CONFIDENTIAL, contact the Imaging Platform to collaborate on the findings herein MAPK1\_WT.2 - in Canonical MAPK How similar is this gene to the other genes? 0.9 0.4 Correlation of the gene to the other genes 0.3 RBPJ\_WT.2 XBP1\_WT.2 CASP8\_WT.1 JUN\_WT.2 GLI1\_WT PPARGC1A\_1 PRKACG 0.0 TGFBR1\_K232R
STK3\_WT.2

KRAS\_WT.1

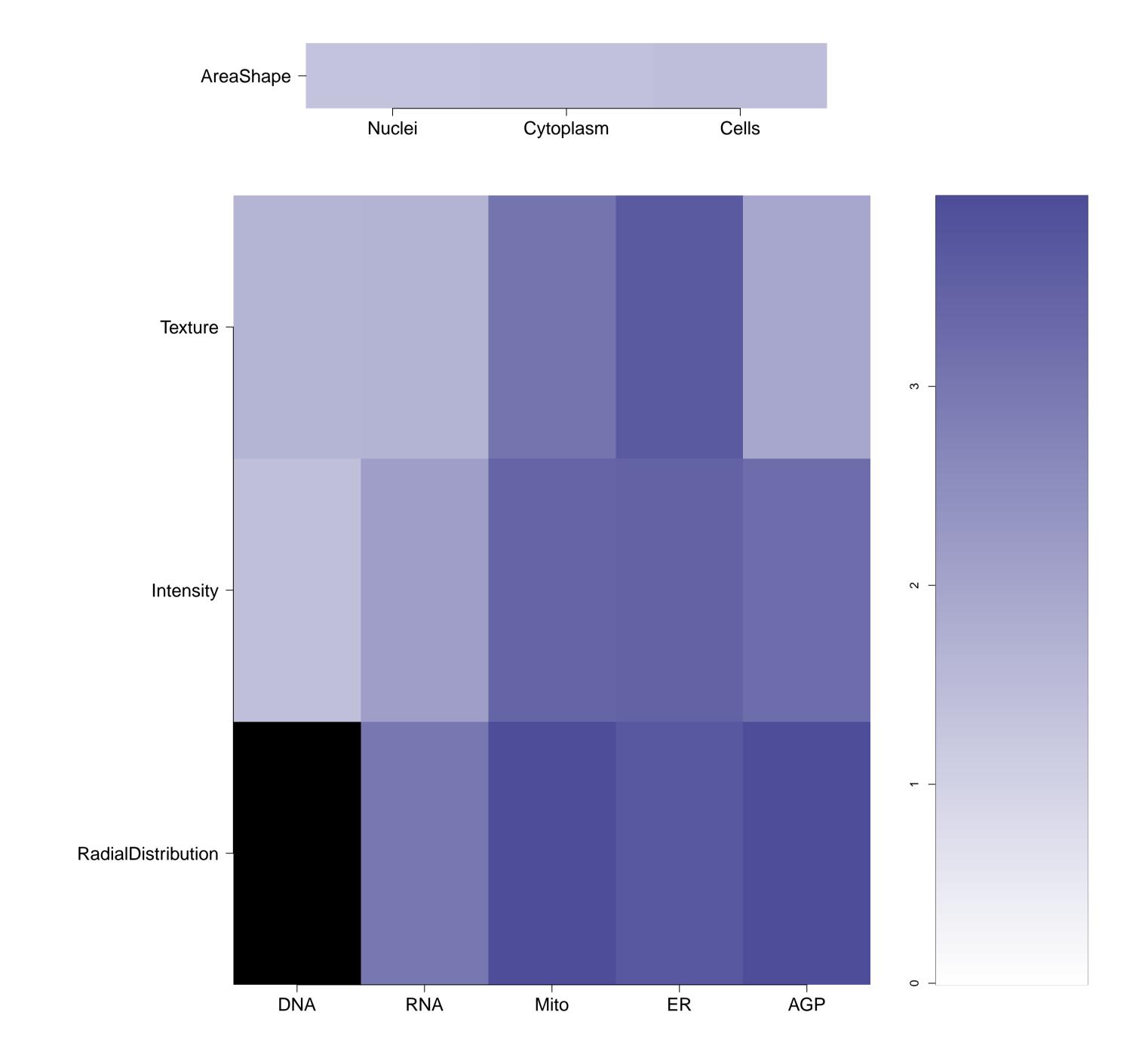
STK3\_WT.1

STK3\_WT.1

STK3\_WT.2

DVL3\_WT CSNK1E\_WT.2
AKT3\_WT.3
JAG1\_WT
DDIT4\_WT

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



Compound

rank when

scored

against the

gene using

L1000

profiling

How similar is the compound signature to the genes in this

experiment? (Yellow and red lines correspond to top/bottom

1st and 5th percentile DMSO correlation to all the genes)

Correlation

between

compound

the gene

Mean pairwise

replicates

correlation of the

compound signature

(95th DMSO

replicate correlation

is 0.52)

Chemical

structure

Mito

AGP

Compound IDs and

common names (where

available); blue/red colored

box means the matching

compound is

positively/negatively

correlated with the cluster

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

Distinguishing individual features for the compound relative to Number of PubChem assays in which

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

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

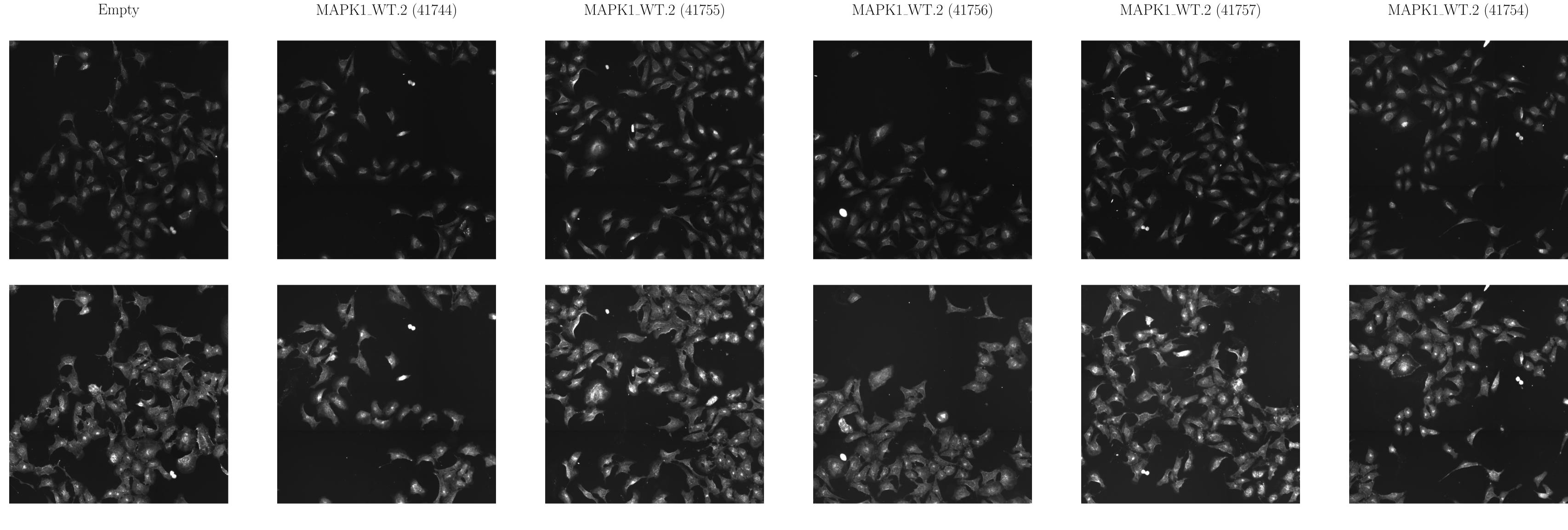
small z-score in magnitude) or oppositely active in the gene

the compound was tested; assays in

which the compound was active are

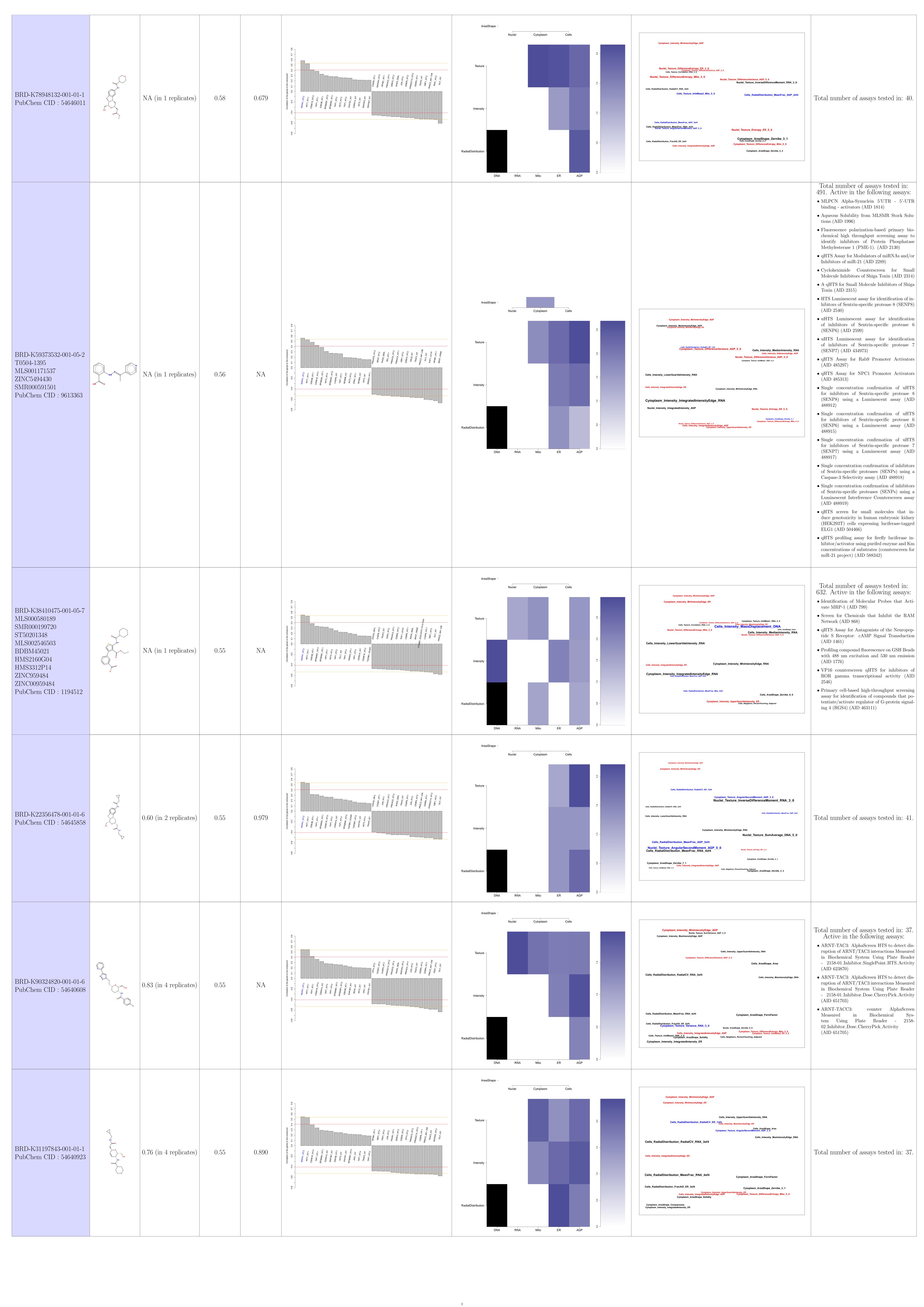
itemized





Common distinguishing feature categories in the compound and

the gene relative to the untreated samples



of Plasmodium falciparum line GB4 (AID 1816) (TRPC6) (AID 2553) (AID 2674)tentiate/activate regulator of G-protein signal-(AID 485317) BRD-K63675182-003-16-0 Flumazin Fluorofen Neoprin Nivoman 1098-60-8 MC 4703 NSC 14959 NSC 17473 SBB058191 AreaShape -CHEBI:9712 Cytoplasm SMR000058517 AC1L24JZ MLS000069672 MLS001148408 MLS002222277 Cells\_RadialDistribution\_RadialCV\_ER\_1of4 Cytoplasm\_Texture\_DifferenceVariance\_AGP\_5\_0 ATF4\_WT2
DKK1\_WT
CEBPA\_WT2
MAP2K4\_WT2
CEBPA\_WT.1
AKT1S1\_WT.1
CCND1\_WT.1
RELB\_WT
XBP1\_WT2
PRKAGG\_WT3
PRKAGG\_WT3
PRKAGG\_WT3
PRKAG\_WT2
COND1\_WT2
CDKZ\_WT2
PRKAGA\_K36BR
CCND1\_WT2
CDKZ\_WT2 T2896 SIGMA Cytoplasm\_Texture\_AngularSecondMoment\_AGP\_3\_0 Cytoplasm\_Texture\_InfoMeas1\_AGP\_5\_0 46976 RIEDEL Cells\_RadialDistribution\_MeanFrac\_AGP\_2of4 9E75N4A5HM 0.57 (in 4 replicates) 0.52Cells\_RadialDistribution\_RadialCV\_AGP\_2of4 46976 FLUKA Intensity · CTK8G3605 Cells\_RadialDistribution\_RadialCV\_AGP\_3of4 HMS1568K07 HMS1922G15 Cytoplasm\_AreaShape\_FormFactor HY-B0909 Tox21 111276 2767AH RadialDistribution -Cells\_Neighbors\_PercentTouching\_Adjacent NSC-14959 NSC-17473 NSC758387 ER CCG-213116 LP01146 NSC-758387 LS-105501 EU-0101146 ST51015135 602449) D00800 T 2896 PubChem CID: 66069 651633)• qHTS for induction of synthetic lethality in tuabsence of CPT (AID 686978) 720552)

Total number of assays tested in: 1138. Active in the following assays: • NCI In Vivo Anticancer Drug Screen. Data for tumor model P388 Leukemia (intraperitoneal) in B6D2F1 (BDF1) mice (AID 328)

• Human A549 Lung Tumor Cell Growth Inhibition Assay (AID 371)

• Fluorescent HTS Cytotoxicity/Cell viability assay (HPDE-C7 cells) (AID 430) • Fluorescent HTS Cytotoxicity/Cell viability as-

say (HPDE-C7K cells) (AID 431) • NFAT Signaling Pathway (AID 444) • Human SK-BR-3 Breast Tumor Cell Growth

Inhibition In a 24- Hour Assay (Pilot Screen) (AID 572)• Primary Cell Based High Throughput Screening Assay for Agonists of the 5-

Hydroxytryptamine Receptor Subtype 1E (5HT1E) (AID 574) • Human H69AR Lung Tumor Cell Growth Inhi-

bition Assay - 86K Screen (AID 598)

• Fluorescent HTS Cytotoxicity/Cell viability assay (HT1080 cells) (AID 620)

• Discovery of novel allosteric modulators of the M1 muscarinic receptor: Antagonist Primary Screen (AID 628)

• Discovery of novel allosteric modulators of the M1 muscarinic receptor: Antagonist Confirmation Screen (AID 677)

• Human Lung Fibroblast Proliferation Assay (AID 719)

• Cell Growth High Content Screening Assay of Human HT29 Colon Tumor Cells (48 Hour Treatment Protocol) (AID 771)

• Discovery of novel allosteric modulators of the M1 muscarinic receptor: Antagonist Dose-Response Assay (AID 859)

• Discovery of novel allosteric modulators of the M1 muscarinic receptor: Antagonist Dose-

Response Counterscreen (AID 860) • Chemical Genetic Screen to Identify Inhibitors of Mitochondrial Fusion - Primary Screen (AID

• Multiplex HTS Assay for Inhibitors of MEK Kinase PB1 Domains, specifically MEK5 binding

to MEK Kinase 2 Wildtype (AID 1531) • Primary cell-based high-throughput screening assay for identification of compounds that

inhibit/block inward-rectifying potassium ion channel Kir2.1 (AID 1672)

• Identification of Novel Modulators of Cl- dependent Transport Process via HTS: Secondary Assay 3 with KCC2 cells (AID 1714)

• qHTS for differential inhibitors of proliferation of Plasmodium falciparum line 7G8 (AID 1815) • qHTS for differential inhibitors of proliferation

• qHTS for differential inhibitors of proliferation of Plasmodium falciparum line D10 (AID 1877) • qHTS for differential inhibitors of proliferation of Plasmodium falciparum line Dd2 (AID 1882) • qHTS for differential inhibitors of proliferation

of Plasmodium falciparum line W2 (AID 1883) • qHTS for differential inhibitors of proliferation of Plasmodium falciparum line HB3 (AID 1886) • A cytotoxicity screen of small molecule inhibitors of the PhoP regulon in Salmonella ty-

phi identified in the primary screen (AID 2252) • A counter screen for small molecule screen for inhibitors of the PhoP regulon in Salmonella typhi (AID 2384)

• High Content Assay for Compounds that inhibit the Assembly of the Perinucleolar Com-

partment (AID 2417) • High throughput screening of inhibitors of transient receptor potential cation channel C6

• HTS for Identification of VLA-4 Allosteric Modulators from Validation Compound Set.

• Confirmation dose response assay for compounds that inhibit transient receptor potential cation channel C6 (TRPC6). (AID 2696) • Second specificity screen against TRPC4 for

compounds that inhibit transient receptor potential cation channel C6 (TRPC6) (AID 2776) • Specificity screen against TRPC4 for com-

pounds that inhibit transient receptor potential cation channel C6 (TRPC6) (AID 2777) • Primary cell-based high-throughput screening assay for identification of compounds that po-

ing 4 (RGS4) (AID 463111) • 96-well format Chlamydomonas reinhardtii Algae Gravitaxis Assay to measure the difference in the absorbance between the small compact plug of WT swimming algae versus the MUT

algae lacking cilia. (AID 463189) • uHTS identification of small molecule inhibitors of tim10-1 yeast via a luminescent as-

say (AID 463190) • 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 • HTS Assay for Allosteric Antagonists of the

Human D2 Dopamine Receptor: Primary Screen for Antagonists (AID 485344)

• uHTS Fluorescent assay for identification of inhibitors of Apaf-1 (AID 489030) • qHTS Assay for Inhibitors of BAZ2B (AID

• Antagonist of Human D 1 Dopamine Receptor: qHTS (AID 504652)

• Allosteric Agonists of the Human D1 Dopamine Receptor: qHTS (AID 504660)

• qHTS profiling for inhibitors of Plasmodium falciparum proliferation (AID 504749) • Primary qHTS for delayed death inhibitors of

the malarial parasite plastid, 96 hour incubation (AID 504834) • Antiplasmodial activity against Plasmodium

falciparum 3D7 after 72 hrs by SYBR green assay (AID 524790) • Antiplasmodial activity against Plasmodium

falciparum 7G8 after 72 hrs by SYBR green assay (AID 524791)

• Antiplasmodial activity against Plasmodium falciparum D10 after 72 hrs by SYBR green assay (AID 524792)

• Antiplasmodial activity against Plasmodium falciparum Dd2 after 72 hrs by SYBR green assay (AID 524793)

• Antiplasmodial activity against Plasmodium falciparum GB4 after 72 hrs by SYBR green assay (AID 524794)

• Antiplasmodial activity against Plasmodium falciparum HB3 after 72 hrs by SYBR green assay (AID 524795)

• Antiplasmodial activity against Plasmodium falciparum W2 after 72 hrs by SYBR green assay (AID 524796)

• qHTS for Inhibitors of binding or entry into cells for Lassa Virus (AID 540256)

• qHTS for inhibitors of binding or entry into cells for Marburg Virus (AID 540276) • qHTS Assay for Small Molecule Inhibitors of the Human hERG Channel Activity (AID

• Fluorescence-based cell-based primary high throughput screening assay to identify antag-

onists of the human M1 muscarinic receptor

(CHRM1) (AID 588852) • uHTS identification of small molecule inhibitors of the mitochondrial permeability tran-

sition pore via an absorbance assay (AID • Fluorescence-based cell-based primary high

throughput screening assay to identify antagonists of the human cholinergic receptor, mus-

carinic 5 (CHRM5) (AID 624040) • Fluorescence-based cell-based primary high

throughput screening assay to identify antagonists of the human cholinergic receptor, muscarinic 4 (CHRM4) (AID 624125)

• 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

• qHTS assay for small molecule agonists of the p53 signaling pathway (AID 651631)

• qHTS assay for small molecule agonists of the p53 signaling pathway - cell viability (AID

• qHTS of D3 Dopamine Receptor Antagonist:

qHTS (AID 652054)

mor cells producing 2HG: qHTS for the HT-1080-NT fibrosarcoma cell line (AID 686970) • qHTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TDP1): qHTS in cells in

• qHTS for Inhibitors of binding or entry into cells for Marburg Virus (AID 720532) • qHTS assay for small molecule agonists of

the p53 signaling pathway: Summary (AID

