A full cycle anti-viral drug screen identifies a clinical compound against adenovirus infection

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Human adenoviruses (HAdVs) are fatal to immune-suppressed people, but no effective anti-HAdV therapy is available. Here, we present a novel image-based high-throughput screening (HTS) platform, which scores the full viral replication cycle from virus entry to dissemination of progeny. We analysed 1,280 small molecular compounds of the Prestwick Chemical Library (PCL) for interference with HAdV-C2 infection in a quadruplicate blinded format, followed by robust image analyses, and hit identification. We present the entire set of image-based screening data including all the images, and the image analysis and data processing pipelines, as deposited at the Image Data repository (IDR) [1] (project number #pending). We identified Nelfinavir mesylate as an inhibitor of HAdV plaque formation, in agreement with the previous notion that Nelfinavir is ineffective in single round HAdV infection assays. Nelfinavir has been FDA-approved for anti-retroviral therapy in humans. Our results underscore the power of image-based multi-round infection assays in identifying viral inhibitors with clinical potential.

Background & Summary:

Human adenoviruses (HAdV) predominantly cause diseases of the respiratory and gastrointestinal tracts. They are a significant cause of acute human disease with morbidity and mortality, especially for immuno-compromised patients [2,3] as indicated by a recent outbreak in the USA killing 12 children. Surprisingly, a recent case of HAdV-C2 caused meningoencephalitis was also reported in a middle-aged woman in the US [4]. HAdV have a high prevalence [5–8] and are broadly used as gene therapy vectors [9] and oncolytic viruses [10,11]. The high seroprevalence of HAdV-C2/5 [12] underlines that HAdV infections are asymptomatic in healthy individuals, but HAdV persist in mucosal lymphocytes, and thereby pose a severe risk for immunosuppressed patients undergoing stem cell transplantation [13].

More than 100 HAdV genotypes have been formally approved [14] and are grouped into seven species based on hemagglutination assay and genome sequences [15]. They exhibit a broad range of tissue tropism, including the respiratory and gastrointestinal tracts, the eye, the kidney, the urogenital tracts and blood cells. While species A, F and G target the gastrointestinal tract, HAdV-B, C and E cause infections of the respiratory tract, and conjunctivitis is mostly associated with species B and D, but also C types. HAdV-B show the broadest spectrum of tropisms, also infecting the kidney and hematopoietic system [7,13].

HAdV is a non-enveloped virus with a double-stranded DNA genome of ~36 kbp tightly packaged into an icosahedral capsid of about 90 nm in diameter [16,17]. The best-studied HAdV are HAdV-C2/5 (species C, type 2 and 5), which are very closely related to each other. HAdV enter cells by receptor mediated endocytosis, penetrate the endosomal membrane by the activation of a viral lytic machinery, and shed virion proteins in a stepwise manner, until they arrive at the nuclear membrane, where they uncoat and release their genome to the nucleus [18,19]. In the nucleus the viral genome gives rise to the immediate early viral mRNA encoding the E1A protein which then transactivates all the subviral promoters and is key to give rise to lytic infection and maintains viral persistence in presence of the innate immune regulator interferon [20]. Mature HAdV progeny is known to be released by cell lysis upon rupture of the nuclear envelope and the plasma membrane, giving rise to cell-free virions [21–23].

To this day, no effective anti-viral therapy is available against HAdV infection For example, the nucleoside analogue Cidofovir is the current standard of care for the treatment of HAdV infections, albeit with poor clinical efficacy [7]. Cidofovir is a general inhibitor of viral DNA polymerases and impairs the replication of viral DNA [24]. The pre-clinical development of novel anti-HAdV agents has been limited by the shortage of a suitable small animal model, although Syrian Hamsters support HAdV-C progeny production, albeit in limited amounts [25].

Here, we developed a data-based approach to identify novel inhibitors of HAdV infection by testing the Prestwick Chemical Library (PCL) to inhibit HAdV-C2 infection in cell cultures. The PCL is commercially available, and comprises a library of 1,280 off-patent FDA-approved small molecules (listed in Supplementary Table 1) covering significant pharmaceutical range. PCL has been successfully used to identify many compounds for repurposing applications ranging from antimicrobial agents[26] to anticancer candidates [27]. For a full list of publications, see [28]. We performed a phenotypic screen for HAdV-C2 infection, as outlined in (Figure 1A, 1B). We took advantage of automated fluorescence microscopy and image-based scoring of the progression of multi-round infections using Plaque2.0 software [29]. This high-throughput screening (HTS) modality was carried out at a 384-well plate format. For representative images, see Figure 1C.

We demonstrate robust imaging methodology, image analysis and data processing routines as concluded from parallel procedures in two teams at independent institutions, the Biomolecular Screening Facility at Ecole Polytechnique Fédérale de Lausanne (EPFL) and the Department of Molecular Life Sciences at University of Zurich (UZH). To score the infection phenotypes, we used five infection assay features obtained from microscopy: the number of nuclei, the number of infected nuclei, the infection index as calculated from the total nuclei and the infected cells, the number of plaques (areas of multi-round infection foci originating from a single infected host cell) and the integrated viral infection marker, in this case the green fluorescence protein (GFP) intensity. All data is available at the Image Data repository (IDR) [1] (project number #pending). The structure of the repository is outlined in Figure 2. Raw and scored infection phenotype features are shown for UZH and EPFL analyses (Supplementary Tables 2 and 3, and Supplementary Tables 4 and 5, respectively). Rigorous assay development ensured a high assay quality as indicated in Figure 3 and by mean Z'-scores of 0.52 for the number of plaques (Table 1). The

screening was performed in four biological replicates at high reproducibility, see Figure 4 and Table 2. We further excluded those PCL compounds that showed significant toxicity in the absence of infection (Table 3 and Figure 5). Imaging, image analysis and scoring by the two independent teams yielded well correlated scores, as depicted in Figure 6.

Our data indicate a high significance of the identified top hit, Nelfinavir mesylate (Figure 1D and 6). We confirmed the efficacy of Nelfinavir as an inhibitor of HAdV infection by biological follow-up studies (submission in preparation).

Methods:

Virus

HAdV-C2-dE3B virus was produced as described [21]. In brief, the virus was generated by exchange of the viral E3B genome region with a reporter cassette harbouring the enhanced green fluorescent protein (GFP) under the immediate early Cytomegalovirus (CMV) promoter. The virus was grown in A549 cells and purified by double caesium chloride gradient centrifugation [30]. Aliquots supplemented with 10% glycerol (v/v) were stored at -80°C. HAdV-C2-dE3B was found to be homogeneous by SDS-PAGE and negative-stain analyses by transmission electron microscopy.

Cell line

A549 (human adenocarcinomic alveolar basal epithelium) cells were obtained from the American Type Culture Collection (ATCC), Manassas, USA. The cells were maintained in full medium: high glucose Dulbecco Modified Eagle Medium (DMEM; Thermo Fisher Scientific, Waltham, USA) containing 7.5% fetal bovine serum (FBS, Invitrogen, Carlsbad, USA), 1% L-glutamine (Sigma-Aldrich, St. Louis, USA) and 1% penicillin streptomycin (Sigma-Aldrich, St. Louis, USA) and subcultured following PBS washing and trypsinisation (Trypsin-EDTA, Sigma-Aldrich, St. Louis, USA) weekly. Cell cultures were grown at standard conditions (37°C, 5% CO_2, 95% humidity) and passage number limited to 20.

Preparation of pre plates

10 µl 0.0125% DMSO in PBS was spotted on all 384 wells each of imaging-compatible 384-well plates (Matrix plates #4332, Thermo Fisher Scientific, Waltham, USA) using a Matrix WellMate dispenser and normal bore Matrix WellMate tubing cartridges (Thermo Fisher Scientific, Waltham, USA). Plates were sealed and stored at -20°C.

Blinding

The PCL compound arrangement as spotted by EPFL across the 4 plates A - D comprising each screening set replicate 1 - 4 was blinded and replaced by UZH with internal identifier (Supplementary Tables 2 and 3, *compoundIdentifier* 1 to 1280). The identity of the compounds was only disclosed (Table 3 and Supplementary Tables 1 and 2, *PCL_ID* Prestw-1 to Prestw-1804 and *compoundName*) after the screening process including hit filtering was finished.

Compounds

The PCL was obtained from Prestwick Chemical (Illkirch, France). 3′-Deoxy-3′-fluorothymidine (DFT, CAS number 25526-93-6) was obtained from Toronto Research Chemical, North York, Canada. All compounds were dissolved in Dimethyl sulfoxide (DMSO, Sigma-Aldrich, St. Louis, USA) at a final stock concentration of 10 mM and stored at -20°C.

Presto-blue toxicity assay

Toxicity of the PCL chemical compounds on A549 in absence of infection was tested using compound concentrations, treatment timing and seeding cell numbers corresponding to the screening protocol, and using the Presto Blue Cell Viability reagent (Thermo Fisher Scientific, Waltham, USA). Briefly, following 3.5-day continuous treatment of A549 cells, 10% final PrestoBlue was added to each well and incubated for 1 h at standard cell incubation conditions. Fluorescence intensity (bottom-read) was then measured using a multi-well plate reader (Tecan Infinite F500, Tecan, Männedorf, Switzerland) with excitation at 560/10 nm, emission at 590/10 nm at a fixed gain. Doxorubicin hydrochloride (Prestw-438, Prestwick Chemical, Illkirch, France) was used as a positive control for cytotoxicity, at a final concentration of 10 µM, and the corresponding volume of DMSO was used as a negative control. The full PCL library was tested on duplicated plates. The EPFL-BSF in-house Laboratory Information Management System (LIMS) was used for data processing and statistical validation. First, raw PrestoBlue readings were normalized per plate to negative control values at 0 and positive controls at 1. Then, the normalized values of the duplicates were averaged. Assay quality was assessed for each plate through the Z' factor calculation. Compounds were considered toxic hits when the normalized value for all replicates was higher than the average + 3σ (standard deviation, SD) of the DMSO negative control for the corresponding plate. Scores and score SD were then calculated for hit compounds by averaging normalized value for all replicates.

Preparation of Z' and screening plates

10 nl of 10 mM PCL compounds, the nucleoside analogue DFT positive control (all dissolved in DMSO) and DMSO only as negative control were pre-spotted on imaging-compatible 384-well plates (Falcon plates, Corning Inc., New York, USA) using an Echo acoustic liquid handling system (Labcyte, San Jose, USA) by the EPFL-BSF, sealed and stored at -20°C. Z' plates consisted of 192 technical replicates of positive and negative control, each, per 384-well plate. Each screening plate set consisted of 4 plates A to D. Each screening plate consisted of 32 technical replicates of positive and negative control, each, and 320 single technical replicate PCL compounds.

Wet-lab screening pipeline

The screening was performed in four independent biological replicates. Wet-lab liquid handling was performed using a Matrix WellMate dispenser and Matrix WellMate tubing cartridges (Thermo Fisher Scientific, Waltham, USA). Prior to usage, tubings were rinsed with 125 ml autoclaved ddH_2O followed by 125 ml autoclaved PBS. Pre-spotted compound plates were thawed at room temperature (RT) for 30 min, briefly centrifuged before compounds were dissolved in 10 µl/ well PBS. 4,000 A549 cells/ well in 60 µl full medium were seeded onto the compounds using standard bore tubing cartridges. Following cell adhesion over night, the cells are inoculated with $1.77*10^5$

genome equivalents per well of HAdV-C2-dE3B in 10 µl full media using bovine serum albumin (BSA, cell-culture grade, Sigma-Aldrich, St. Louis, USA)-blocked small bore tubing cartridges. Final compound concentration was 1.25 µM at 0.0125% DMSO. Infection was allowed to progress over multiple infection rounds for 72 h giving rise to foci of infected cells originating from a single first round infected cell termed plaque. Cells were fixed for 1 h at RT by addition of 26.6 µL 16% PFA and 4 µg/ml Hoechst 33342 (Sigma-Aldrich, St. Louis, USA) in PBS using standard bore tubing cartridges. Cells were washed 3 times with PBS before PBS supplemented with 0.02% N_3 was added and plates were sealed for long-term storage at 4°C. Following usage, tubings were rinse with 125 ml autoclaved ddH_2O followed by 125 ml autoclaved PBS and autoclaved for re-usage.

Imaging

Nuclei (DAPI channel) and viral GFP (FITC channel) were imaged on two devices. At UZH, plates were imaged on an IXM-C automated high-throughput fluorescence microscope (Molecular Devices, San Jose, USA) using MetaXpress (version 6.2, Molecular Devices, San Jose, USA) and a 4x air objective (Nikon S Fluor, 0.20 NA, 15.5 mm WD, Nikon Instruments, Minato, Japan) at widefield mode. Image size $2{,}048^2$ px at 1.72 µm/px resolution acquired on an Andor sCMOS camera (Oxford Instruments, Abingdon, UK). Exposure times: DAPI 150 ms, FITC 20 ms. At EPFL, images were acquired on a IN Cell 2200 automated high-throughput florescence microscope (GE Healthcare, Chicago, USA) using IN Cell Analyzer (version 6.2, GE Healthcare, Chicago, USA) and a 4x air objective (Nikon Plan Apo, 0.20 NA, 15.7 mm WD, Nikon Instruments, Minato, Japan) at widefield mode. Image size $2{,}048^2$ px at 1.625 µm/px resolution acquired on an Andor sCMOS camera. Exposure times: DAPI 300 ms, FITC 40 ms.

Image analysis

The infection phenotype for each well was quantified by Plaque2.0 [29] (https://github.com/plaque2/matlab/tree/antivir) via five read-outs: number of nuclei, number of infected nuclei, the ratio between infected and total nuclei referred to as infection index, number of multi-round infection foci termed plaques (plaque forming units, pfu) and the integrated viral transgenic GFP intensity. Plaque2.0 parameters were optimized independently at UZH and EPFL for the data acquired at the respective institution.

Z'-score calculation

The Z'-score was computed using R version 3.3.2 [31] according to Equation (1)

$$Z' = 1 - \frac{(3\sigma_+ + 3\sigma_-)}{|\mu_+ - \mu_-|} \quad (1)$$

where σ_+ is the SD of the positive control, σ_- is the SD of the negative control, μ_+ the mean of the positive control and μ_- the mean of the negative control.

Screening data processing

Plaque2.0 results were further independently processed and filtered. At UZH, results were processed in R version 3.3.2 [31], EPFL used KNIME version 3.4.0 [32] as well as the EPFL-BSF in-house LIMS. Mean infection scores over the Plaque2.0 read-outs of the four biological replicates of each PCL compound and the 16 biological replicates containing each 16 technical replicates

of positive and negative control, each, were calculated. Each compound's scores were normalized by the mean score of the DMSO negative control of the respective plate. Only non-toxic, effective PCL compounds were considered as HAdV inhibitor candidates. Non-toxic compounds were filtered by applying an inclusive μ_+ (mean of the negative control) $\pm 2\sigma$ (SD of the negative control) threshold for number of nuclei. Efficacy was filtered by applying an excluding $\mu_+ \pm 3\sigma$ threshold for the infection scores (number of infected nuclei, infection index, number of plaques or integrated GFP intensity).

Data Records:

Data structure and repository

The HAdV screening data comprise the information collected during assay development, including stability, quality and the PCL screening itself. The latter two have been imaged on two different microscopes. We provide the parameters used for Plaque2.0 image analysis, and the code for the subsequent hit filtering in R. The data structure as available at the IDR [1] , project number #pending) is structures as outlined in Figure 2.

Data sets and file types

The provided data consists of four data sets 1 to 4.

- *1-prePlates* contains layouts (.csv), images (.tif), Plaque2.0 image analysis parameters (.mat) and results (.csv) for the assay stability test plates performed at UZH prior to Z' plates (*preZ*) and the AntiVir screen (*preScreen*).
- *2-ZPlates* contains layouts (.csv), images (.tif), Plaque2.0 image analysis parameters (.mat) and results (.csv) for the two Z' plates a and b as imaged and analysed at (*Data_UZH*) and EPFL (*Data_EPFL*).
- *3-Screen* contains layouts (.csv), images (.tif), Plaque2.0 image analysis parameters (.mat) and results (.csv) for the 16 screening plates (4 biological replicas 1 - 4 each consisting of a set of 4 plates A - D) as imaged and analysed at UZH (*Data_UZH*) and EPFL (*Data_EPFL*). Moreover, *Analysis* contains the Plaque2.0 batch processing (*AntiVir_batchprocessing.m*) and hit filtering pipeline (*AntiVir_hitfiltering.R*) used by UZH.
- *4-Toxicity* contains the Presto-blue raw results (.csv) for toxicity in absence of infection.

Technical Validation:

Assay stability

The wet-lab screening pipeline was optimized regarding liquid handling, cell seeding, virus inoculum, positive and negative control, time line, imaging and image analysis to ensure high assay stability and reproducibility. Furthermore, all compounds, especially media and supplements, the BSA for tubing saturation, PFA- and Hoechst-supplemented fixative were prepared as large batch from a single LOT and stored as single-use aliquots. Assay stability with respect to cell and infection phenotype was tested following the established wet-lab, imaging and image analysis pipeline prior to every experiment on pre plates. Since the solvent control had already been spotted in 10 µl PBS, no further PBS was added prior to cell seeding. If infection

scores were found to be low due to limited stability of viral stocks, the virus stock dilution in the subsequent experiment was decreased.

Independent analysis

Imaging, image analysis and screening data processing was performed by two independent research teams from two independent institutions at UZH and EPFL. Both dry-lab pipelines confirmed the high assay quality (Table 1). As summarized in Figure 6 left panel, both scores are strongly correlated with R^2 between 0.6870 - 0.9870. Both approaches yielded identical top scored compounds (Figure 6 right panel), of which Prestw-1764, Nelfinavir mesylate, was the top hit.

Assay quality determination: Z'-score

The assay's effect size was assessed following the established wet-lab, imaging and image analysis pipeline for two independently performed Z' plates (Table 1 and Figure 2). 3σ Z'-scores of *numberOfInfectedNuclei*, *infectionIndex* and *numberOfPlaques* were in the range of 0.30 to 0.57 and thus good to excellent. *totalVirusIntensity* (Z' scores between -0.07 to 0.08) are not suitable to identify HAdV infection inhibitors, while *numberOfNuclei* (Z' scores between -1.11 to -8.10) is not relevant either. Additionally, the Z'-scores were determined for each of the 16 screening plates (Table 2 and Figure 3). 3σ Z'-scores of *numberOfInfectedNuclei*, *infectionIndex* and *numberOfPlaques* were again good to excellent (0.27 to 0.57).

<u>Usage Notes:</u>

Infection scoring using the Plaque2.0 GUI

A detailed manual for Plaque2.0-based infection phenotype scoring is available at http://plaque2.github.io/. No MATLAB license is necessary.

Five parameters were quantified for each well: the number of nuclei (*numberOfNuclei*), number of infected nuclei (*numberOfInfectedNuclei*), the ratio between number of infected and total nuclei (*infectionIndex*), the number of multi-round infection foci termed plaques (*numberOfPlaques*) and the extend of viral GFP reporter expression as integrated GFP intensity *totalVirusIntensity*).

To analyse the HAdV screening data by Plaque2.0, the following setting should be used:
<u>Input/Output:</u>
Processing Folder: Path to folder containing the images (e.g. *ScreenA /3-Screen/Data_EPFL/Screen/ BSF018292_1A*).
filename pattern Data_UZH: *.* (?<wellName>[A-Z][0-9]*)_(?<channelName>w[0-9]*).TIF*
filename pattern Data_EPFL: *.* (?<wellName>[A-Z] - [0-9]+)[(]fld 1 wv (?<channel>[A-Z]{4}) .*.tif*
Plate name: Name of the plate to be analysed (e.g. *BSF018292_1A*)
Result Output Folder: Path to the results folder in the respective Data folder (e.g. *ScreenA/3-Screen/Data_EPFL/Results*).
<u>Stitch:</u> Stitching of the images is not necessary, since every 384-well is imaged in a single site. Do not activate the tab.
<u>Mask:</u>

Custom Mask File: Path to the manually defined mask file (e.g. *ScreenA/3-Screen/Data_UZH/Parameters*).

Monolayer:

Channel: Nuclei were imaged in channel 1.

Plaque:

Channel: Viral GFP reporter signal was imaged in channel 2.

Code Availability:

Plaque2.0 batch image analysis for infection scoring

The MATLAB (version R2016b, The MathWorks, Natick, USA) script *AntiVir_batchprocessing.m* used by UZH for image analysis is provided at IDR #pending under *ScreenA/3-Screen/Analysis*. It is based on the Plaque2.0 software available on GitHub: https://github.com/plaque2/matlab under GPLv3 open source license.

To batch analyse the HAdV screening data by Plaque2.0, fork or download the Plaque2.0 AntiVir code from GitHub: https://github.com/plaque2/matlab/tree/antivir. Place the *AntiVir_batchprocessing.m* file from *ScreenA/3-Screen/Analysis* into the *Plaque2/matlab* folder and follow the instructions in *AntiVir_batchprocessing.m*. A MATLAB license is required.

Hit filtering using R

The R[31] (version 3.6.1 (2019-07-05)) script *AntiVir_hitfiltering* used by UZH for data processing and hit filtering is provided at IDR #pending under *ScreenA/3-Screen/Analysis*.

Acknowledgements, Author Contributions & Competing Interests

Author Contributions:

UFG, VA, AY conceived the screening idea. FG designed the experiments, and with UFG coordinated the project. FK prepared the PCL-spotted plates. FG and RW performed the experiments. FG and FK acquired the data. FG and VA analysed the imaging data. LM and FG processed the data. GT organized and supervised the screening project at the EPFL-BSF. FG, FK and UFG wrote manuscript, with input from all the co-authors.

Acknowledgements:

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Competing Interests:

The authors declare no conflict of interest.

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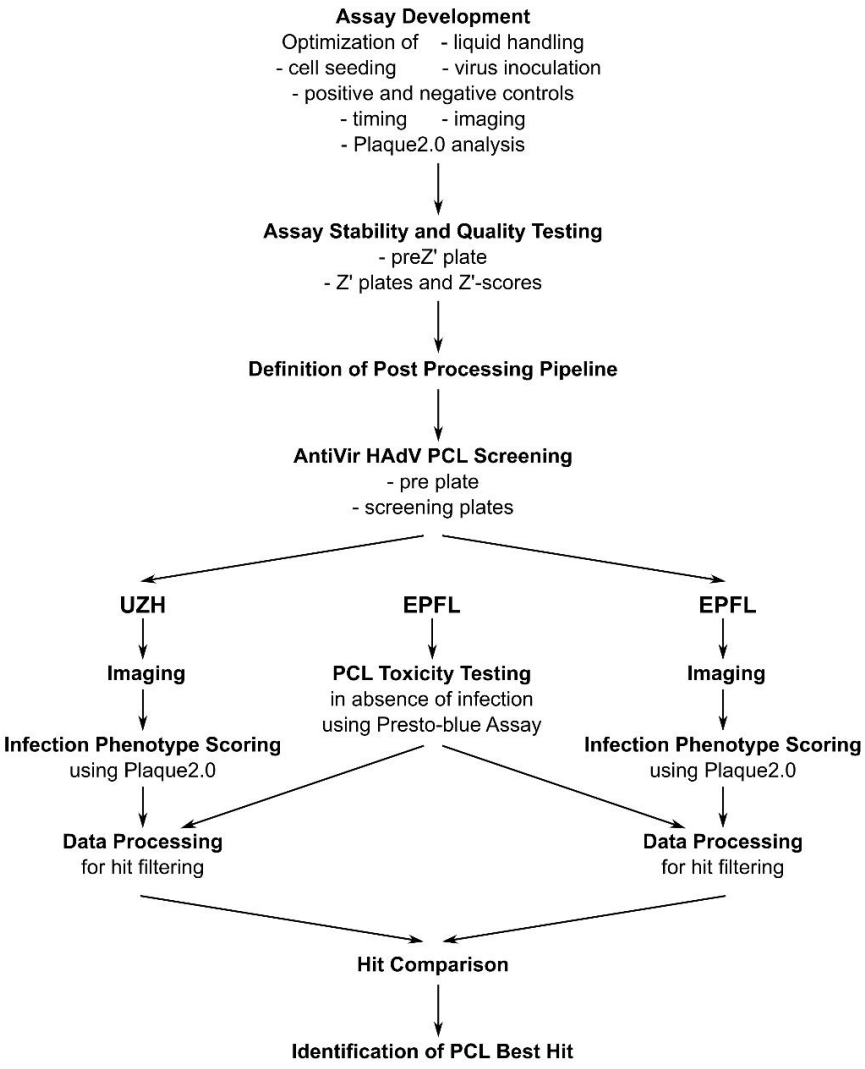
Abbreviations:

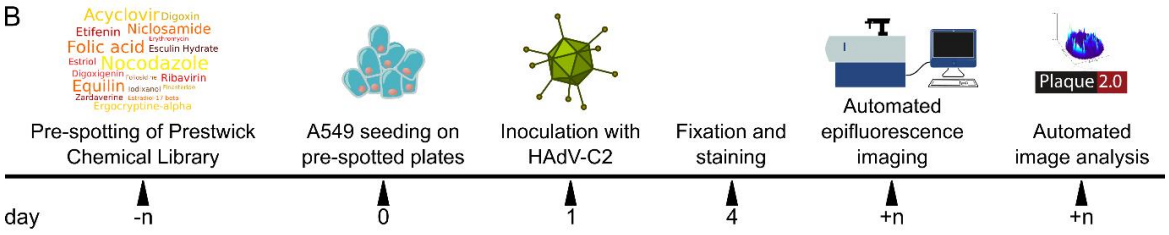
BSA, bovine serum albumin;
BSF, Biomolecular Screening Facility;
CMV, Cytomegalovirus;
DFT, 3′-Deoxy-3′-fluorothymidine;
DMEM, Dulbecco Modified Eagle medium;
DMSO, Dimethyl sulfoxide;
dpi, days post infection;
EPFL, Ecole Polytechnique Fédérale de Lausanne;
FBS, fetal bovine serum;
GFP, green fluorescent protein;
HAdV, Human adenovirus;
hpi, hours post infection;
HTS, high-throughput screening;
IDR, The Image Data Resource;
LIMS, Laboratory Information Management System;
LUT, Look up table;
PCL, Prestwick Chemical Library;
PFA, para-formaldehyde;
pfu, plaque forming units;
RT, room temperature;
SE, standard error;
SD, standard deviation;
UZH, University of Zurich

Figures & Tables

A



B



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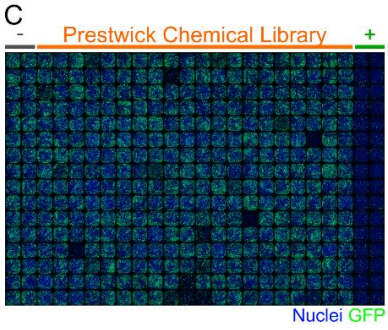

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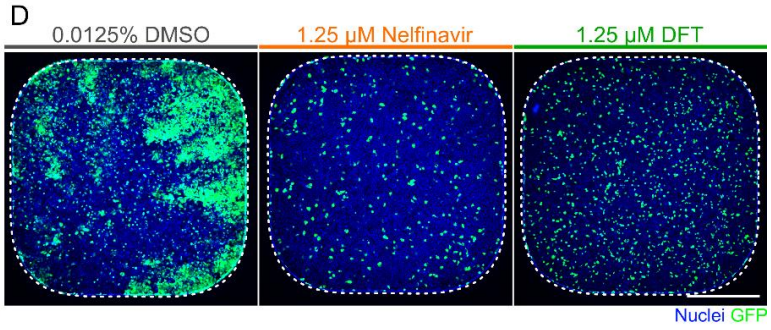

Fig. 1: The HAdV screening procedure. A Following assay development, stability and quality testing, the HAdV screening of the PCL was performed. Imaging, image analysis and data processing was performed independently at UZH and EPFL, before ranked hits were compared. **B** Schematic overview of the wet-lab pipeline. PCL compounds and DFT positive control in DMSO as well as DMSO alone as negative control were pre-spotted onto 384-well imaging plates by Echo acoustic liquid handling at 10 nl corresponding to a final concentration of 1.25 µM in 80 µl assay volume/ well and stored at -20°C. Compound-blinded plates were thawed and 4,000 A549 cells/ wells seeded. The following day, the cells were inoculated with HAdV-C2-dE3B at $1.77*10^5$ genome equivalents / well. Allowing for multiple viral replication rounds, the cells were PFA-fixed at 72 hpi and the nuclei stained using Hoechst. The infection phenotype was imaged using an epifluorescence HT microscope and score using Plaque2.0. The data of the four technical replicates was further processed in R or through EPFL-BSF LIMS. **C** Exemplary epifluorescence microscopy 384-well images stitched to a screening plate overview of consistent of 16 replicates of negative (two most left columns) and positive control (two most right columns) and 320 blinded PCL compounds (centre 20 columns). Hoechst-stained nuclei are shown in blue, viral GFP in green. **D** Representative 384-well epifluorescence microscopy images of the DMSO negative control (most left), the DFT positive control (most right) and the top hit Nelfinavir mesylate (centre). Hoechst-stained nuclei are shown in blue, viral GFP in green. Scale bar is 5 mm.

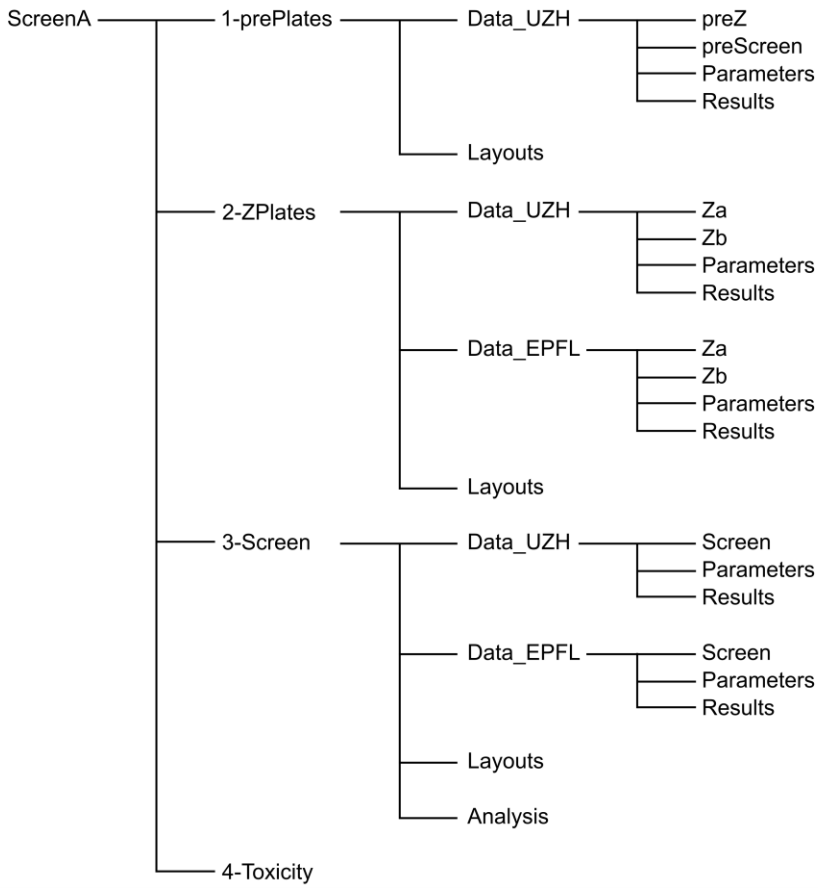

Fig. 2. HAdV data structure provided as project #pending at IDR.

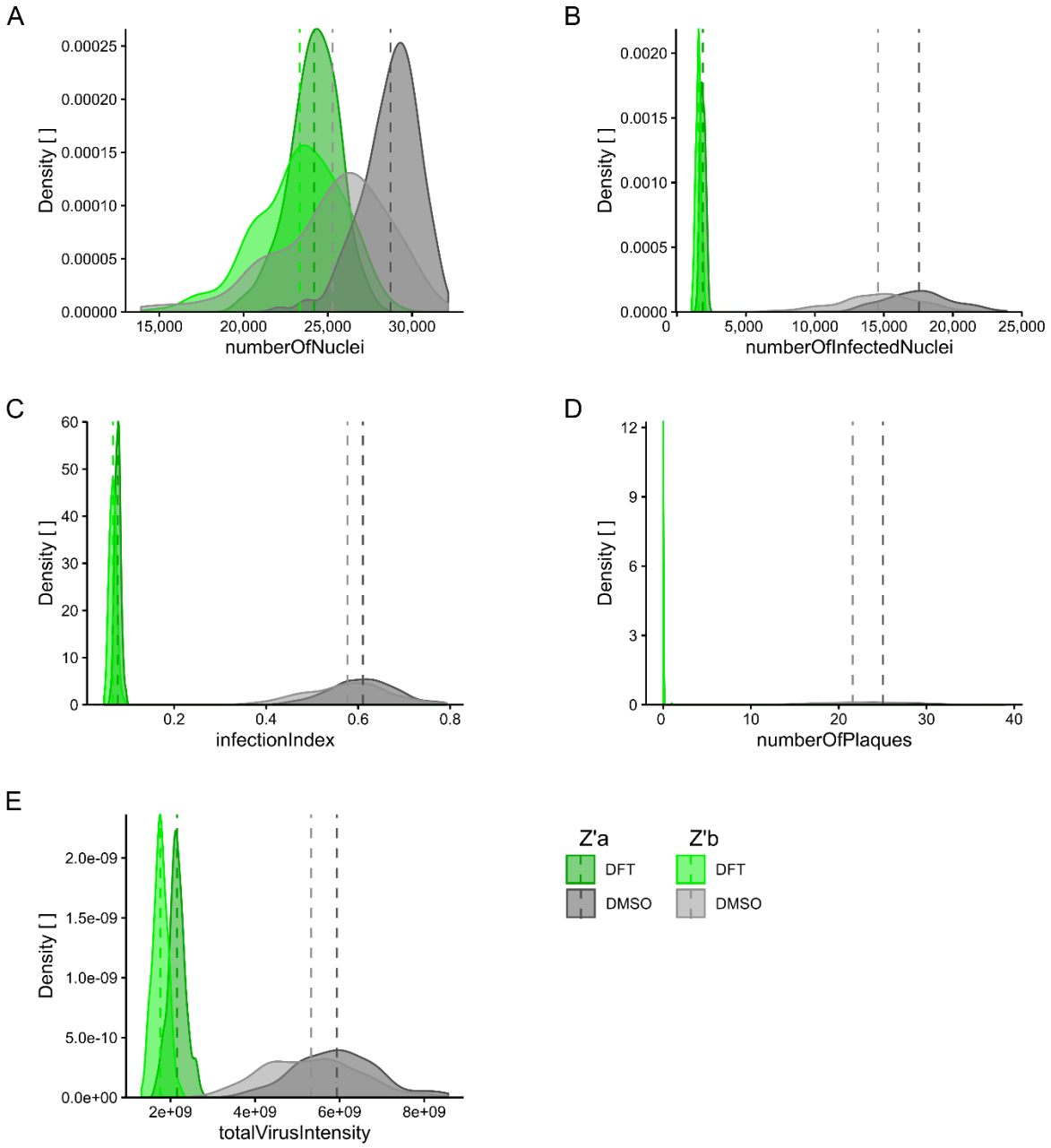

Fig. 3: Infection score density of positive and negative controls across Z' plates. Distribution of **A** *numberOfNuclei,* **B** *numberOfInfectedNuclei*, **C** *infectionIndex*, **D** *numberOfPlaques* and **E** *totalVirusIntensity* in negative control (0.0125% DMSO) compared to positive control-treated (1.25 µM DFT) samples of the two Z' plates. Dark green and dark grey indicates Z' plate a, light green and grey show Z' plate b. Dashed vertical lines mark mean of 192 technical replicas.

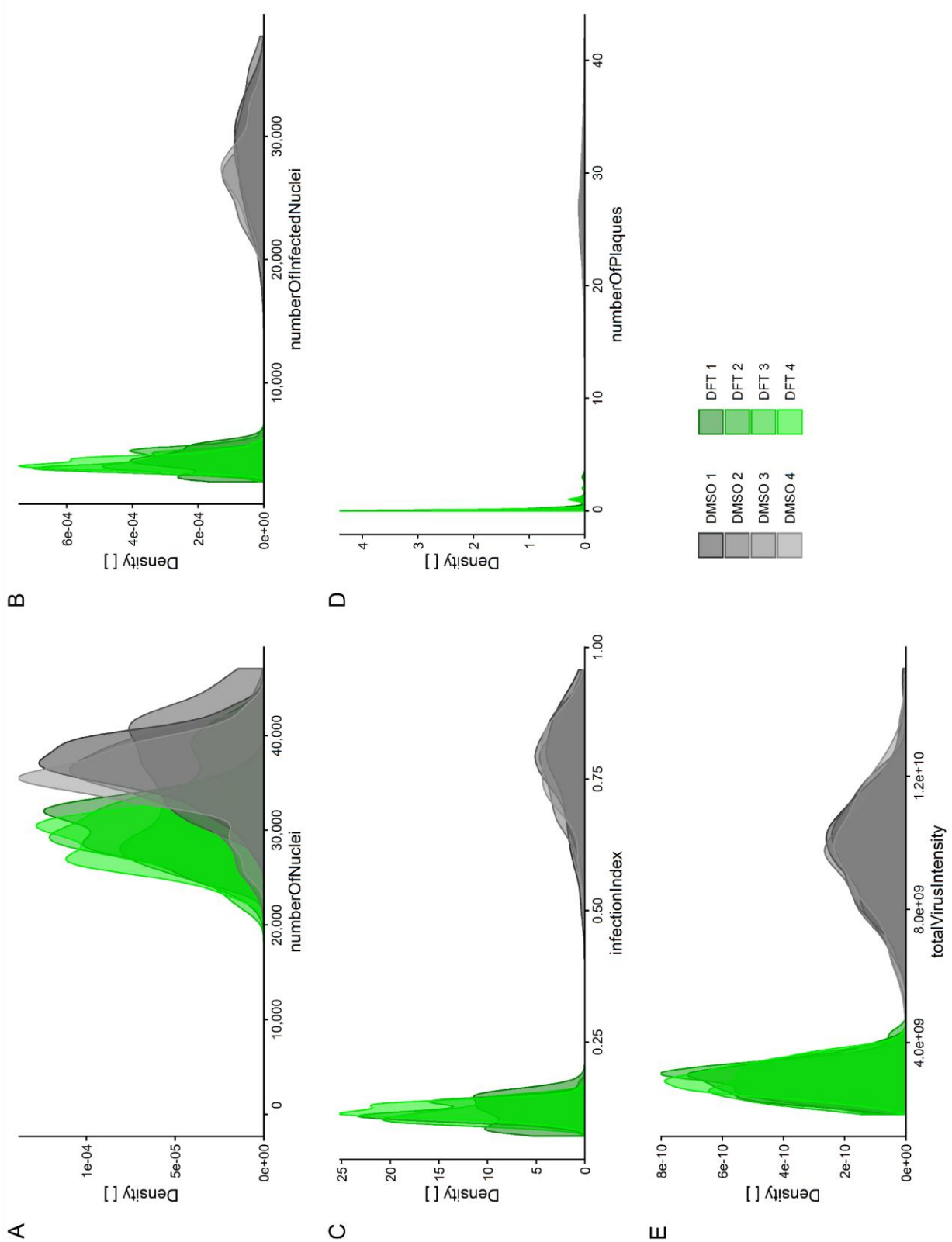

Fig. 4: Infection score density of positive and negative controls across screening replicates. Distribution of **A** *numberOfNuclei,* **B** *numberOfInfectedNuclei*, **C** *infectionIndex*, **D** *numberOfPlaques* and **E** *totalVirusIntensity* in negative control (0.0125% DMSO in grey) compared to positive control-treated (1.25

µM DFT in green) samples of the screening sets. Each set 1 to 4 indicated by colour shading is comprised of four plates containing 32 technical replicas per control.

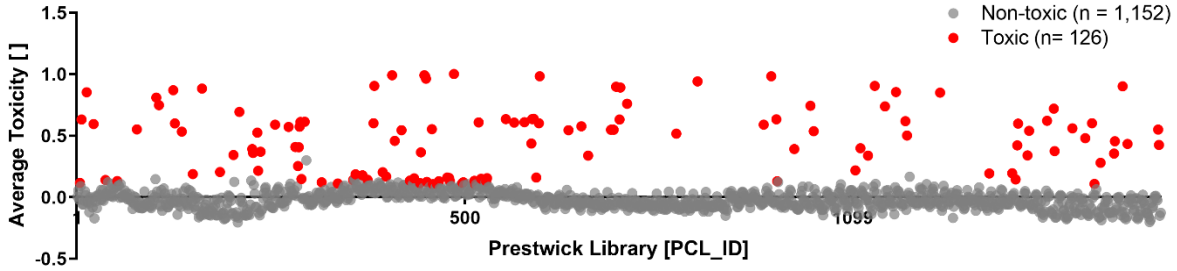

Fig. 5: PCL Toxicity in absence of infection. Of the 1,278 PCL compounds tested, 126 PCL compounds (shown in red, listed in Table 3) were found to be toxic.

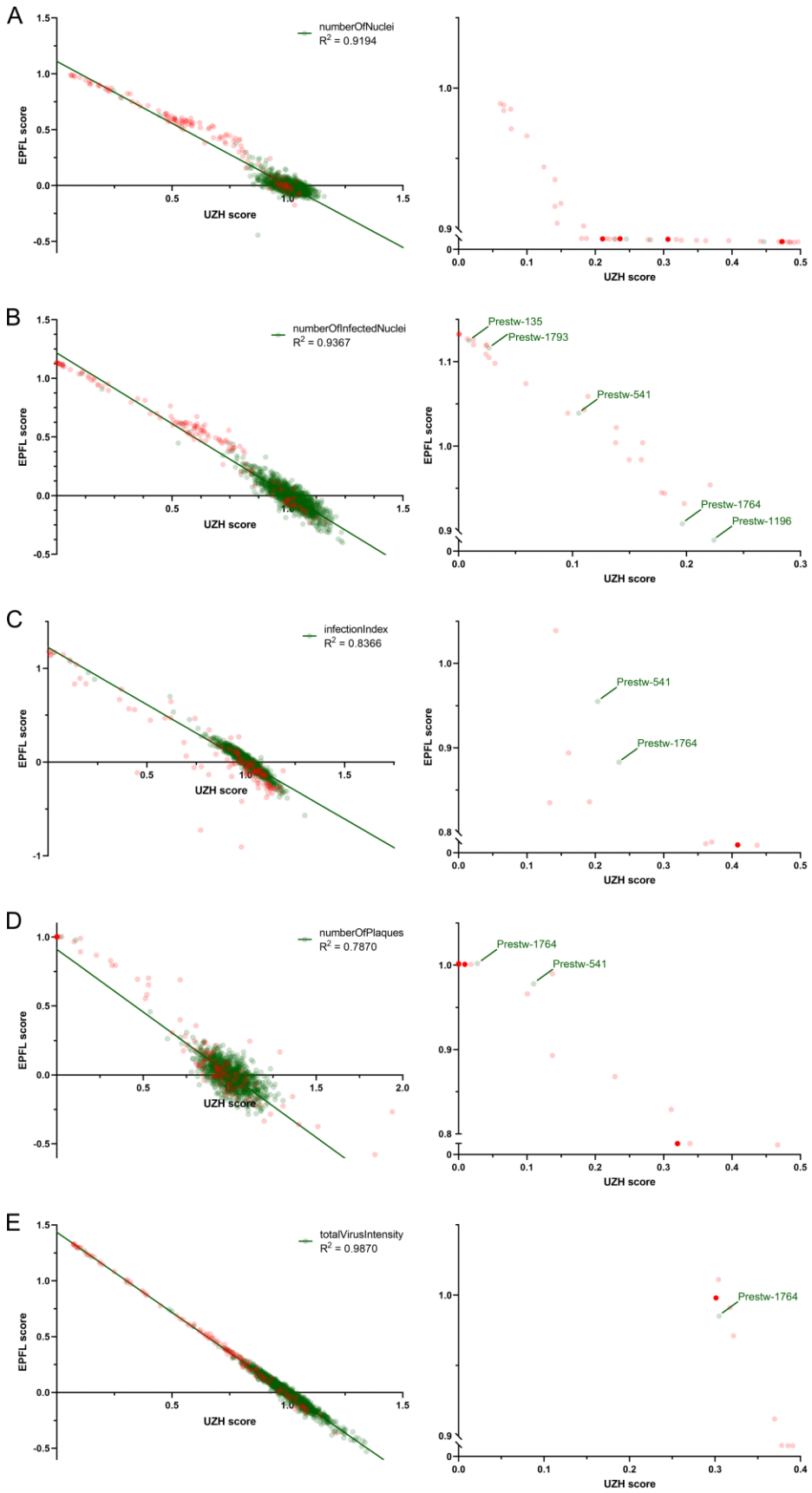
A
numberOfNuclei
R^2 = 0.9194
EPFL score
UZH score
B
numberOfInfectedNuclei
R^2 = 0.9367
Prestw-135
Prestw-1793
Prestw-541
Prestw-1764
Prestw-1196
C
infectionIndex
R^2 = 0.8366
Prestw-541
Prestw-1764
D
numberOfPlaques
R^2 = 0.7870
Prestw-1764
Prestw-541
E
totalVirusIntensity
R^2 = 0.9870
Prestw-1764

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Fig. 6: Correlation between PCL scores from independent dry-lab pipelines. Imaging, image analysis and data processing was performed independently at UZH and EPFL. PCL-treated infection phenotypes from 4 biological replicates were averaged and normalized against the DMSO solvent control. Obtained scores for **A** *numberOfNuclei*, **B** *numberOfInfectedNuclei*, **C** *infectionIndex*, **D** *numberOfPlaques* and **E** *totalVirusIntensity* of the 1,278 tested PCL compounds from UZH and EPFL are correlated via linear regression (green line), R^2 was calculated using GraphPad Prism 8.2.1. Highest scoring compounds are shown on the right and *PCL_ID* of non-toxic compounds indicated. Red dots indicate toxicity in the absence of infection, non-toxic compounds are shown in green.

Tab. 1: Z'-scores of Z plates.

The quality of the screening platform was assessed prior to screening the PCL by two independent Z' plates containing 192 technical replicas of both positive control- (1.25 µM DFT) and negative solvent only control-treated (0.0125% DMSO). Z'-scores for the five Plaque2.0 read-outs [29] obtained by independent analysis at UZH and EPFL were calculated according to Equation 1 for 3 and 2σ.

		UZH					EPFL				
		3 sigma					3 sigma				
Barcode	Plate	numberOf Nuclei	numberOf Infected Nuclei	infection Index	numberOf Plaques	totalVirus Intensity	numberOf Nuclei	numberOf Infected Nuclei	infection Index	numberOf Plaques	totalVirus Intensity
BSF018104	Za	-1.11	0.50	0.57	0.50	0.07	-1.20	0.36	0.47	0.52	0.08
BSF018105	Zb	-8.10	0.30	0.45	0.39	-0.07	-1.23	0.27	0.32	0.44	-0.04
Mean		-4.61	0.40	0.51	0.44	0.00	-1.22	0.32	0.40	0.48	0.02

		UZH					EPFL				
		2 sigma					2 sigma				
Barcode	Plate	numberOf Nuclei	numberOf Infected Nuclei	infection Index	numberOf Plaques	totalVirus Intensity	numberOf Nuclei	numberOf Infected Nuclei	infection Index	numberOf Plaques	totalVirus Intensity
BSF018104	Za	-0.41	0.67	0.71	0.67	0.07	-0.47	0.58	0.64	0.68	0.38
BSF018105	Zb	-5.07	0.53	0.63	0.59	-0.07	-0.49	0.52	0.55	0.63	0.31
Mean		-2.74	0.60	0.67	0.63	0.00	-0.48	0.55	0.60	0.66	0.35

Tab. 2: Z'-scores of screening plates.

The quality of the screening data was quantified for each screening plate based on the 32 technical replicas of both positive control- (1.25 µM DFT) and negative solvent only control-treated (0.0125% DMSO) included in each plate. Z'-scores for the five Plaque2.0 read-outs [29] obtained by independent analysis at UZH and EPFL were calculated according to Equation (1) for 3σ.

		UZH					EPFL				
		3 sigma					3 sigma				
Barcode	Plate	numberOf Nuclei	numberOf Infected Nuclei	infection Index	numberOf Plaques	totalVirus Intensity	numberOf Nuclei	numberOf Infected Nuclei	infection Index	numberOf Plaques	totalVirus Intensity
BSF018292	1A	-0.13	0.58	0.58	0.59	0.35	-0.14	0.51	0.49	0.58	0.31
BSF018293	1B	-0.88	0.58	0.65	0.55	0.34	-0.35	0.51	0.52	0.51	0.35
BSF018294	1C	-1.01	0.62	0.62	0.63	0.33	-0.74	0.52	0.50	0.66	0.32
BSF018295	1D	-0.34	0.56	0.54	0.45	0.16	-0.21	0.43	0.38	0.46	0.19
BSF018296	2A	-1.35	0.64	0.67	0.55	0.30	-0.20	0.57	0.55	0.55	0.28
BSF018297	2B	-3.63	0.56	0.52	0.45	0.14	-1.20	0.45	0.39	0.40	0.12
BSF018298	2C	-1.81	0.60	0.58	0.49	0.24	-0.38	0.52	0.42	0.52	0.19
BSF018299	2D	-1.94	0.57	0.57	0.57	0.24	-0.22	0.50	0.43	0.63	0.20
BSF018300	3A	-1.74	0.64	0.66	0.56	0.36	-0.54	0.55	0.51	0.59	0.34
BSF018301	3B	-1.13	0.60	0.68	0.58	0.40	-0.09	0.52	0.57	0.59	0.40
BSF018302	3C	-4.02	0.66	0.68	0.48	0.42	-1.07	0.63	0.60	0.50	0.41
BSF018303	3D	-2.36	0.55	0.63	0.51	0.36	-0.10	0.58	0.54	0.52	0.35
BSF018304	4A	-0.68	0.70	0.74	0.42	0.37	-0.29	0.56	0.58	0.48	0.36
BSF018305	4B	-0.17	0.71	0.74	0.51	0.50	-0.50	0.63	0.67	0.50	0.50
BSF018306	4C	-0.44	0.61	0.62	0.50	0.28	-0.28	0.50	0.48	0.47	0.26
BSF018307	4D	-0.77	0.63	0.70	0.42	0.41	-0.22	0.54	0.56	0.36	0.39
Mean		-1.40	0.61	0.64	0.52	0.32	-0.41	0.53	0.51	0.52	0.31

Tab. 3: PCL compounds excluded due to toxicity in absence of infection. Presto-blue raw data is available at *ScreenA/4-Toxicity*.

PCL_ID	Compound	Score	ScoreSD	Toxic	PCL_ID	Compound	Score	ScoreSD	Toxic
Prestw-100	Nocodazole	0.75	0.02	yes	Prestw-347	Thioguanosine	0.18	0.03	yes
Prestw-1020	Rimexolone	0.39	0.08	yes	Prestw-353	Moclobemide	0.14	0.02	yes
Prestw-1040	Pyrvinium pamoate	0.74	0.03	yes	Prestw-362	Betamethasone	0.60	0.03	yes
Prestw-1044	Prednicarbate	0.54	0.00	yes	Prestw-363	Colchicine	0.91	0.00	yes
Prestw-1104	Clonixin Lysinate	0.22	0.05	yes	Prestw-373	Amethopterin (R,S)	0.20	0.01	yes
Prestw-1110	Parbendazole	0.40	0.02	yes	Prestw-377	Nafronyl oxalate	0.17	0.03	yes
Prestw-1119	Clocortolone pivalate	0.34	0.04	yes	Prestw-385	Mitoxantrone dihydrochloride	0.99	0.00	yes
Prestw-1134	Cytarabine	0.91	0.00	yes	Prestw-388	Dequalinium dichloride	0.46	0.00	yes
Prestw-1159	Sibutramine HCl	0.74	0.06	yes	Prestw-396	Etoposide	0.55	0.02	yes
Prestw-118	Nalbuphine hydrochloride	0.87	0.00	yes	Prestw-4	Metformin hydrochloride	0.12	0.00	yes
Prestw-1180	Docetaxel	0.86	0.03	yes	Prestw-409	Amiodarone hydrochloride	0.14	0.02	yes
Prestw-1196	Topotecan	0.62	0.04	yes	Prestw-419	Bisacodyl	0.15	0.01	yes
Prestw-1198	Tranilast	0.50	0.02	yes	Prestw-430	Cisapride	0.12	0.02	yes
Prestw-12	Benzonatate	0.85	0.06	yes	Prestw-432	Corticosterone	0.37	0.01	yes
Prestw-120	Triamcinolone	0.60	0.03	yes	Prestw-436	Digitoxigenin	0.99	0.00	yes
Prestw-1266	Gemcitabine	0.85	0.01	yes	Prestw-437	Digoxin	0.98	0.00	yes
Prestw-130	Dexamethasone acetate	0.53	0.02	yes	Prestw-438	Doxorubicin hydrochloride	0.96	0.00	yes
Prestw-1362	Vorinostat	0.19	0.01	yes	Prestw-439	Carbimazole	0.13	0.00	yes
Prestw-1408	Etoricoxib	0.20	0.03	yes	Prestw-447	Hydrocortisone base	0.55	0.02	yes
Prestw-1415	Floxuridine	0.15	0.04	yes	Prestw-448	Hydroxytacrine maleate (R,S)	0.11	0.00	yes
Prestw-1417	Fluconazole	0.42	0.01	yes	Prestw-456	Meclocycline sulfosalicylate	0.11	0.01	yes
Prestw-1419	Fluocinolone acetonide	0.60	0.03	yes	Prestw-457	Meclozine dihydrochloride	0.11	0.02	yes
Prestw-143	Chlorhexidine	0.19	0.02	yes	Prestw-458	Melatonin	0.13	0.01	yes
Prestw-1435	Melengestrol acetate	0.34	0.05	yes	Prestw-476	Primaquine diphosphate	0.16	0.01	yes
Prestw-1443	Misoprostol	0.54	0.05	yes	Prestw-478	Felodipine	0.16	0.01	yes
Prestw-1476	Amcinonide	0.62	0.02	yes	Prestw-48	Dicyclomine hydrochloride	0.13	0.03	yes
Prestw-1484	Cladribine	0.72	0.03	yes	Prestw-481	Serotonin hydrochloride	0.13	0.01	yes
Prestw-1486	Cortisol acetate	0.38	0.08	yes	Prestw-487	Daunorubicin hydrochloride	1.00	0.00	yes
Prestw-1509	Deflazacort	0.56	0.01	yes	Prestw-497	Vancomycin hydrochloride	0.12	0.02	yes
Prestw-155	Paclitaxel	0.88	0.02	yes	Prestw-498	Artemisinin	0.12	0.00	yes
Prestw-1704	Desonide	0.48	0.06	yes	Prestw-513	Norcyclobenzaprine	0.13	0.00	yes
Prestw-1712	Flumethasone pivalate	0.60	0.02	yes	Prestw-514	Pyrazinamide	0.11	0.01	yes
Prestw-1715	Algestone acetophenide	0.11	0.00	yes	Prestw-518	Budesonide	0.61	0.00	yes
Prestw-1722	Azatadine maleate	0.28	0.13	yes	Prestw-522	Thiostrepton	0.15	0.01	yes
Prestw-1740	Besifloxacin hydrochloride	0.36	0.09	yes	Prestw-529	Mesoridazine besylate	0.13	0.00	yes
Prestw-1741	Loteprednol etabonate	0.46	0.05	yes	Prestw-530	Trolox	0.16	0.00	yes
Prestw-1752	Epirubicin hydrochloride	0.90	0.02	yes	Prestw-553	Pentamidine isethionate	0.64	0.01	yes
Prestw-176	Iproniazide phosphate	0.21	0.11	yes	Prestw-572	Mometasone furoate	0.61	0.00	yes
Prestw-1761	Rizatriptan benzoate	0.43	0.00	yes	Prestw-6	Isoflupredone acetate	0.63	0.01	yes
Prestw-1801	Ciclesonide	0.55	0.03	yes	Prestw-619	Diflorasone Diacetate	0.61	0.00	yes
Prestw-1802	Darunavir	0.43	0.06	yes	Prestw-641	Sulmazole	0.44	0.01	yes
Prestw-192	Thalidomide	0.34	0.09	yes	Prestw-643	Flunisolide	0.64	0.01	yes
Prestw-20	Minoxidil	0.60	0.01	yes	Prestw-645	Flurandrenolide	0.64	0.01	yes
Prestw-200	Camptothecine (S,+)	0.69	0.02	yes	Prestw-652	Picrotoxinin	0.16	0.07	yes
Prestw-216	Tiapride hydrochloride	0.39	0.02	yes	Prestw-655	Halcinonide	0.60	0.01	yes
Prestw-217	Mebendazole	0.36	0.02	yes	Prestw-656	Lanatoside C	0.98	0.00	yes
Prestw-222	Antimycin A	0.53	0.08	yes	Prestw-718	Fluorometholone	0.55	0.03	yes
Prestw-223	Xylometazoline hydrochloride	0.22	0.09	yes	Prestw-72	Imipramine hydrochloride	0.55	0.00	yes
Prestw-226	Griseofulvin	0.37	0.07	yes	Prestw-734	Flumethasone	0.58	0.04	yes
Prestw-244	Glutethimide, para-amino	0.59	0.00	yes	Prestw-743	Medrysone	0.34	0.01	yes
Prestw-260	Praziquantel	0.57	0.05	yes	Prestw-771	Alclometasone dipropionate	0.55	0.02	yes
Prestw-268	Vinpocetine	0.41	0.01	yes	Prestw-774	Fluocinonide	0.55	0.03	yes
Prestw-271	Vincamine	0.25	0.00	yes	Prestw-777	Alexidine dihydrochloride	0.90	0.00	yes
Prestw-272	Indomethacin	0.41	0.00	yes	Prestw-781	Clobetasol propionate	0.63	0.00	yes
Prestw-273	Cortisone	0.57	0.01	yes	Prestw-782	Podophyllotoxin	0.89	0.00	yes
Prestw-274	Prednisolone	0.61	0.00	yes	Prestw-790	Cycloheximide	0.76	0.01	yes
Prestw-275	Fenofibrate	0.15	0.01	yes	Prestw-855	Beclomethasone dipropionate	0.52	0.02	yes
Prestw-279	Methylprednisolone, 6-alpha	0.61	0.00	yes	Prestw-883	Digoxigenin	0.94	0.00	yes
Prestw-299	Mifepristone	0.12	0.01	yes	Prestw-97	Disulfiram	0.81	0.04	yes
Prestw-318	Quinacrine dihydrochloride dihydrate	0.11	0.03	yes	Prestw-975	Naftopidil dihydrochloride	0.59	0.01	yes
Prestw-337	Procainamide hydrochloride	0.14	0.01	yes	Prestw-986	Proscillaridin A	0.98	0.00	yes
Prestw-339	Guanfacine hydrochloride	0.19	0.01	yes	Prestw-997	Fluticasone propionate	0.63	0.02	yes
Prestw-34	Triamterene	0.14	0.00	yes	Prestw-998	Zuclopenthixol hydrochloride	0.13	0.01	yes

Tab. 4: Summary of screening controls and top hits. Compounds were scored toxic, if they showed significant toxicity in either of the assays. Mean correspond to means over four biological replicates of PCL compound and 16 biological replicates each carrying 16 technical replicates for each control. Neg. ctr. refers to negative control (DMSO), pos. ctr. to positive control (DFT). Normalized indicates each compound's mean read-outs relative to the mean of the positive control. Toxicity was accessed by presto-blue assay of 72 h treatment of non-infected A549 cells as well as by the nuclei Z'-score in the screen. Hits were selected for low toxicity and high inhibitory effect compared to solvent control.

						Mean read-outs					Normalized mean read-outs					Hit				
PCL_ID	compound Identifier	Compound	Group	Toxic	Analysis	Nuclei	Infected nuclei	Infection index	Plaques	Virus intensity [AU]	Nuclei	Infected nuclei	Infection index	Plaques	Virus intensity [AU]	Nuclei	Infected nuclei	Infection index	Plaques	Virus intensity [AU]
DMSO	DMSO	DMSO	neg. ctr.	no	UZH	36'399	27'911	0.77	27.32	9.79E+09	1.00	1.00	1.00	1.00	1.00	-	-	-	-	-
					EPFL	29'749	15'156	0.51	21.11	5.02E+09	1.00	1.00	1.00	1.00	1.00					
DFT	DFT	DFT	pos. ctr.	no	UZH	30'204	3'595	0.12	0.12	2.90E+09	0.83	0.13	0.15	0.00	0.30					
					EPFL	20'745	1'776	0.09	0.03	1.62E+09	0.70	0.12	0.17	0.00	0.32					
Prestw-1764	497	Nelfinavir mesylate	PCL	no	UZH	30'908	5'479	0.18	0.75	2.98E+09	0.85	0.20	0.23	0.03	0.30	no	yes	yes	yes	yes
					EPFL	21'895	2'988	0.14	0.00	1.68E+09	0.74	0.20	0.27	0.00	0.33	no	yes	yes	yes	yes
Prestw-388	763	Dequalinium dichloride	PCL	yes	UZH	28'763	13'751	0.48	14.00	3.62E+09	0.79	0.49	0.62	0.51	0.37	no	yes	yes	yes	yes
					EPFL	21'247	4'988	0.23	9.25	1.92E+09	0.71	0.33	0.46	0.44	0.38	yes	yes	yes	yes	yes
Prestw-1717	452	Aminacrine	PCL	no	UZH	31'723	14'689	0.47	20.50	4.88E+09	0.87	0.53	0.62	0.75	0.50	no	yes	yes	no	yes
					EPFL	42'191	9'057	0.22	14.25	2.54E+09	1.42	0.60	0.42	0.67	0.51	no	no	yes	no	yes
Prestw-925	1214	Thonzonium bromide	PCL	no	UZH	30'644	15'057	0.49	14.75	4.77E+09	0.84	0.54	0.63	0.54	0.49	no	yes	yes	no	yes
					EPFL	24'093	6'849	0.28	11.75	2.51E+09	0.81	0.45	0.56	0.56	0.50	no	yes	no	no	no

Suppl. Tab. 1: PCL compounds tested in the screening procedure. PCL catalogue IDs (*PCL_ID*), compound names (*CompoundName*) and spottability flag (*SpottabilityFlag*) for the 1,280 compounds of the PCL. Two compounds, namely Prestw-354 (Clopamide) and Prestw-410 (Amphotericine B) could not be successfully transferred via acoustic dispensing e.g. due to precipitation and were therefore not included in the screening.

Suppl. Tab. 2: UZH HAdV screening infection scores.

Suppl. Tab. 3: Scored UZH PCL-treated HAdV infection phenotype.

Suppl. Tab. 4: EPFL HAdV screening infection scores.

Suppl. Tab. 5: Scored EPFL PCL-treated HAdV infection phenotype.

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		UZH 3 sigma					EPFL 3 sigma				
Barcode	Plate	numberOf Nuclei	numberOf Infected Nuclei		infection Index	numberOf Plaques	numberOf Nuclei	numberOf Infected Nuclei		infection Index	numberOf Plaques
BSF018104	Za	-1.11	0.50	0.57	0.50	0.07	-1.20	0.36	0.47	0.52	0.08
BSF018105	Zb	-8.10	0.30	0.45	0.39	-0.07	-1.23	0.27	0.32	0.44	-0.04
Mean		-4.61	0.40	0.51	0.44	0.00	-1.22	0.32	0.40	0.48	0.02

		UZH 2 sigma					EPFL 2 sigma				
Barcode	Plate	numberOf Nuclei	numberOf Infected Nuclei		infection Index	numberOf Plaques	numberOf Nuclei	numberOf Infected Nuclei		infection Index	numberOf Plaques
BSF018104	Za	-0.41	0.67	0.71	0.67	0.07	-0.47	0.58	0.64	0.68	0.38
BSF018105	Zb	-5.07	0.53	0.63	0.59	-0.07	-0.49	0.52	0.55	0.63	0.31
Mean		-2.74	0.60	0.67	0.63	0.00	-0.48	0.55	0.60	0.66	0.35

	UZH					EPFL					
	3 sigma					3 sigma					
Barcode	Plate	numberOf Nuclei		numberOf Infected Nuclei			infection				
Index	numberOf Plaques	totalVirus		Intensity		numberOf Nuclei		numberOf			
Infected Nuclei		infection Index		numberOf Plaques		totalVirus		Intensity			
BSF018292	1A	-0.13	0.58	0.58	0.59	0.35	-0.14	0.51	0.49	0.58	0.31
BSF018293	1B	-0.88	0.58	0.65	0.55	0.34	-0.35	0.51	0.52	0.51	0.35
BSF018294	1C	-1.01	0.62	0.62	0.63	0.33	-0.74	0.52	0.50	0.66	0.32
BSF018295	1D	-0.34	0.56	0.54	0.45	0.16	-0.21	0.43	0.38	0.46	0.19
BSF018296	2A	-1.35	0.64	0.67	0.55	0.30	-0.20	0.57	0.55	0.55	0.28
BSF018297	2B	-3.63	0.56	0.52	0.45	0.14	-1.20	0.45	0.39	0.40	0.12
BSF018298	2C	-1.81	0.60	0.58	0.49	0.24	-0.38	0.52	0.42	0.52	0.19
BSF018299	2D	-1.94	0.57	0.57	0.57	0.24	-0.22	0.50	0.43	0.63	0.20
BSF018300	3A	-1.74	0.64	0.66	0.56	0.36	-0.54	0.55	0.51	0.59	0.34
BSF018301	3B	-1.13	0.60	0.68	0.58	0.40	-0.09	0.52	0.57	0.59	0.40
BSF018302	3C	-4.02	0.66	0.68	0.48	0.42	-1.07	0.63	0.60	0.50	0.41
BSF018303	3D	-2.36	0.55	0.63	0.51	0.36	-0.10	0.58	0.54	0.52	0.35
BSF018304	4A	-0.68	0.70	0.74	0.42	0.37	-0.29	0.56	0.58	0.48	0.36
BSF018305	4B	-0.17	0.71	0.74	0.51	0.50	-0.50	0.63	0.67	0.50	0.50
BSF018306	4C	-0.44	0.61	0.62	0.50	0.28	-0.28	0.50	0.48	0.47	0.26
BSF018307	4D	-0.77	0.63	0.70	0.42	0.41	-0.22	0.54	0.56	0.36	0.39
Mean		-1.40	0.61	0.64	0.52	0.32	-0.41	0.53	0.51	0.52	0.31

PCL_ID	Compound	Score	ScoreSD	Toxic
Prestw-1	Azaguanine-8			no
Prestw-10	Sulfaguanidine			no
Prestw-100	Nocodazole	0.749439938	0.015000825	yes
Prestw-1000	Lymecycline			no
Prestw-1001	Alfadolone acetate			no
Prestw-1002	Alfaxalone			no
Prestw-1003	Azapropazone			no
Prestw-1004	Meptazinol hydrochloride			no
Prestw-1005	Apramycin			no
Prestw-1007	Fursultiamine Hydrochloride			no
Prestw-1008	Gabexate mesilate			no
Prestw-1009	Pivampicillin			no
Prestw-101	R(-) Apomorphine hydrochloride hemihydrate			no
Prestw-1011	Flucloxacillin sodium			no
Prestw-1012	Trapidil			no
Prestw-1013	Deptropine citrate			no
Prestw-1014	Sertraline			no
Prestw-1015	Ethamsylate			no
Prestw-1016	Moxonidine			no
Prestw-1017	Etilefrine hydrochloride			no
Prestw-1018	Alprostadil			no
Prestw-1019	Tribenoside			no
Prestw-102	Amoxapine			no
Prestw-1020	Rimexolone	0.392103742	0.075804134	yes
Prestw-1021	Isradipine			no
Prestw-1023	Isometheptene mucate			no
Prestw-1024	Nifurtimox			no
Prestw-1025	Letrozole			no
Prestw-1026	Arbutin			no
Prestw-1027	Tocainide hydrochloride			no
Prestw-1028	Benzathine benzylpenicillin			no
Prestw-1029	Risperidone			no
Prestw-103	Cyproheptadine hydrochloride			no
Prestw-1030	Torsemide			no

Prestw-1031	Halofantrine hydrochloride			no
Prestw-1032	Articaine hydrochloride			no
Prestw-1033	Nomegestrol acetate		no	
Prestw-1034	Pancuronium bromide		no	
Prestw-1035	Molindone hydrochloride			no
Prestw-1036	Alcuronium chloride		no	
Prestw-1037	Zalcitabine	no		
Prestw-1038	Methyldopate hydrochloride			no
Prestw-1039	Levocabastine hydrochloride			no
Prestw-104	Famotidine	no		
Prestw-1040	Pyrvinium pamoate	0.743404425	0.032474443	yes
Prestw-1041	Etomidate	no		
Prestw-1042	Tridihexethyl chloride		no	
Prestw-1043	Penbutolol sulfate		no	
Prestw-1044	Prednicarbate	0.537113537	0.00162552	yes
Prestw-1045	Sertaconazole nitrate		no	
Prestw-1046	Repaglinide	no		
Prestw-1047	Piretanide	no		
Prestw-1048	Piperacetazine		no	
Prestw-1049	Oxyphenbutazone		no	
Prestw-105	Danazol	no		
Prestw-1050	Quinethazone		no	
Prestw-1051	Moricizine hydrochloride			no
Prestw-1052	Iopanoic acid		no	
Prestw-1053	Pivmecillinam hydrochloride			no
Prestw-1054	Levopropoxyphene napsylate			no
Prestw-1055	Piperidolate hydrochloride			no
Prestw-1056	Trifluridine		no	
Prestw-1057	Oxprenolol hydrochloride			no
Prestw-1058	Ondansetron Hydrochloride			no

Prestw-1059	Propoxycaine hydrochloride			no	
Prestw-106	Nicorandil	no			
Prestw-1060	Oxaprozin	no			
Prestw-1061	Phensuximide		no		
Prestw-1062	Ioxaglic acid		no		
Prestw-1063	Naftifine hydrochloride			no	
Prestw-1064	Meprylcaine hydrochloride			no	
Prestw-1065	Milrinone	no			
Prestw-1066	Methantheline bromide			no	
Prestw-1067	Ticarcillin sodium			no	
Prestw-1068	Thiethylperazine dimalate			no	
Prestw-1069	Mesalamine	no			
Prestw-1071	Imidurea	no			
Prestw-1072	Lansoprazole		no		
Prestw-1073	Bethanechol chloride			no	
Prestw-1074	Cyproterone acetate			no	
Prestw-1075	(R)-Propranolol hydrochloride				no
Prestw-1076	Ciprofibrate		no		
Prestw-1078	Benzylpenicillin sodium			no	
Prestw-108	Nomifensine maleate			no	
Prestw-1080	Methiazole	no			
Prestw-1081	(S)-propranolol hydrochloride				no
Prestw-1082	(-)-Eseroline fumarate salt			no	
Prestw-1086	D-cycloserine		no		
Prestw-1088	(+,-)-Synephrine		no		
Prestw-1089	(S)-(-)-Cycloserine			no	
Prestw-109	Dizocilpine maleate			no	
Prestw-1090	Homosalate	no			
Prestw-1091	Spaglumic acid		no		
Prestw-1092	Ranolazine	no			
Prestw-1094	Sulfadoxine	no			

Prestw-1095	Cyclopentolate hydrochloride			no
Prestw-1096	Estriol			no
Prestw-1097	(-)-Isoproterenol hydrochloride			no
Prestw-1099	Nialamide			no
Prestw-11	Meticrane			no
Prestw-110	Acenocoumarol			no
Prestw-1101	Perindopril			no
Prestw-1102	Fexofenadine HCl			no
Prestw-1104	Clonixin Lysinate	0.219176883	0.047610971	yes
Prestw-1105	Verteporfin			no
Prestw-1106	Meropenem			no
Prestw-1107	Ramipril			no
Prestw-1108	Mephenytoin			no
Prestw-1109	Rifabutin			no
Prestw-111	Naloxone hydrochloride			no
Prestw-1110	Parbendazole	0.398402496	0.018663349	yes
Prestw-1111	Mecamylamine hydrochloride			no
Prestw-1112	Procarbazine hydrochloride			no
Prestw-1113	Viomycin sulfate			no
Prestw-1114	Saquinavir mesylate			no
Prestw-1115	Ronidazole			no
Prestw-1116	Dorzolamide hydrochloride			no
Prestw-1117	Azaperone			no
Prestw-1118	Cefepime hydrochloride			no
Prestw-1119	Clocortolone pivalate	0.338538784	0.042248856	yes
Prestw-112	Metolazone			no
Prestw-1120	Nadifloxacin			no
Prestw-1121	Carbadox			no
Prestw-1125	Oxiconazole Nitrate			no
Prestw-1127	Acipimox			no
Prestw-1129	Benazepril HCl			no
Prestw-113	Ciprofloxacin hydrochloride hydrate			no
Prestw-1130	Azelastine HCl			no
Prestw-1132	Celiprolol HCl			no

Prestw-1134 Cytarabine 0.905540871 0.00431943 yes

Prestw-1136 Doxofylline no
Prestw-1137 Esmolol hydrochloride no

Prestw-1139 Itraconazole no

Prestw-114 Ampicillin trihydrate no

Prestw-1140 Liranaftate no
Prestw-1144 Mirtazapine no
Prestw-1147 Modafinil no
Prestw-115 Haloperidol no
Prestw-1152 Nefazodone HCl no

Prestw-1154 Nilvadipine no
Prestw-1156 Oxcarbazepine no

Prestw-1157 Rifapentine no
Prestw-1158 Ropinirole HCl no

Prestw-1159 Sibutramine HCl 0.738620234 0.064731141 yes

Prestw-116 Naltrexone hydrochloride dihydrate no

Prestw-1161 Stanozolol no
Prestw-1162 Zonisamide no
Prestw-1165 Acitretin no
Prestw-1166 Rebamipide no
Prestw-1167 Diacerein no
Prestw-1169 Miglitol no
Prestw-117 Chlorpheniramine maleate no

Prestw-1170 Venlafaxine no
Prestw-1173 Irsogladine maleate no

Prestw-1174 Acarbose no
Prestw-1177 Carbidopa no
Prestw-1178 Aniracetam no
Prestw-1179 Busulfan no
Prestw-118 Nalbuphine hydrochloride 0.870454735 0.004500787 yes

Prestw-1180 Docetaxel 0.856343595 0.032520001 yes

Prestw-1181 Tibolone no
Prestw-1182 Tizanidine HCl no

Prestw-1183 Temozolomide no

Prestw-1184 Tioconazole no
Prestw-1187 Granisetron no
Prestw-1188 Ziprasidone Hydrochloride no

Prestw-1189 Montelukast no

Prestw-119	Picotamide monohydrate			no
Prestw-1190	Olmesartan		no	
Prestw-1192	Oxandrolone		no	
Prestw-1195	Toltrazuril		no	
Prestw-1196	Topotecan	0.61923066	0.043792234	yes
Prestw-1197	Toremifene		no	
Prestw-1198	Tranilast	0.502083509	0.024539976	yes
Prestw-1199	Tripelennamine hydrochloride			no
Prestw-12	Benzonatate	0.853668407	0.055294598	yes
Prestw-120	Triamcinolone	0.600492086	0.025733241	yes
Prestw-1202	4-aminosalicylic acid			no
Prestw-1203	5-fluorouracil		no	
Prestw-1206	Acetylcysteine		no	
Prestw-1207	Acetylsalicylic acid			no
Prestw-121	Bromocryptine mesylate			no
Prestw-1210	Alendronate sodium			no
Prestw-1211	Alfacalcidol		no	
Prestw-1213	Allopurinol		no	
Prestw-1217	Amisulpride		no	
Prestw-1219	Amlodipine		no	
Prestw-1222	Anastrozole		no	
Prestw-1223	Anethole-trithione			no
Prestw-1224	Anthralin		no	
Prestw-1228	Argatroban		no	
Prestw-1229	Aripiprazole		no	
Prestw-123	Dehydrocholic acid			no
Prestw-1231	Asenapine maleate		no	
Prestw-1232	Atorvastatin		no	
Prestw-1233	Auranofin		no	
Prestw-1234	Azithromycin		no	
Prestw-1236	Benztropine mesylate			no
Prestw-1239	Bicalutamide		no	
Prestw-1241	Bifonazole		no	

Prestw-1242	Erlotinib	no		
Prestw-1244	Bosentan	no		
Prestw-1246	Bromhexine hydrochloride			no
Prestw-1249	Famciclovir	no		
Prestw-125	Perphenazine		no	
Prestw-1251	Butalbital	no		
Prestw-1252	Butenafine Hydrochloride			no
Prestw-1253	Butylscopolammonium (n-) bromide			no
Prestw-1254	Fentiazac	no		
Prestw-1256	Caffeine	no		
Prestw-1257	Calcipotriene		no	
Prestw-1258	Candesartan	no		
Prestw-1259	Canrenone	no		
Prestw-126	Mefloquine hydrochloride			no
Prestw-1261	Carprofen	no		
Prestw-1262	Carvedilol	no		
Prestw-1263	Cefdinir	no		
Prestw-1265	Gatifloxacin		no	
Prestw-1266	Gemcitabine	0.8506899	0.006780787	yes
Prestw-1267	Gestrinone	no		
Prestw-1268	Guaiacol	no		
Prestw-1269	Haloprogin	no		
Prestw-127	Isoconazole	no		
Prestw-1270	Gefitinib	no		
Prestw-1271	Escitalopram		no	
Prestw-1274	Emedastine	no		
Prestw-1279	Stavudine	no		
Prestw-128	Spironolactone		no	
Prestw-1280	Mepivacaine hydrochloride			no
Prestw-1282	Methenamine	no		
Prestw-1283	Buspirone hydrochloride			no
Prestw-1284	Hydroxychloroquine sulfate			no
Prestw-1285	Ibandronate sodium		no	
Prestw-1286	Ibudilast	no		
Prestw-1288	Idebenone	no		
Prestw-129	Pirenzepine dihydrochloride			no
Prestw-1290	Imatinib	no		
Prestw-1291	Imiquimod	no		
Prestw-1292	Ipsapirone	no		

Prestw-1294	Isosorbide mononitrate		no	
Prestw-1295	Itopride	no		
Prestw-1297	Lacidipine	no		
Prestw-1298	Lamivudine	no		
Prestw-13	Hydroflumethiazide		no	
Prestw-130	Dexamethasone acetate	0.534246176	0.016683283	yes
Prestw-1303	Pefloxacine	no		
Prestw-1307	Olopatadine hydrochloride			no
Prestw-1308	Phentermine hydrochloride			no
Prestw-131	Glipizide	no		
Prestw-1310	Phenylbutazone		no	
Prestw-1314	Pioglitazone		no	
Prestw-1315	Potassium clavulanate		no	
Prestw-1316	Pramipexole	no		
Prestw-1317	Pranlukast	no		
Prestw-1318	Pranoprofen	no		
Prestw-1319	Pravastatin	no		
Prestw-132	Loxapine succinate		no	
Prestw-1321	Prothionamide		no	
Prestw-1322	Pyridostigmine iodid		no	
Prestw-1323	Quetiapine	no		
Prestw-1325	Raclopride	no		
Prestw-1328	Reboxetine mesylate		no	
Prestw-133	Hydroxyzine dihydrochloride			no
Prestw-1331	Rimantadine Hydrochloride			no
Prestw-1334	Rivastigmine		no	
Prestw-1336	Rofecoxib	no		
Prestw-1337	Rosiglitazone Hydrochloride			no
Prestw-1338	Rufloxacin	no		
Prestw-1339	Sarafloxacin		no	
Prestw-134	Diltiazem hydrochloride			no
Prestw-1340	Secnidazole	no		
Prestw-1341	Sertindole	no		
Prestw-1342	Sildenafil	no		
Prestw-1343	Sparfloxacin		no	

Prestw-1345	Sulbactam	no		
Prestw-1346	Sumatriptan succinate		no	
Prestw-1349	Tazobactam	no		
Prestw-135	Methotrexate		no	
Prestw-1350	Telmisartan	no		
Prestw-1351	Tenatoprazole		no	
Prestw-1352	Tulobuterol	no		
Prestw-1353	Tylosin	no		
Prestw-1356	Vardenafil	no		
Prestw-1358	Vatalanib	no		
Prestw-1359	Vecuronium bromide		no	
Prestw-136	Astemizole	no		
Prestw-1361	Viloxazine hydrochloride			no
Prestw-1362	Vorinostat	0.194967444	0.014823239	yes
Prestw-1363	Warfarin	no		
Prestw-1364	Zafirlukast	no		
Prestw-1365	Zileuton	no		
Prestw-1367	Zopiclone	no		
Prestw-1368	Zotepine	no		
Prestw-1369	Zaleplon	no		
Prestw-137	Clindamycin hydrochloride			no
Prestw-1371	Celecoxib	no		
Prestw-1374	Chlormadinone acetate		no	
Prestw-1376	Cilnidipine	no		
Prestw-1378	Clarithromycin		no	
Prestw-1379	Clinafloxacin		no	
Prestw-138	Terfenadine	no		
Prestw-1380	Clobutinol hydrochloride			no
Prestw-1383	Clofibrate	no		
Prestw-1385	Closantel	no		
Prestw-1387	Tetraethylenepentamine pentahydrochloride			no
Prestw-139	Cefotaxime sodium salt		no	
Prestw-1390	Desloratadine		no	
Prestw-1392	Dexfenfluramine hydrochloride			no
Prestw-1393	Dibenzepine hydrochloride			no
Prestw-1394	Diclazuril	no		
Prestw-1398	Dopamine hydrochloride		no	

Prestw-1399	Doxycycline hydrochloride			no
Prestw-14	Sulfacetamide sodic hydrate			no
Prestw-140	Tetracycline hydrochloride			no
Prestw-1400	Efavirenz		no	
Prestw-1401	Enoxacin		no	
Prestw-1403	Entacapone		no	
Prestw-1405	Ethinylestradiol			no
Prestw-1407	Etofenamate		no	
Prestw-1408	Etoricoxib	0.196053034	0.033370342	yes
Prestw-1409	Etretinate		no	
Prestw-141	Verapamil hydrochloride			no
Prestw-1410	Exemestane		no	
Prestw-1414	Fleroxacin		no	
Prestw-1415	Floxuridine	0.145511021	0.04436541	yes
Prestw-1416	Flubendazol		no	
Prestw-1417	Fluconazole	0.42186662	0.00949002	yes
Prestw-1419	Fluocinolone acetonide		0.598570483	0.027322461 yes
Prestw-142	Dipyridamole			no
Prestw-1420	Formestane		no	
Prestw-1421	Formoterol fumarate			no
Prestw-1423	Fosinopril		no	
Prestw-1424	Fulvestrant		no	
Prestw-1427	Levetiracetam			no
Prestw-1429	Linezolid		no	
Prestw-143	Chlorhexidine	0.189885893	0.018482317	yes
Prestw-1430	Lofexidine		no	
Prestw-1431	Loracarbef		no	
Prestw-1432	Loratadine		no	
Prestw-1433	Losartan		no	
Prestw-1435	Melengestrol acetate		0.340764251	0.046314669 yes
Prestw-144	Loperamide hydrochloride			no
Prestw-1441	Mevastatin		no	
Prestw-1443	Misoprostol	0.541210393	0.046498969	yes
Prestw-1444	Mitotane		no	
Prestw-1446	Moxifloxacin			no
Prestw-1447	Nalidixic acid sodium salt			no

Prestw-1449 Nicotinamide no

Prestw-145 Chlortetracycline hydrochloride no

Prestw-1452 Norgestimate no

Prestw-1454 Nylidrin no
Prestw-1455 Olanzapine no
Prestw-1456 Opipramol dihydrochloride no

Prestw-1459 Oxfendazol no
Prestw-146 Tamoxifen citrate no

Prestw-1460 Oxibendazol no
Prestw-1463 Tomoxetine hydrochloride no

Prestw-1464 Tosufloxacin hydrochloride no

Prestw-1465 Tramadol hydrochloride no

Prestw-1467 Troglitazone no

Prestw-1469 Mercaptopurine no

Prestw-147 Nicergoline no
Prestw-1471 Amfepramone hydrochloride no

Prestw-1472 Hexachlorophene no

Prestw-1473 Estradiol Valerate no

Prestw-1474 Chloroxine no
Prestw-1475 Oxacillin sodium no

Prestw-1476 Amcinonide 0.622636517 0.015692533 yes

Prestw-1477 Penicillamine no

Prestw-1478 Rifaximin no
Prestw-1479 Triclosan no
Prestw-148 Canrenoic acid potassium salt no

Prestw-1480 Racepinephrine HCl no

Prestw-1481 Cyclophosphamide no

Prestw-1482 Valproic acid no

Prestw-1483 Fludarabine no
Prestw-1484 Cladribine 0.720890411 0.028504044 yes

Prestw-1486 Cortisol acetate 0.376061648 0.082147287 yes

Prestw-1487 Mesna no

Prestw-1488	Penciclovir			no
Prestw-1489	Amifostine			no
Prestw-149	Thioproperazine dimesylate			no
Prestw-1490	Nalmefene hydrochloride			no
Prestw-1491	Pentobarbital			no
Prestw-1492	Lamotrigine			no
Prestw-1493	Topiramate			no
Prestw-1494	Irinotecan Hydrochloride			no
Prestw-1495	Rabeprazole Sodium salt			no
Prestw-1497	Ambrisentan			no
Prestw-1498	Camylofine chlorhydrate			no
Prestw-1499	Fomepizole			no
Prestw-15	Heptaminol hydrochloride			no
Prestw-150	Dihydroergotamine tartrate			no
Prestw-1500	Voriconazole			no
Prestw-1501	Fenipentol			no
Prestw-1502	Acamprosate calcium			no
Prestw-1503	Diosmin			no
Prestw-1505	Valacyclovir hydrochloride			no
Prestw-1506	Mizolastine			no
Prestw-1507	Acefylline			no
Prestw-1508	Ibutilide fumarate			no
Prestw-1509	Deflazacort	0.56116229	0.005447151	yes
Prestw-151	Erythromycin			no
Prestw-1510	Dolasetron mesilate			no
Prestw-1511	Aceclidine Hydrochloride			no
Prestw-1512	Abacavir Sulfate			no
Prestw-1514	Darifenacin hydrobromide			no
Prestw-1516	Levalbuterol hydrochloride			no
Prestw-153	Didanosine			no
Prestw-154	Josamycin			no
Prestw-155	Paclitaxel	0.883419652	0.019851781	yes
Prestw-156	Ivermectin			no

Prestw-157	Gallamine triethiodide			no
Prestw-158	Neomycin sulfate		no	
Prestw-159	Dihydrostreptomycin sulfate			no
Prestw-16	Sulfathiazole		no	
Prestw-160	Gentamicine sulfate			no
Prestw-1600	Aprepitant	no		
Prestw-1601	Pinaverium bromide			no
Prestw-1602	Indatraline hydrochloride			no
Prestw-1603	Pemirolast potassium			no
Prestw-1604	(-)-Emtricitabine		no	
Prestw-161	Isoniazid	no		
Prestw-162	Pentylenetetrazole			no
Prestw-163	Chlorzoxazone		no	
Prestw-164	Ornidazole	no		
Prestw-165	Ethosuximide		no	
Prestw-166	Mafenide hydrochloride			no
Prestw-167	Riluzole hydrochloride			no
Prestw-168	Nitrofurantoin		no	
Prestw-169	Hydralazine hydrochloride			no
Prestw-17	Levodopa	no		
Prestw-170	Phenelzine sulfate			no
Prestw-1700	Histamine dihydrochloride			no
Prestw-1701	Clopidogrel	no		
Prestw-1702	Trimetozine	no		
Prestw-1703	1,8-Dihydroxyanthraquinone			no
Prestw-1704	Desonide	0.480247318	0.055471432	yes
Prestw-1705	Diatrizoic acid dihydrate			no
Prestw-1706	Donepezil hydrochloride			no
Prestw-1707	Doxapram hydrochloride			no
Prestw-1708	(R)-Duloxetine hydrochloride			no

Prestw-1709	Estramustine	no		
Prestw-171	Tranexamic acid	no		
Prestw-1710	Ethoxzolamide	no		
Prestw-1711	Felbamate	no		
Prestw-1712	Flumethasone pivalate	0.602259043	0.020548598	yes
Prestw-1713	Fenoldopam	no		
Prestw-1714	Adapalene	no		
Prestw-1715	Algestone acetophenide	0.10931683	0.003425235	yes
Prestw-1716	Altrenogest	no		
Prestw-1717	Aminacrine	no		
Prestw-1718	Amlexanox	no		
Prestw-1719	Amorolfine hydrochloride	no		
Prestw-172	Etofylline	no		
Prestw-1720	Anagrelide	no		
Prestw-1721	Avobenzone	no		
Prestw-1722	Azatadine maleate	0.28020354	0.129728397	yes
Prestw-1723	Benzoxiquine	no		
Prestw-1726	Cefpiramide	no		
Prestw-1727	Cefpodoxime proxetil	no		
Prestw-1728	Cefprozil	no		
Prestw-1729	Ceftibuten	no		
Prestw-173	Tranylcypromine hydrochloride	no		
Prestw-1730	Cefuroxime axetil	no		
Prestw-1731	Zoledronic acid hydrate	no		
Prestw-1732	Tolcapone	no		
Prestw-1733	Nitazoxanide	no		
Prestw-1734	Rasagiline	no		
Prestw-1735	Valsartan	no		
Prestw-1736	Irbesartan	no		
Prestw-1737	Indinavir sulfate	no		
Prestw-1738	Risedronic acid monohydrate	no		
Prestw-1739	Nevirapine	no		
Prestw-174	Alverine citrate salt	no		
Prestw-1740	Besifloxacin hydrochloride	0.356621139	0.093303577	yes
Prestw-1741	Loteprednol etabonate	0.455770914	0.050619797	yes
Prestw-1743	Dofetilide	no		

Prestw-1744	Tolterodine tartrate		no	
Prestw-1745	Cisatracurium besylate		no	
Prestw-1746	Lodoxamide	no		
Prestw-1748	Nateglinide	no		
Prestw-1749	Silodosin	no		
Prestw-175	Aceclofenac	no		
Prestw-1750	Terbinafine	no		
Prestw-1751	Brimonidine L-Tartrate		no	
Prestw-1752	Epirubicin hydrochloride	0.902839264	0.016524502	yes
Prestw-1753	Tegafur	no		
Prestw-1756	Lofepramine	no		
Prestw-1758	Pantoprazole sodium		no	
Prestw-1759	Valdecoxib	no		
Prestw-176	Iproniazide phosphate	0.205675223	0.111130671	yes
Prestw-1760	Tegaserod maleate	no		
Prestw-1761	Rizatriptan benzoate	0.433665551	0.001547144	yes
Prestw-1762	Ezetimibe	no		
Prestw-1763	Actarit	no		
Prestw-1764	Nelfinavir mesylate		no	
Prestw-1765	Latanoprost	no		
Prestw-1766	Benidipine hydrochloride			no
Prestw-1768	Triclabendazole	no		
Prestw-1769	Enalaprilat dihydrate		no	
Prestw-177	Sulfamethoxazole	no		
Prestw-1770	Perospirone	no		
Prestw-1771	Carmofur	no		
Prestw-1772	Ampiroxicam	no		
Prestw-1773	Ipriflavone	no		
Prestw-1774	Nifekalant	no		
Prestw-1775	Lomerizine hydrochloride			no
Prestw-1776	Phenprobamate	no		
Prestw-1777	Trimebutine	no		
Prestw-1778	Troxipide	no		
Prestw-178	Mephenesin	no		
Prestw-1780	Oxymetholone	no		
Prestw-1781	Alosetron hydrochloride			no
Prestw-1782	Ritonavir	no		

Prestw-1783	Palonosetron hydrochloride			no
Prestw-1784	Ubenimex	no		
Prestw-1785	Phenothiazine		no	
Prestw-1786	Enrofloxacin		no	
Prestw-1787	Homoveratrylamine		no	
Prestw-1788	Milnacipran hydrochloride			no
Prestw-179	Phenformin hydrochloride			no
Prestw-1791	Pregabalin	no		
Prestw-1792	Pidotimod	no		
Prestw-1793	Raltitrexed	no		
Prestw-1794	Pemetrexed disodium			no
Prestw-1795	Mupirocin	no		
Prestw-1796	Delavirdine	no		
Prestw-1797	Grepafloxacin		no	
Prestw-1798	Mirabegron	no		
Prestw-1799	Tigecycline	no		
Prestw-18	Idoxuridine	no		
Prestw-180	Flutamide	no		
Prestw-1800	Zolmitriptan		no	
Prestw-1801	Ciclesonide	0.550239421	0.033851547	yes
Prestw-1802	Darunavir	0.42653591	0.063667248	yes
Prestw-1803	Methicillin sodium			no
Prestw-1804	Nelarabine	no		
Prestw-181	Ampyrone	no		
Prestw-182	Levamisole hydrochloride			no
Prestw-183	Pargyline hydrochloride			no
Prestw-184	Methocarbamol		no	
Prestw-185	Aztreonam	no		
Prestw-186	Cloxacillin sodium salt			no
Prestw-187	Catharanthine		no	
Prestw-188	Pentolinium bitartrate			no
Prestw-189	Aminopurine, 6-benzyl			no
Prestw-19	Captopril	no		
Prestw-190	Tolbutamide	no		

Prestw-191	Midodrine hydrochloride			no
Prestw-192	Thalidomide	0.344191967	0.089259533	yes
Prestw-193	Oxolinic acid			no
Prestw-194	Nimesulide			no
Prestw-196	Pentoxifylline			no
Prestw-197	Metaraminol bitartrate			no
Prestw-198	Salbutamol			no
Prestw-199	Prilocaine hydrochloride			no
Prestw-2	Allantoin			no
Prestw-20	Minoxidil	0.595790897	0.008462418	yes
Prestw-200	Camptothecine (S,+)	0.693495492	0.017802016	yes
Prestw-201	Ranitidine hydrochloride			no
Prestw-202	Tiratricol, 3,3',5-triiodothyroacetic acid			no
Prestw-203	Flufenamic acid			no
Prestw-204	Flumequine			no
Prestw-205	Tolfenamic acid			no
Prestw-206	Meclofenamic acid sodium salt monohydrate			no
Prestw-208	Trimethoprim			no
Prestw-209	Metoclopramide monohydrochloride			no
Prestw-21	Sulfaphenazole			no
Prestw-210	Fenbendazole			no
Prestw-211	Piroxicam			no
Prestw-212	Pyrantel tartrate			no
Prestw-213	Fenspiride hydrochloride			no
Prestw-214	Gemfibrozil			no
Prestw-215	Mefexamide hydrochloride			no
Prestw-216	Tiapride hydrochloride	0.391945138	0.023910398	yes
Prestw-217	Mebendazole	0.360975753	0.020675576	yes
Prestw-218	Fenbufen			no
Prestw-219	Ketoprofen			no
Prestw-22	Panthenol (D)			no

Prestw-220	Indapamide			no
Prestw-221	Norfloxacin			no
Prestw-222	Antimycin A	0.526173916	0.078294325	yes
Prestw-223	Xylometazoline hydrochloride	0.215555951	0.08506239	yes
Prestw-224	Oxymetazoline hydrochloride			no
Prestw-225	Nifenazone			no
Prestw-226	Griseofulvin	0.370865398	0.066871042	yes
Prestw-227	Clemizole hydrochloride			no
Prestw-228	Tropicamide			no
Prestw-229	Nefopam hydrochloride			no
Prestw-23	Sulfadiazine			no
Prestw-230	Phentolamine hydrochloride			no
Prestw-231	Etodolac			no
Prestw-232	Scopolamin-N-oxide hydrobromide			no
Prestw-233	Hyoscyamine (L)			no
Prestw-234	Chlorphensin carbamate			no
Prestw-236	Dilazep dihydrochloride			no
Prestw-237	Ofloxacin			no
Prestw-238	Lomefloxacin hydrochloride			no
Prestw-239	Orphenadrine hydrochloride			no
Prestw-24	Norethynodrel			no
Prestw-240	Proglumide			no
Prestw-241	Mexiletine hydrochloride			no
Prestw-242	Flavoxate hydrochloride			no
Prestw-243	Bufexamac			no
Prestw-244	Glutethimide, para-amino	0.590640799	0.004495793	yes
Prestw-245	Dropropizine (R,S)			no
Prestw-246	Pinacidil			no
Prestw-247	Albendazole			no
Prestw-248	Clonidine hydrochloride			no
Prestw-249	Bupropion hydrochloride			no
Prestw-25	Thiamphenicol			no

Prestw-250	Alprenolol hydrochloride			no
Prestw-251	Chlorothiazide			no
Prestw-252	Diphenidol hydrochloride			no
Prestw-253	Norethindrone			no
Prestw-254	Nortriptyline hydrochloride			no
Prestw-255	Niflumic acid			no
Prestw-256	Isotretinoin			no
Prestw-257	Retinoic acid			no
Prestw-258	Antazoline hydrochloride			no
Prestw-259	Ethacrynic acid			no
Prestw-26	Cimetidine			no
Prestw-260	Praziquantel	0.572807813	0.04518284	yes
Prestw-261	Ethisterone			no
Prestw-262	Triprolidine hydrochloride			no
Prestw-263	Doxepin hydrochloride			no
Prestw-264	Dyclonine hydrochloride			no
Prestw-265	Dimenhydrinate			no
Prestw-266	Disopyramide			no
Prestw-267	Clotrimazole			no
Prestw-268	Vinpocetine	0.408765577	0.014497286	yes
Prestw-269	Clomipramine hydrochloride			no
Prestw-27	Doxylamine succinate			no
Prestw-270	Fendiline hydrochloride			no
Prestw-271	Vincamine	0.253500604	0.000173832	yes
Prestw-272	Indomethacin	0.40760967	0.001655721	yes
Prestw-273	Cortisone	0.573403865	0.009975833	yes
Prestw-274	Prednisolone	0.612821653	0.004544576	yes
Prestw-275	Fenofibrate	0.149090539	0.007268135	yes

Prestw-276	Bumetanide	no		
Prestw-277	Labetalol hydrochloride		no	
Prestw-278	Cinnarizine	no		
Prestw-279	Methylprednisolone, 6-alpha	0.613370634	0.004055706	yes
Prestw-28	Ethambutol dihydrochloride		no	
Prestw-280	Quinidine hydrochloride monohydrate			no
Prestw-281	Fludrocortisone acetate		no	
Prestw-282	Fenoterol hydrobromide		no	
Prestw-283	Homochlorcyclizine dihydrochloride			no
Prestw-284	Diethylcarbamazine citrate		no	
Prestw-285	Chenodiol	no		
Prestw-286	Perhexiline maleate		no	
Prestw-287	Oxybutynin chloride		no	
Prestw-288	Spiperone	no		
Prestw-289	Pyrilamine maleate		no	
Prestw-29	Antipyrine	no		
Prestw-290	Sulfinpyrazone		no	
Prestw-291	Dantrolene sodium salt		no	
Prestw-292	Trazodone hydrochloride		no	
Prestw-293	Glafenine hydrochloride		no	
Prestw-294	Pimethixene maleate		no	
Prestw-295	Pergolide mesylate		no	
Prestw-296	Acemetacin	no		
Prestw-297	Benzydamine hydrochloride		no	
Prestw-298	Fipexide hydrochloride		no	
Prestw-299	Mifepristone	0.122510375	0.005380019	yes
Prestw-3	Acetazolamide		no	
Prestw-30	Antipyrine, 4-hydroxy		no	
Prestw-300	Diperodon hydrochloride		no	
Prestw-301	Lisinopril	no		

Prestw-302 Lincomycin hydrochloride no

Prestw-303 Telenzepine dihydrochloride no

Prestw-304 Econazole nitrate no

Prestw-305 Bupivacaine hydrochloride no

Prestw-306 Clemastine fumarate no

Prestw-307 Oxytetracycline dihydrate no

Prestw-308 Pimozide no
Prestw-309 Amodiaquin dihydrochloride dihydrate no

Prestw-31 Chloramphenicol no

Prestw-310 Mebeverine hydrochloride no

Prestw-311 Ifenprodil tartrate no

Prestw-312 Flunarizine dihydrochloride no

Prestw-313 Trifluoperazine dihydrochloride no

Prestw-314 Enalapril maleate no

Prestw-315 Minocycline hydrochloride no

Prestw-316 Glibenclamide no

Prestw-317 Guanethidine sulfate no

Prestw-318 Quinacrine dihydrochloride dihydrate 0.112868076
0.026711166 yes
Prestw-319 Clofilium tosylate no

Prestw-32 Epirizole no
Prestw-320 Fluphenazine dihydrochloride no

Prestw-321 Streptomycin sulfate no

Prestw-322 Alfuzosin hydrochloride no

Prestw-323 Chlorpropamide no

Prestw-324 Phenylpropanolamine hydrochloride no

Prestw-325 Ascorbic acid no

Prestw-326 Methyldopa (L,-) no

Prestw-327 Cefoperazone dihydrate no

Prestw-328	Zoxazolamine			no
Prestw-329	Tacrine hydrochloride			no
Prestw-33	Diprophylline			no
Prestw-330	Bisoprolol fumarate			no
Prestw-331	Tremorine dihydrochloride			no
Prestw-332	Practolol		no	
Prestw-333	Zidovudine, AZT			no
Prestw-334	Sulfisoxazole			no
Prestw-335	Zaprinast		no	
Prestw-336	Chlormezanone			no
Prestw-337	Procainamide hydrochloride	0.137586477	0.007951479	yes
Prestw-338	N6-methyladenosine			no
Prestw-339	Guanfacine hydrochloride	0.187986194	0.011159652	yes
Prestw-34	Triamterene	0.141584474	0.002094588	yes
Prestw-340	Domperidone		no	
Prestw-341	Furosemide		no	
Prestw-342	Methapyrilene hydrochloride			no
Prestw-343	Desipramine hydrochloride			no
Prestw-344	Clorgyline hydrochloride			no
Prestw-345	Clenbuterol hydrochloride			no
Prestw-346	Maprotiline hydrochloride			no
Prestw-347	Thioguanosine	0.179913987	0.031786184	yes
Prestw-348	Chlorprothixene hydrochloride			no
Prestw-349	Ritodrine hydrochloride			no
Prestw-35	Dapsone		no	
Prestw-350	Clozapine		no	
Prestw-351	Chlorthalidone			no
Prestw-352	Dobutamine hydrochloride			no
Prestw-353	Moclobemide	0.142220859	0.021919493	yes
Prestw-355	Hycanthone		no	

Prestw-356	Adenosine 5'-monophosphate monohydrate			no
Prestw-357	Amoxicillin			no
Prestw-359	Dextromethorphan hydrobromide monohydrate			no
Prestw-36	Troleandomycin			no
Prestw-360	Droperidol			no
Prestw-361	Bambuterol hydrochloride			no
Prestw-362	Betamethasone	0.602803979	0.032068404	yes
Prestw-363	Colchicine	0.905055715	0.002997195	yes
Prestw-364	Metergoline			no
Prestw-365	Brinzolamide			no
Prestw-366	Ambroxol hydrochloride			no
Prestw-367	Benfluorex hydrochloride			no
Prestw-368	Bepridil hydrochloride			no
Prestw-369	Meloxicam			no
Prestw-37	Pyrimethamine			no
Prestw-370	Benzbromarone			no
Prestw-371	Ketotifen fumarate			no
Prestw-372	Debrisoquin sulfate			no
Prestw-373	Amethopterin (R,S)	0.204253877	0.009370681	yes
Prestw-374	Methylergometrine maleate			no
Prestw-375	Methiothepin maleate			no
Prestw-376	Clofazimine			no
Prestw-377	Nafronyl oxalate	0.169009561	0.029886225	yes
Prestw-378	Bezafibrate			no
Prestw-38	Hexamethonium dibromide dihydrate			no
Prestw-380	Clebopride maleate			no
Prestw-381	Lidoflazine			no
Prestw-382	Betaxolol hydrochloride			no
Prestw-383	Nicardipine hydrochloride			no
Prestw-384	Probucol			no
Prestw-385	Mitoxantrone dihydrochloride	0.991694132	0.000573566	yes

Prestw-386	GBR 12909 dihydrochloride			no
Prestw-387	Carbetapentane citrate			no
Prestw-388	Dequalinium dichloride	0.459536573	0.004539056	yes
Prestw-389	Ketoconazole			no
Prestw-39	Diflunisal			no
Prestw-390	Fusidic acid sodium salt			no
Prestw-391	Terbutaline hemisulfate			no
Prestw-392	Ketanserin tartrate hydrate			no
Prestw-393	Hemicholinium bromide			no
Prestw-394	Kanamycin A sulfate			no
Prestw-395	Amikacin hydrate			no
Prestw-396	Etoposide	0.545076873	0.015578586	yes
Prestw-397	Clomiphene citrate (Z,E)			no
Prestw-398	Oxantel pamoate			no
Prestw-399	Prochlorperazine dimaleate			no
Prestw-4	Metformin hydrochloride	0.117062894	0.000250737	yes
Prestw-40	Niclosamide			no
Prestw-400	Hesperidin			no
Prestw-401	Testosterone propionate			no
Prestw-403	Thyroxine (L)			no
Prestw-405	Pepstatin A			no
Prestw-407	Adamantamine fumarate			no
Prestw-408	Butoconazole nitrate			no
Prestw-409	Amiodarone hydrochloride	0.135560563	0.016230909	yes
Prestw-41	Procaine hydrochloride			no
Prestw-411	Androsterone			no
Prestw-413	Carbarsone			no
Prestw-416	Bacampicillin hydrochloride			no
Prestw-418	Biotin			no
Prestw-419	Bisacodyl	0.153803101	0.011345262	yes

Prestw-42	Moxisylyte hydrochoride			no
Prestw-421	Suloctidil			no
Prestw-423	Carisoprodol			no
Prestw-424	Cephalosporanic acid, 7-amino			no
Prestw-425	Chicago sky blue 6B			no
Prestw-426	Buflomedil hydrochloride			no
Prestw-428	Roxatidine Acetate HCl			no
Prestw-43	Betazole hydrochloride			no
Prestw-430	Cisapride	0.115164789	0.018744489	yes
Prestw-432	Corticosterone	0.366129081	0.013359203	yes
Prestw-433	Cyanocobalamin			no
Prestw-434	Cefadroxil			no
Prestw-435	Cyclosporin A			no
Prestw-436	Digitoxigenin	0.992747505	0.000204895	yes
Prestw-437	Digoxin	0.984748688	0.000178533	yes
Prestw-438	Doxorubicin hydrochloride	0.964578971	0.002854986	yes
Prestw-439	Carbimazole	0.125199625	0.002194123	yes
Prestw-44	Isoxicam			no
Prestw-440	Epiandrosterone			no
Prestw-441	Estradiol-17 beta			no
Prestw-443	Gabazine bromide			no
Prestw-445	Cyclobenzaprine hydrochloride			no
Prestw-446	Carteolol hydrochloride			no
Prestw-447	Hydrocortisone base	0.553541859	0.021775587	yes
Prestw-448	Hydroxytacrine maleate (R,S)	0.107538381	0.003603812	yes
Prestw-449	Pilocarpine nitrate			no
Prestw-45	Naproxen			no
Prestw-450	Dicloxacillin sodium salt hydrate			no
Prestw-451	Alizapride HCl			no

Prestw-455	Mebhydroline 1,5-naphtalenedisulfonate			no
Prestw-456	Meclocycline sulfosalicylate	0.107156782	0.011836131	yes
Prestw-457	Meclozine dihydrochloride	0.113507415	0.017087115	yes
Prestw-458	Melatonin	0.13160938	0.006597583	yes
Prestw-46	Naphazoline hydrochloride			no
Prestw-460	Dinoprost trometamol			no
Prestw-461	Tropisetron HCl			no
Prestw-462	Cefixime			no
Prestw-463	Metrizamide			no
Prestw-468	Neostigmine bromide			no
Prestw-469	Niridazole			no
Prestw-47	Ticlopidine hydrochloride			no
Prestw-470	Ceforanide			no
Prestw-473	Cefotetan			no
Prestw-475	Brompheniramine maleate			no
Prestw-476	Primaquine diphosphate	0.161620847	0.011225059	yes
Prestw-477	Progesterone			no
Prestw-478	Felodipine	0.156799322	0.007799217	yes
Prestw-48	Dicyclomine hydrochloride	0.132347475	0.02511396	yes
Prestw-481	Serotonin hydrochloride	0.132305018	0.005810307	yes
Prestw-482	Cefotiam hydrochloride			no
Prestw-484	Benperidol			no
Prestw-485	Cefaclor hydrate			no
Prestw-486	Colistin sulfate			no
Prestw-487	Daunorubicin hydrochloride	1.002834608	0.00290379	yes
Prestw-488	Dosulepin hydrochloride			no
Prestw-489	Ceftazidime pentahydrate			no
Prestw-49	Amyleine hydrochloride			no
Prestw-490	Iobenguane sulfate			no
Prestw-491	Metixene hydrochloride			no

Prestw-492	Nitrofural	no		
Prestw-493	Omeprazole	no		
Prestw-494	Propylthiouracil	no		
Prestw-495	Terconazole	no		
Prestw-496	Tiaprofenic acid	no		
Prestw-497	Vancomycin hydrochloride	0.117319101	0.02199845	yes
Prestw-498	Artemisinin	0.122977377	0.004564096	yes
Prestw-499	Propafenone hydrochloride	no		
Prestw-5	Atracurium besylate	no		
Prestw-50	Lidoca? hydrochloride	no		
Prestw-500	Ethamivan	no		
Prestw-501	Vigabatrin	no		
Prestw-502	Biperiden hydrochloride	no		
Prestw-503	Cetirizine dihydrochloride	no		
Prestw-504	Etifenin	no		
Prestw-505	Metaproterenol sulfate, orciprenaline sulfate	no		
Prestw-506	Sisomicin sulfate	no		
Prestw-509	Bromperidol	no		
Prestw-510	Cyclizine hydrochloride	no		
Prestw-511	Fluoxetine hydrochloride	no		
Prestw-512	Iohexol	no		
Prestw-513	Norcyclobenzaprine	0.133914745	0.003222051	yes
Prestw-514	Pyrazinamide	0.107208754	0.013354302	yes
Prestw-515	Trimethadione	no		
Prestw-516	Lovastatin	no		
Prestw-517	Nystatine	no		
Prestw-518	Budesonide	0.609531215	0.003357572	yes
Prestw-519	Imipenem	no		
Prestw-52	Carbamazepine	no		
Prestw-520	Sulfasalazine	no		
Prestw-522	Thiostrepton	0.150332354	0.010142501	yes
Prestw-524	Tiabendazole	no		
Prestw-525	Rifampicin	no		

Prestw-526	Ethionamide	no		
Prestw-527	Tenoxicam	no		
Prestw-528	Triflusal	no		
Prestw-529	Mesoridazine besylate	0.131310604	0.001900833	yes
Prestw-53	Triflupromazine hydrochloride			no
Prestw-530	Trolox	0.155439272	0.00338611	yes
Prestw-531	Pirenperone	no		
Prestw-533	Phenacetin	no		
Prestw-534	Atovaquone	no		
Prestw-535	Methoxamine hydrochloride			no
Prestw-536	(R)-(+)-Atenolol		no	
Prestw-537	Piracetam	no		
Prestw-538	Phenindione	no		
Prestw-539	Thiocolchicoside		no	
Prestw-54	Mefenamic acid		no	
Prestw-540	Clorsulon	no		
Prestw-541	Ciclopirox ethanolamine			no
Prestw-542	Probenecid	no		
Prestw-543	Betahistine mesylate			no
Prestw-544	Tobramycin	no		
Prestw-545	Tetramisole hydrochloride			no
Prestw-546	Pregnenolone		no	
Prestw-547	Molsidomine	no		
Prestw-548	Chloroquine diphosphate			no
Prestw-549	Trimetazidine dihydrochloride			no
Prestw-55	Acetohexamide		no	
Prestw-550	Parthenolide		no	
Prestw-551	Hexetidine	no		
Prestw-552	Selegiline hydrochloride			no
Prestw-553	Pentamidine isethionate		0.635144006	0.005485571 yes
Prestw-554	Tolazamide	no		
Prestw-555	Nifuroxazide		no	
Prestw-557	Dirithromycin		no	
Prestw-558	Gliclazide	no		
Prestw-559	DO 897/99	no		

Prestw-56	Sulpiride	no		
Prestw-560	Prenylamine lactate		no	
Prestw-565	Atropine sulfate monohydrate			no
Prestw-566	Eserine sulfate, physostigmine sulfate			no
Prestw-57	Benoxinate hydrochloride			no
Prestw-571	Tetraca? hydrochloride		no	
Prestw-572	Mometasone furoate	0.60798789	0.00123881	yes
Prestw-574	Dacarbazine	no		
Prestw-576	Acetopromazine maleate salt			no
Prestw-58	Oxethazaine	no		
Prestw-583	Papaverine hydrochloride			no
Prestw-584	Yohimbine hydrochloride			no
Prestw-587	Cilostazol	no		
Prestw-588	Galanthamine hydrobromide			no
Prestw-59	Pheniramine maleate		no	
Prestw-594	Diclofenac sodium		no	
Prestw-598	Xylazine	no		
Prestw-6	Isoflupredone acetate	0.632408562	0.005865799	yes
Prestw-60	Tolazoline hydrochloride			no
Prestw-607	Eburnamonine (-)		no	
Prestw-61	Morantel tartrate		no	
Prestw-616	Demecarium bromide		no	
Prestw-617	Quipazine dimaleate salt			no
Prestw-619	Diflorasone Diacetate	0.610204817	0.001675959	yes
Prestw-62	Homatropine hydrobromide (R,S)			no
Prestw-623	Pyridoxine hydrochloride			no
Prestw-626	Racecadotril		no	
Prestw-627	Folic acid	no		
Prestw-63	Nifedipine	no		
Prestw-630	Dimethisoquin hydrochloride			no

Prestw-631	Thiamine hydrochloride			no
Prestw-632	Dipivefrin hydrochloride			no
Prestw-633	Thiorphan			no
Prestw-64	Chlorpromazine hydrochloride			no
Prestw-641	Sulmazole	0.436896596	0.005633171	yes
Prestw-643	Flunisolide	0.635876191	0.008417054	yes
Prestw-644	N-Acetyl-DL-homocysteine Thiolactone			no
Prestw-645	Flurandrenolide	0.636960415	0.007943442	yes
Prestw-649	Etanidazole			no
Prestw-65	Diphenhydramine hydrochloride			no
Prestw-651	Glimepiride			no
Prestw-652	Picrotoxinin	0.160261438	0.069339383	yes
Prestw-653	Mepenzolate bromide			no
Prestw-654	Benfotiamine			no
Prestw-655	Halcinonide	0.60231122	0.014767943	yes
Prestw-656	Lanatoside C	0.984812221	0.000400162	yes
Prestw-657	Benzamil hydrochloride			no
Prestw-658	Suxibuzone			no
Prestw-659	6-Furfurylaminopurine			no
Prestw-66	Minaprine dihydrochloride			no
Prestw-660	Avermectin B1a			no
Prestw-666	Nisoldipine			no
Prestw-67	Miconazole			no
Prestw-671	Dydrogesterone			no
Prestw-676	Beta-Escin			no
Prestw-68	Isoxsuprine hydrochloride			no
Prestw-683	Pempidine tartrate			no
Prestw-688	Estropipate			no
Prestw-69	Acebutolol hydrochloride			no
Prestw-692	Citalopram Hydrobromide			no
Prestw-693	Promazine hydrochloride			no

Prestw-694	Sulfamerazine			no
Prestw-696	Ethotoin			no
Prestw-697	3-alpha-Hydroxy-5-beta-androstan-17-one			no
Prestw-698	Tetrahydrozoline hydrochloride			no
Prestw-699	Hexestrol			no
Prestw-7	Amiloride hydrochloride dihydrate			no
Prestw-70	Tolnaftate			no
Prestw-700	Cefmetazole sodium salt			no
Prestw-701	Trihexyphenidyl-D,L Hydrochloride			no
Prestw-702	Succinylsulfathiazole			no
Prestw-703	Famprofazone			no
Prestw-704	Bromopride			no
Prestw-705	Methyl benzethonium chloride			no
Prestw-706	Chlorcyclizine hydrochloride			no
Prestw-707	Diphenylpyraline hydrochloride			no
Prestw-708	Benzethonium chloride			no
Prestw-709	Trioxsalen			no
Prestw-71	Todralazine hydrochloride			no
Prestw-711	Sulfabenzamide			no
Prestw-712	Benzocaine			no
Prestw-713	Dipyrone			no
Prestw-714	Isosorbide dinitrate			no
Prestw-715	Sulfachloropyridazine			no
Prestw-716	Pramoxine hydrochloride			no
Prestw-717	Finasteride			no
Prestw-718	Fluorometholone	0.546621819	0.026697765	yes
Prestw-719	Cephalothin sodium salt			no
Prestw-72	Imipramine hydrochloride	0.552337921	0.001220565	yes
Prestw-720	Cefuroxime sodium salt			no
Prestw-721	Althiazide			no
Prestw-722	Isopyrin hydrochloride			no

Prestw-723	Phenethicillin potassium salt			no
Prestw-724	Sulfamethoxypyridazine			no
Prestw-725	Deferoxamine mesylate			no
Prestw-726	Mephentermine hemisulfate			no
Prestw-728	Sulfadimethoxine			no
Prestw-729	Sulfanilamide			no
Prestw-73	Sulindac			no
Prestw-730	Balsalazide Sodium			no
Prestw-731	Sulfaquinoxaline sodium salt			no
Prestw-732	Streptozotocin			no
Prestw-733	Metoprolol-(+,-) (+)-tartrate salt			no
Prestw-734	Flumethasone	0.578328937	0.035894338	yes
Prestw-735	Flecainide acetate			no
Prestw-736	Cefazolin sodium salt			no
Prestw-738	Folinic acid calcium salt			no
Prestw-739	Levonordefrin			no
Prestw-74	Amitryptiline hydrochloride			no
Prestw-740	Ebselen			no
Prestw-741	Nadide			no
Prestw-742	Sulfamethizole			no
Prestw-743	Medrysone	0.339177425	0.010461615	yes
Prestw-744	Flunixin meglumine			no
Prestw-745	Spiramycin			no
Prestw-746	Glycopyrrolate			no
Prestw-748	Monensin sodium salt			no
Prestw-749	Isoetharine mesylate salt			no
Prestw-75	Adiphenine hydrochloride			no
Prestw-750	Mevalonic-D, L acid lactone			no
Prestw-751	Terazosin hydrochloride			no

Prestw-752	Phenazopyridine hydrochloride			no
Prestw-753	Demeclocycline hydrochloride			no
Prestw-754	Fenoprofen calcium salt dihydrate			no
Prestw-755	Piperacillin sodium salt			no
Prestw-756	Diethylstilbestrol			no
Prestw-757	Chlorotrianisene			no
Prestw-758	Ribostamycin sulfate salt			no
Prestw-759	Methacholine chloride			no
Prestw-76	Dibucaine			no
Prestw-760	Pipenzolate bromide			no
Prestw-761	Butamben			no
Prestw-762	Sulfapyridine			no
Prestw-763	Meclofenoxate hydrochloride			no
Prestw-764	Furaltadone hydrochloride			no
Prestw-765	Ethoxyquin			no
Prestw-766	Tinidazole			no
Prestw-767	Guanadrel sulfate			no
Prestw-768	Vidarabine			no
Prestw-769	Sulfameter			no
Prestw-77	Prednisone			no
Prestw-770	Isopropamide iodide			no
Prestw-771	Alclometasone dipropionate	0.548857471	0.019210964	yes
Prestw-772	Leflunomide			no
Prestw-773	Norgestrel-(-)-D			no
Prestw-774	Fluocinonide	0.548669847	0.033125277	yes
Prestw-775	Sulfamethazine sodium salt			no
Prestw-776	Guaifenesin			no
Prestw-777	Alexidine dihydrochloride	0.899746757	0.004763748	yes
Prestw-778	Proadifen hydrochloride			no
Prestw-779	Zomepirac sodium salt			no
Prestw-78	Thioridazine hydrochloride			no
Prestw-780	Cinoxacin			no

Prestw-781	Clobetasol propionate	0.632383559	0.001669832	yes
Prestw-782	Podophyllotoxin	0.891825686	0.004025029	yes
Prestw-783	Clofibric acid			no
Prestw-784	Bendroflumethiazide			no
Prestw-785	Dicumarol			no
Prestw-786	Methimazole			no
Prestw-787	Merbromin			no
Prestw-788	Hexylcaine hydrochloride			no
Prestw-789	Drofenine hydrochloride			no
Prestw-79	Diphemanil methylsulfate			no
Prestw-790	Cycloheximide	0.760396853	0.010900281	yes
Prestw-791	(R) -Naproxen sodium salt			no
Prestw-792	Propidium iodide			no
Prestw-793	Cloperastine hydrochloride			no
Prestw-794	Eucatropine hydrochloride			no
Prestw-795	Isocarboxazid			no
Prestw-796	Lithocholic acid			no
Prestw-797	Methotrimeprazine maleat salt			no
Prestw-798	Dienestrol			no
Prestw-799	Pridinol methanesulfonate salt			no
Prestw-8	Amprolium hydrochloride			no
Prestw-80	Trimethobenzamide hydrochloride			no
Prestw-800	Amrinone			no
Prestw-801	Carbinoxamine maleate salt			no
Prestw-802	Methazolamide			no
Prestw-803	Pyrithyldione			no
Prestw-804	Spectinomycin dihydrochloride			no
Prestw-805	Piromidic acid			no
Prestw-806	Trimipramine maleate salt			no

Prestw-807	Chloropyramine hydrochloride				no
Prestw-808	Furazolidone		no		
Prestw-809	Dichlorphenamide		no		
Prestw-81	Metronidazole		no		
Prestw-810	Sulconazole nitrate			no	
Prestw-812	Cromolyn disodium salt			no	
Prestw-813	Bucladesine sodium salt				no
Prestw-814	Cefsulodin sodium salt			no	
Prestw-815	Fosfosal	no			
Prestw-816	Suprofen	no			
Prestw-818	Nadolol	no			
Prestw-819	Moxalactam disodium salt				no
Prestw-820	Aminophylline		no		
Prestw-821	Azlocillin sodium salt			no	
Prestw-822	Clidinium bromide		no		
Prestw-823	Sulfamonomethoxine			no	
Prestw-824	Benzthiazide		no		
Prestw-825	Trichlormethiazide			no	
Prestw-826	Oxalamine citrate salt			no	
Prestw-827	Propantheline bromide			no	
Prestw-829	Dimethadione		no		
Prestw-83	Edrophonium chloride			no	
Prestw-830	Ethaverine hydrochloride				no
Prestw-831	Butacaine	no			
Prestw-832	Cefoxitin sodium salt			no	
Prestw-833	Ifosfamide	no			
Prestw-834	Novobiocin sodium salt			no	
Prestw-836	Indoprofen	no			
Prestw-837	Carbenoxolone disodium salt				no
Prestw-838	Iocetamic acid		no		

Prestw-839	Ganciclovir	no		
Prestw-84	Moroxidine hydrochloride		no	
Prestw-840	Ethopropazine hydrochloride		no	
Prestw-842	Trimeprazine tartrate		no	
Prestw-843	Nafcillin sodium salt monohydrate			no
Prestw-844	Procyclidine hydrochloride		no	
Prestw-845	Amiprilose hydrochloride		no	
Prestw-846	Ethynylestradiol 3-methyl ether			no
Prestw-847	(-) -Levobunolol hydrochloride			no
Prestw-848	Iodixanol	no		
Prestw-85	Baclofen (R,S)		no	
Prestw-850	Equilin	no		
Prestw-851	Paroxetine Hydrochloride		no	
Prestw-853	Liothyronine		no	
Prestw-854	Roxithromycin		no	
Prestw-855	Beclomethasone dipropionate	0.516796469	0.01912019	yes
Prestw-856	Tolmetin sodium salt dihydrate			no
Prestw-857	(+) -Levobunolol hydrochloride			no
Prestw-858	Doxazosin mesylate		no	
Prestw-859	Fluvastatin sodium salt		no	
Prestw-86	Acyclovir	no		
Prestw-860	Methylhydantoin-5-(L)		no	
Prestw-861	Gabapentin	no		
Prestw-862	Raloxifene hydrochloride		no	
Prestw-864	Methylhydantoin-5-(D)		no	
Prestw-865	Simvastatin	no		
Prestw-866	Azacytidine-5		no	
Prestw-867	Paromomycin sulfate		no	
Prestw-868	Acetaminophen		no	
Prestw-869	Phthalylsulfathiazole		no	

Prestw-87	Diazoxide	no		
Prestw-870	Luteolin	no		
Prestw-871	Iopamidol	no		
Prestw-872	Iopromide	no		
Prestw-873	Theophylline monohydrate			no
Prestw-874	Theobromine	no		
Prestw-875	Reserpine	no		
Prestw-877	Scopolamine hydrochloride			no
Prestw-878	Ioversol	no		
Prestw-88	Amidopyrine	no		
Prestw-880	Carbachol	no		
Prestw-881	Niacin	no		
Prestw-882	Bemegride	no		
Prestw-883	Digoxigenin	0.942413923	0.003460901	yes
Prestw-884	Meglumine	no		
Prestw-886	Clioquinol	no		
Prestw-887	Oxybenzone	no		
Prestw-888	Promethazine hydrochloride			no
Prestw-893	Felbinac	no		
Prestw-894	Butylparaben		no	
Prestw-895	Aminohippuric acid			no
Prestw-896	N-Acetyl-L-leucine			no
Prestw-897	Pipemidic acid		no	
Prestw-898	Dioxybenzone		no	
Prestw-899	Adrenosterone		no	
Prestw-9	Hydrochlorothiazide			no
Prestw-90	Pindolol	no		
Prestw-900	Methylatropine nitrate			no
Prestw-901	Hymecromone	no		
Prestw-903	Diloxanide furoate			no
Prestw-904	Metyrapone	no		
Prestw-905	Urapidil hydrochloride			no
Prestw-906	Fluspirilen	no		
Prestw-907	S-(+)-ibuprofen		no	
Prestw-908	Ethynodiol diacetate			no
Prestw-909	Nabumetone	no		
Prestw-91	Khellin	no		

Prestw-910 Nisoxetine hydrochloride no

Prestw-911 (+)-Isoproterenol (+)-bitartrate salt no

Prestw-912 Monobenzone no
Prestw-913 2-Aminobenzenesulfonamide no

Prestw-914 Estrone no
Prestw-915 Lorglumide sodium salt no

Prestw-916 Nitrendipine no

Prestw-917 Flurbiprofen no

Prestw-918 Nimodipine no
Prestw-919 Bacitracin no
Prestw-92 Zimelidine dihydrochloride monohydrate no

Prestw-920 L(-)-vesamicol hydrochloride no

Prestw-921 Nizatidine no
Prestw-922 Thioperamide maleate no

Prestw-923 Xamoterol hemifumarate no

Prestw-924 Rolipram no
Prestw-925 Thonzonium bromide no

Prestw-926 Idazoxan hydrochloride no

Prestw-927 Quinapril HCl no

Prestw-928 Nilutamide no
Prestw-929 Ketorolac tromethamine no

Prestw-93 Azacyclonol no
Prestw-930 Protriptyline hydrochloride no

Prestw-931 Propofol no
Prestw-932 S(-)Eticlopride hydrochloride no

Prestw-933 Primidone no
Prestw-934 Flucytosine no
Prestw-935 (-)-MK 801 hydrogen maleate no

Prestw-936 Bephenium hydroxynaphthoate no

Prestw-937 Dehydroisoandosterone 3-acetate no

Prestw-938 Benserazide hydrochloride no

Prestw-939 Iodipamide no
Prestw-94 Azathioprine no

Prestw-941	Pentetic acid		no		
Prestw-942	Bretylium tosylate			no	
Prestw-943	Pralidoxime chloride			no	
Prestw-944	Phenoxybenzamine hydrochloride				no
Prestw-945	Salmeterol	no			
Prestw-946	Altretamine	no			
Prestw-947	Prazosin hydrochloride			no	
Prestw-948	Timolol maleate salt			no	
Prestw-949	(+,-)-Octopamine hydrochloride				no
Prestw-95	Lynestrenol	no			
Prestw-951	Crotamiton	no			
Prestw-953	(S)-(-)-Atenolol		no		
Prestw-954	Tyloxapol	no			
Prestw-955	Florfenicol	no			
Prestw-956	Megestrol acetate		no		
Prestw-957	Deoxycorticosterone			no	
Prestw-958	Urosiol	no			
Prestw-959	Proparacaine hydrochloride				no
Prestw-96	Guanabenz acetate		no		
Prestw-960	Aminocaproic acid		no		
Prestw-961	Denatonium benzoate			no	
Prestw-963	Enilconazole		no		
Prestw-964	Methacycline hydrochloride				no
Prestw-966	Sotalol hydrochloride			no	
Prestw-968	Decamethonium bromide			no	
Prestw-97	Disulfiram	0.810974666	0.041945599	yes	
Prestw-971	Remoxipride Hydrochloride				no
Prestw-972	THIP Hydrochloride			no	
Prestw-973	Pirlindole mesylate			no	
Prestw-974	Pronethalol hydrochloride				no

Prestw-975	Naftopidil dihydrochloride	0.590302611	0.008627842	yes
Prestw-976	Tracazolate hydrochloride			no
Prestw-977	Zardaverine			no
Prestw-978	Memantine Hydrochloride			no
Prestw-979	Ozagrel hydrochloride			no
Prestw-98	Acetylsalicylsalicylic acid			no
Prestw-980	Piribedil hydrochloride			no
Prestw-981	Nitrocaramiphen hydrochloride			no
Prestw-982	Nandrolone			no
Prestw-983	Dimaprit dihydrochloride			no
Prestw-986	Proscillaridin A	0.984088825	0.000202303	yes
Prestw-99	Mianserine hydrochloride			no
Prestw-991	Gliquidone			no
Prestw-992	Pizotifen malate			no
Prestw-993	Ribavirin			no
Prestw-994	Cyclopenthiazide			no
Prestw-995	Fluvoxamine maleate			no
Prestw-997	Fluticasone propionate	0.633845979	0.017135343	yes
Prestw-998	Zuclopenthixol hydrochloride	0.131241358	0.009244257	yes
Prestw-999	Proguanil hydrochloride			no

Compound Group Toxic Mean read-outs
Normalized mean read-outs Hit

PCL_ID compoundIdentifier Analysis Nuclei
Infected nuclei Infection index Plaques Virus intensity [AU]
Nuclei Infected nuclei Infection index Plaques Virus
intensity [AU] Nuclei Infected nuclei Infection index Plaques
Virus intensity [AU]
DMSO DMSO DMSO neg. ctr. no UZH 36’399 27’911 0.77
27.32 9.79E+09 1.00 1.00 1.00 1.00 1.00 - - - -
-
EPFL 29’749 15’156 0.51 21.11
5.02E+09 1.00 1.00 1.00 1.00 1.00
DFT DFT DFT pos. ctr. no UZH 30’204 3’595 0.12 0.12
2.90E+09 0.83 0.13 0.15 0.00 0.30 - - - - -
EPFL 20’745 1’776 0.09 0.03
1.62E+09 0.70 0.12 0.17 0.00 0.32
Prestw-1764 497 Nelfinavir mesylate PCL no UZH 30’908
5’479 0.18 0.75 2.98E+09 0.85 0.20 0.23 0.03 0.30 no yes
yes yes yes
EPFL 21’895 2’988 0.14 0.00
1.68E+09 0.74 0.20 0.27 0.00 0.33 no yes yes yes yes
Prestw-388 763 Dequalinium dichloride PCL yes UZH 28’763
13’751 0.48 14.00 3.62E+09 0.79 0.49 0.62 0.51 0.37 no yes
yes yes yes
EPFL 21’247 4’988 0.23 9.25
1.92E+09 0.71 0.33 0.46 0.44 0.38 yes yes yes yes yes
Prestw-1717 452 Aminacrine PCL no UZH 31’723 14’689 0.47
20.50 4.88E+09 0.87 0.53 0.62 0.75 0.50 no yes yes no
yes
EPFL 42’191 9’057 0.22 14.25
2.54E+09 1.42 0.60 0.42 0.67 0.51 no no yes no yes
Prestw-925 1214 Thonzonium bromide PCL no UZH 30’644
15’057 0.49 14.75 4.77E+09 0.84 0.54 0.63 0.54 0.49 no yes
yes no yes
EPFL 24’093 6’849 0.28 11.75
2.51E+09 0.81 0.45 0.56 0.56 0.50 no yes no no no