCND1_WT.2	Canonical Cell Cycle	Activator	-0.58	0.08	
	$CDK2_WT.1$	Canonical Cell Cycle	Activator	-0.49	0.11	
	$\mathrm{DDIT4}_{-}\mathrm{WT}$	Canonical TOR	Inhibitor	-0.49	0.07	
	PER1 WT 2	Circadian Bhythm	Activator	-0.49	0.09	

AKT1_E17K AKT1S1_WT.1 BRAF_WT.1 CCND1_WT.1 CDKN1A_WT CEBPA_WT.1 CSNK1A1_WT.3 CXXC4_WT DVL3_WT GLI1_WT MAP3K2_WT.1 MYD88_L265P PRKCZ_K281R RBPJ_WT.1 WWTR1_WT AKT3_E17K AKT1S1_WT.2 BRAF_WT.2 CCND1_WT.2 HRAS_G12V CEBPA_WT.2 MAPKAP1_WT STK3_WT.1 TGFBR1_K232R PRKACA_WT.1 MAP3K2_WT.2 MYD88_WT PRKCZ_WT.1 RBPJ_WT.2 YAP1_WT.1 AKT3_WT.2 ATS4_WT.2 MOS_WT.2 MAP2K4_WT.2 MOS_WT.2 STK3_WT.2 STK3_WT.2 STK3_WT.2 TGFBR1_WT.2 PRKACA_WT.2 TRAF5_WT SDHA_WT PRKCZ_WT.2 SMAD3_WT.1 YAP1_WT.3 PRKCA_K368R RAF1_WT.2 MAP2K4_WT.1 MAP2K6_WT.1 MAP2K4_WT.1 MAP2K6_WT.1 MAP2

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?

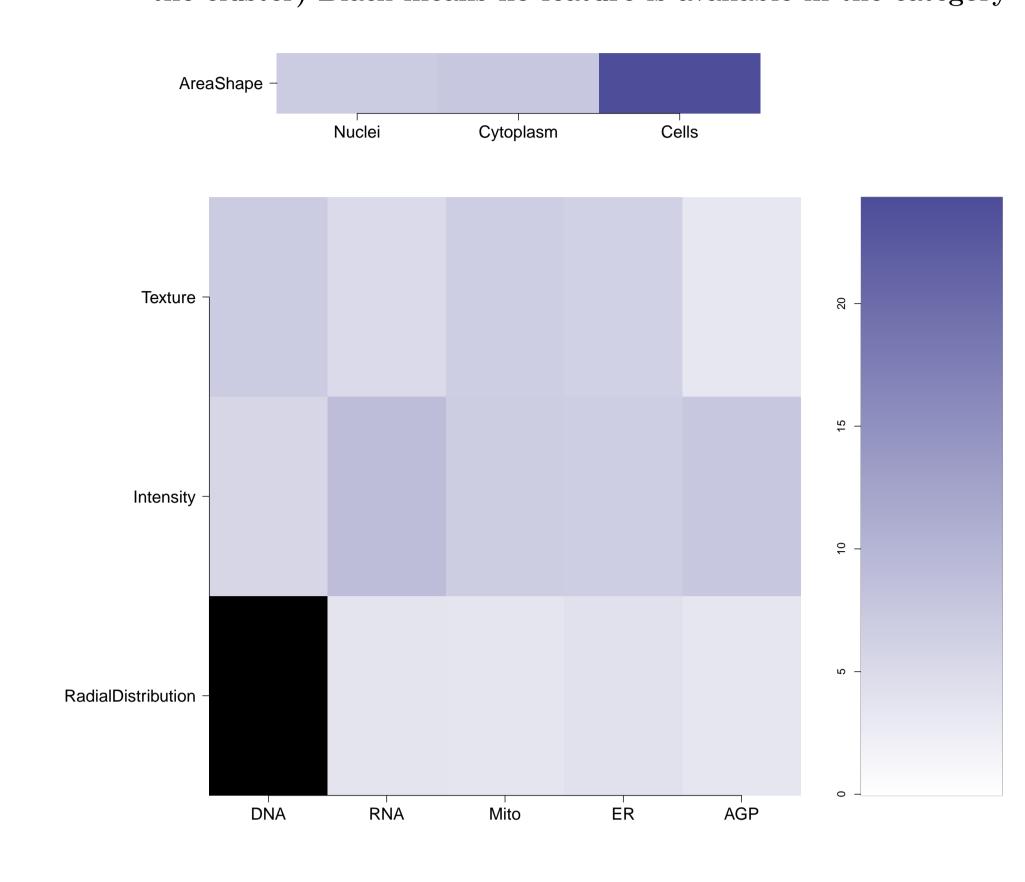
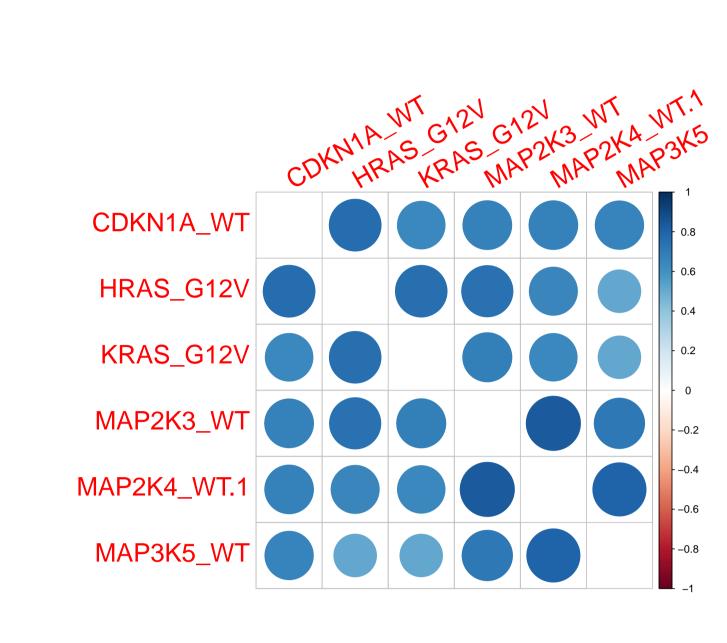
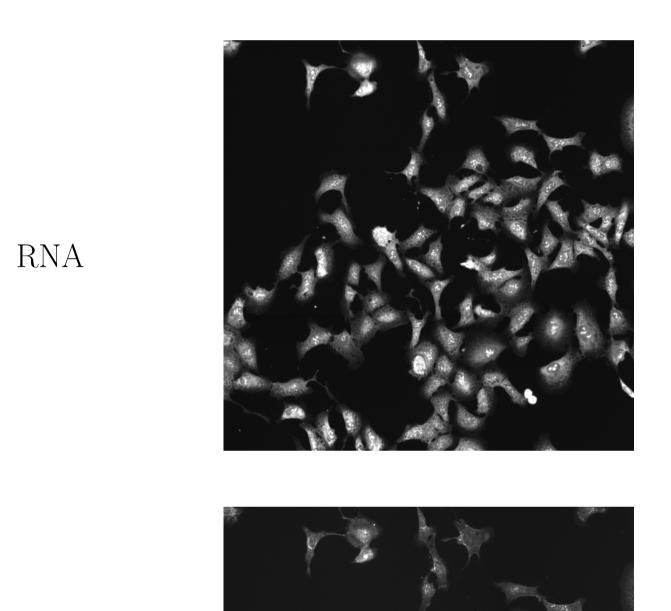


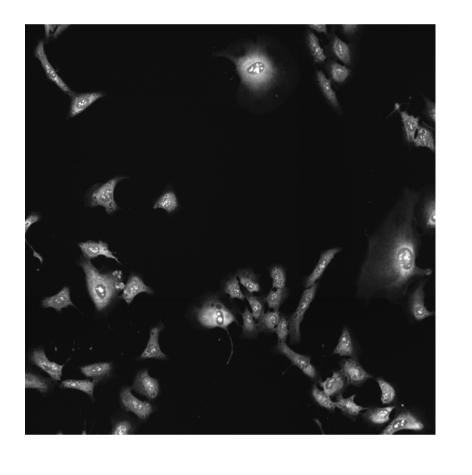


Plate: 41744 - Genes in the Cluster (Channels are sorted based on their dominance in the grid plot)

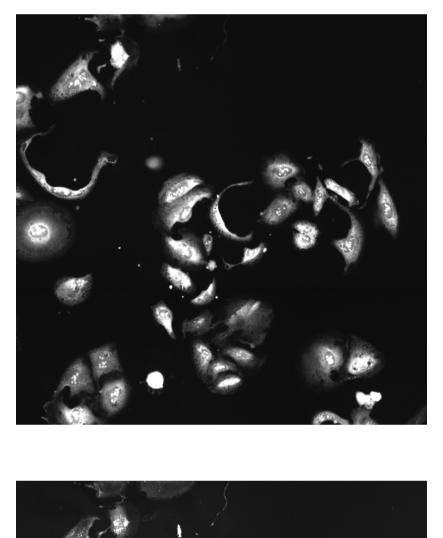




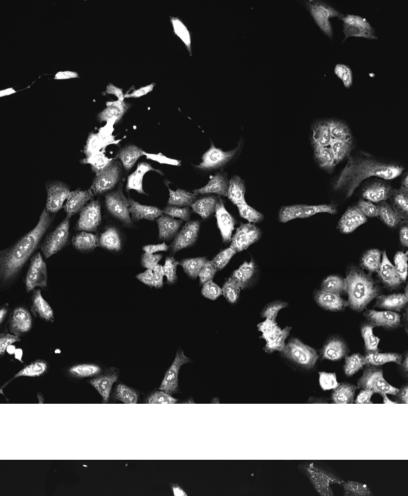
Empty



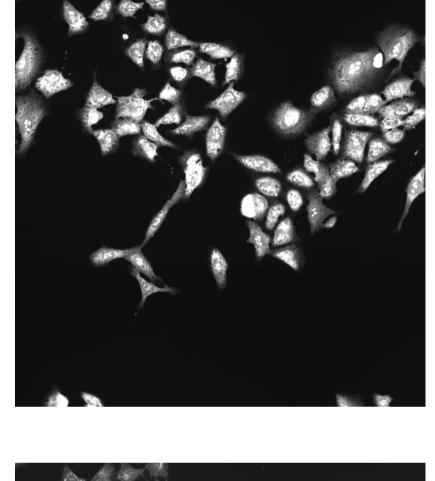
CDKN1A_WT



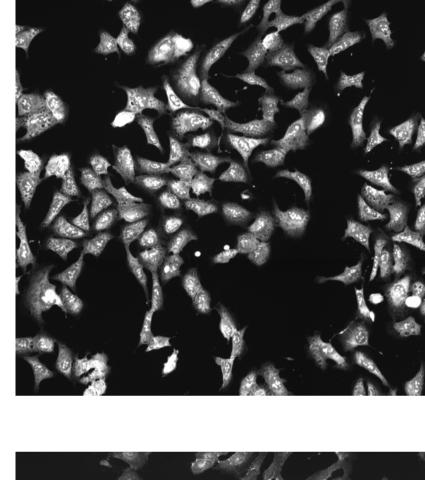
 $HRAS_{-}G12V$



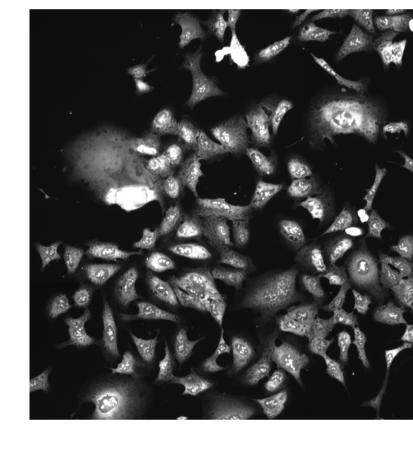
KRAS_G12V



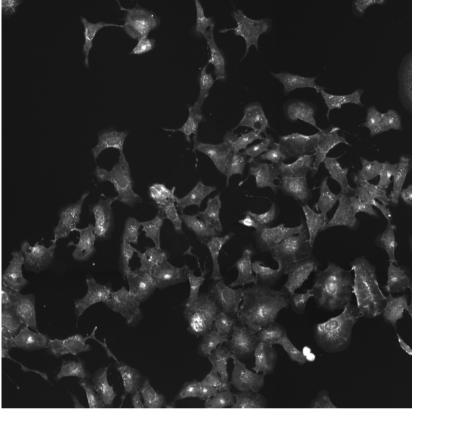
 $MAP2K3_WT$

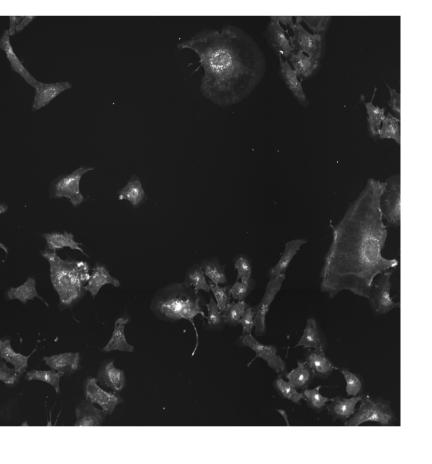


MAP2K4_WT.1



 $MAP3K5_WT$





compound

rank when

scored

against genes

in cluster

using L1000

profiling \pm

standard

deviation;

for individual

Mean \pm

standard

deviation

correlation

between

compound

and each

gene in

cluster;

contain data

for individual

 0.69 ± 0.09

Treatment Score
CDKN1A_WT 0.80

HRAS_G12V 0.76 KRAS_G12V 0.53 MAP2K3_WT 0.64 MAP2K4_WT.1 0.68 MAP3K5_WT 0.71

0.90 (in 3 replicates)

Mean pairwise

replicates

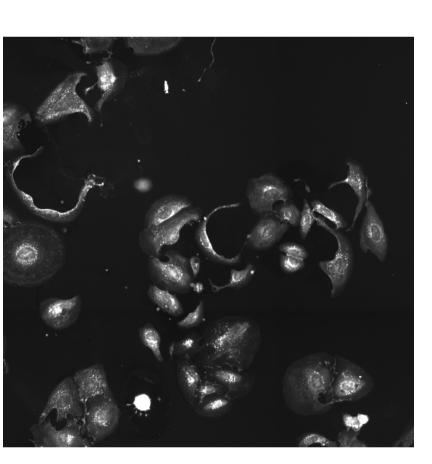
correlation of the

compound signature

(95th DMSO

replicate correlation

is 0.52)

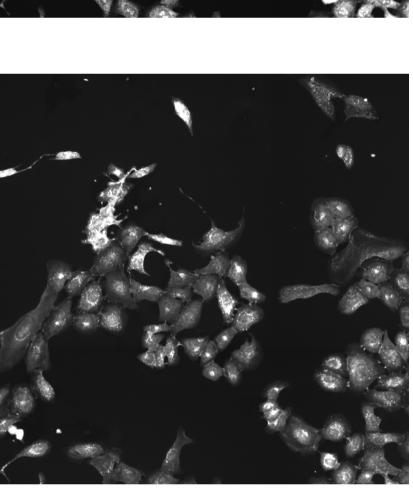


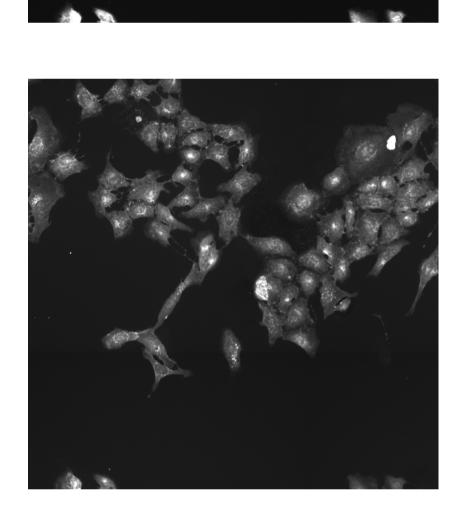
How similar is the compound signature to the gene clusters in

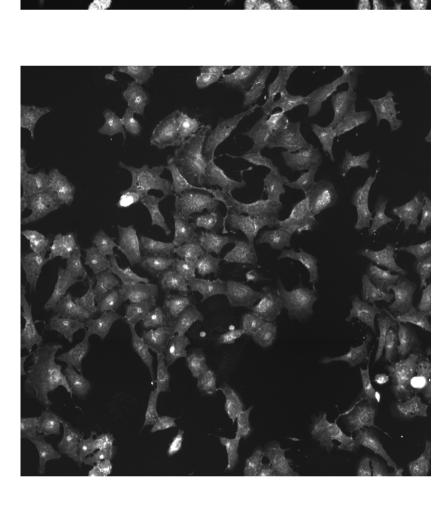
this experiment? (Yellow and red lines correspond to

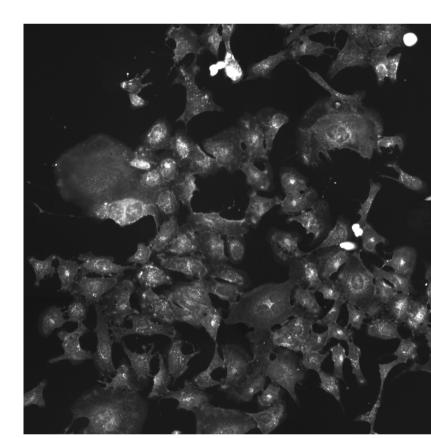
top/bottom 1st and 5th percentile DMSO correlation to all

the genes)









Compound IDs and common names (where available); blue/red colored box means the matching compound is positively/negatively correlated with the cluster	Chemic
BRD-A81850691-001-05-0 F1734-0091 AC1NJT6B MLS000697333 HMS2580B04 SMR000238009 ST50110788 PubChem CID: 4902407	

BRD-K40926874-001-06-3

PubChem CID: 6902822

T6051781

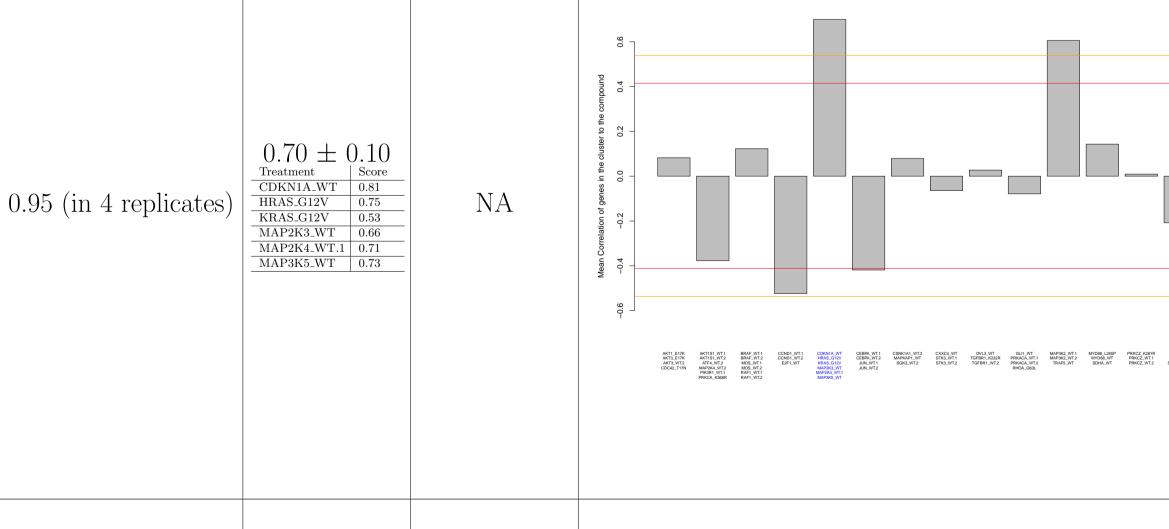
AC1OBTHD

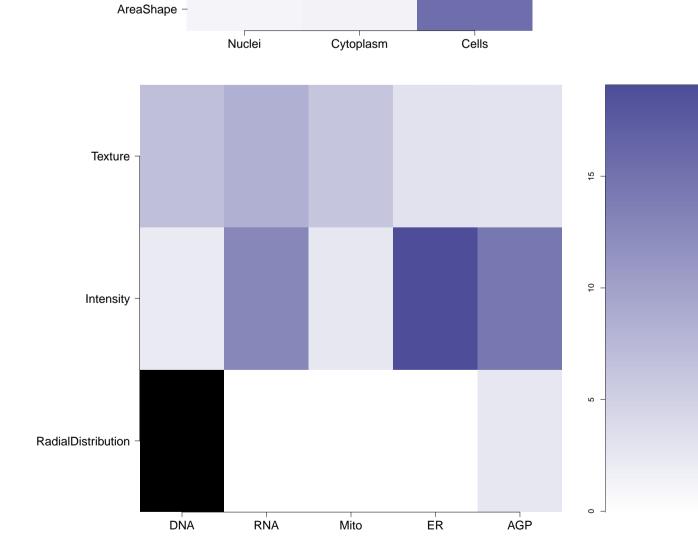
MLS000516321

ZINC12727563

SMR000372882

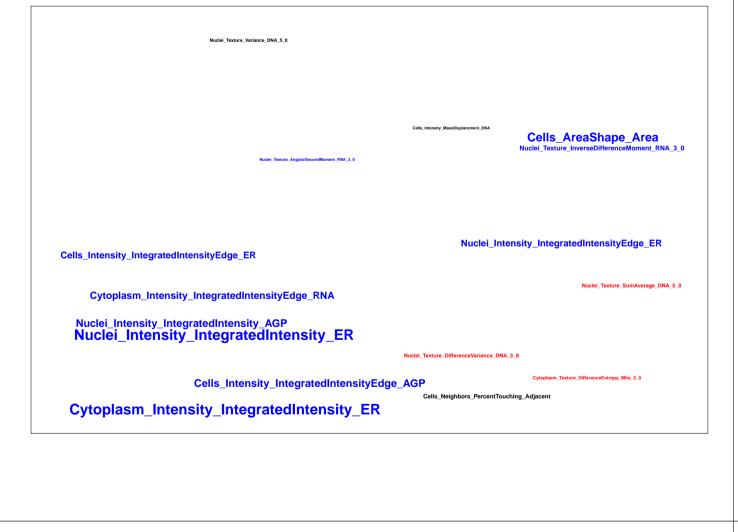
AGP





Common distinguishing feature categories in the compound and

genes in the cluster relative to the untreated samples

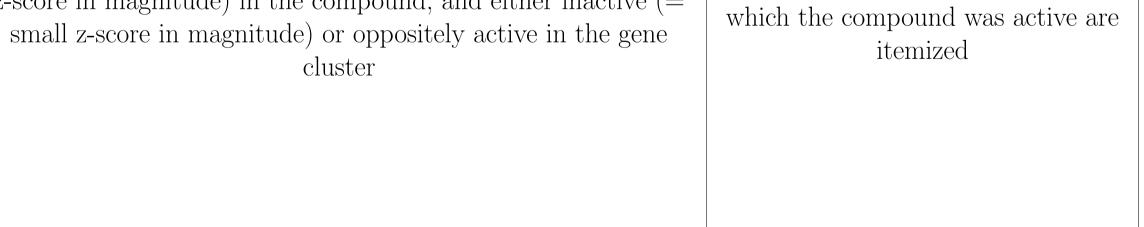


Distinguishing individual features for the compound relative to

untreated samples. Black means a mismatch; i.e. active (= high

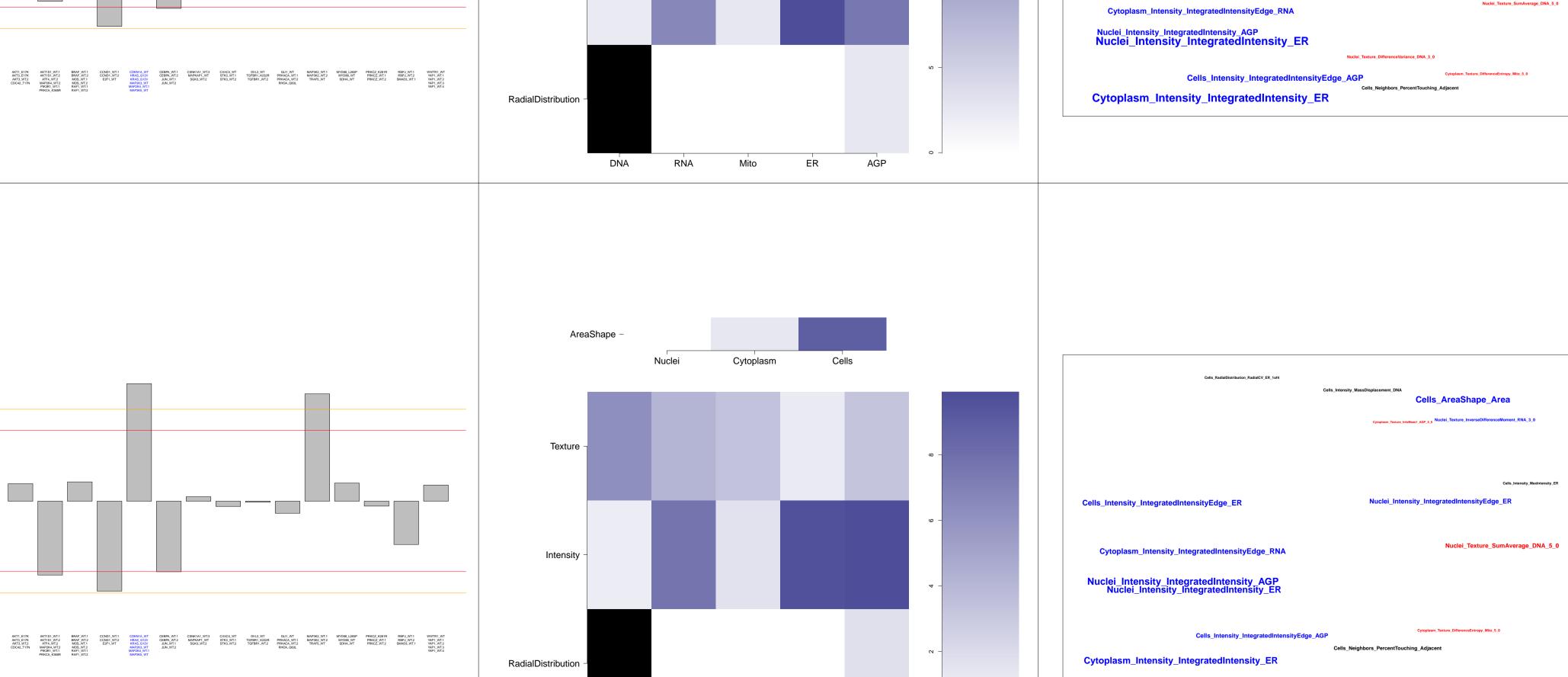
z-score in magnitude) in the compound, and either inactive (=

cluster



Number of PubChem assays in which

the compound was tested; assays in



- Total number of assays tested in: 639. Active in the following assays: • Fluorescence Cell-Free Homogeneous Primary HTS to Identify Inhibitors of the RanGTP-
- Importin-beta complex (AID 2216) • High Content Assay for Compounds that inhibit the Assembly of the Perinucleolar Compartment (AID 2417)
- Primary biochemical fluorescence polarizationbased high throughput screening assay to identify inhibitors of protein arginine methyltransferase 1 (PRMT1) (AID 652257)
- Total number of assays tested in: 636. Active in the following assays: • qHTS Assay for Inhibitors of Aldehyde Dehy-
- drogenase 1 (ALDH1A1) (AID 1030) • qHTS Assay for Inhibitors of Bacillus subtilis Sfp phosphopantetheinyl transferase (PPTase)
- VP16 counterscreen qHTS for inhibitors of ROR gamma transcriptional activity (AID

(AID 1490)

- qHTS for inhibitors of ROR gamma transcriptional activity (AID 2551)
- uHTS identification of small molecule inhibitors of tim10-1 yeast via a luminescent assay (AID 463190)
- uHTS identification of small molecule inhibitors of tim23-1 yeast via a luminescent assay (AID 463212)
- Single concentration confirmation of small molecule inhibitors of tim10-1 yeast via a lu-
- minescent assay (AID 463213) • Single concentration confirmation of small
- molecule inhibitors of tim23-1 yeast via a luminescent assay (AID 463218) • 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)
- qHTS Assay for Inhibitors of Histone Lysine Methyltransferase G9a (AID 504332)

