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 patients²,³ 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 US⁴. HAdV have a high prevalence⁵-⁸ and are broadly used as gene therapy vectors⁹ and oncolytic viruses¹⁰,¹¹. The high seroprevalence of HAdV-C2/5¹² 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 transplantation¹³.

More than 100 HAdV genotypes have been formally approved¹⁴ and are grouped into seven species based on hemagglutination assay and genome sequences¹⁵. 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 system⁷,¹³.
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. 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. 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. 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.

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. Cidofovir is a general inhibitor of viral DNA polymerases and impairs the replication of viral DNA. 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.

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 to anticancer candidates. For a full list of publications, see. 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. 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) (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).
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. 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. 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% CO₂, 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 ddH₂O 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*10⁵
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 was added and plates were sealed for long-term storage at 4°C. Following usage, tubings were rinse with 125 ml autoclaved ddH2O 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 Fluar, 0.20 NA, 15.5 mm WD, Nikon Instruments, Minato, Japan) at widefield mode. Image size 2,048² 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 2,048² 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 (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 according to Equation (1)

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

where \( \sigma_+ \) is the SD of the positive control, \( \sigma_- \) is the SD of the negative control, \( \mu_+ \) the mean of the positive control and \( \mu_- \) 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, EPFL used KNIME version 3.4.0 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 \( \mu_n \pm 2\sigma \) (mean of the negative control) threshold for number of nuclei. Efficacy was filtered by applying an excluding \( \mu_n \pm 3\sigma \) 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 \( \mu l \) 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).

**Usage Notes:**

**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:

**Input/Output:**

| 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). |
| Stitch: | Stitching of the images is not necessary, since every 384-well is imaged in a single site. |
| Mask: | Do not activate the tab. |
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\(^3\) (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:
We thank the entire Greber lab for fruitful discussions and critical assessment of the data.

Competing Interests:
The authors declare no conflict of interest.

Funding:
The work was supported by the Swiss National Science Foundation to UFG (Grant numbers 316030_170799 / 1 and 31003A_179256 / 1), and to GT (National Research Program “NCCR chemical biology”).

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

Assay Development
- Optimization of:
  - liquid handling
  - cell seeding
  - virus inoculation
  - positive and negative controls
  - timing
  - imaging
  - Plaque2.0 analysis

Assay Stability and Quality Testing
- preZ plate
- Z’ plates and Z’-scores

Definition of Post Processing Pipeline

AntiVir HAdV PCL Screening
- pre plate
- screening plates

UZH
- Imaging
- Infection Phenotype Scoring using Plaque2.0
- Data Processing for hit filtering

EPFL
- PCL Toxicity Testing in absence of infection using Presto-blue Assay
- Infection Phenotype Scoring using Plaque2.0
- Data Processing for hit filtering

Hit Comparison

Identification of PCL Best Hit

B

| Pre-spotting of Prestwick Chemical Library | A549 seeding on pre-spotted plates | Inoculation with HAdV-C2 | Fixation and staining | Automated epifluorescence imaging | Automated image analysis |
|------------------------------------------|----------------------------------|------------------------|----------------------|-------------------------------|-------------------------|
| day                                      | -n                               | 0                      | 1                    | +n                            | +n                      |

C

Prestwick Chemical Library +

D

0.0125% DMSO 1.25 μM Nelfinavir 1.25 μM DFT

Nuclei GFP
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.
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.
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 obtained by independent analysis at UZH and EPFL were calculated according to Equation 1 for 3 and 2σ.

| Barcode | Plate | UZH 3 σ | UZH 3 σ | EPFL 3 σ | EPFL 3 σ |
|---------|-------|---------|---------|---------|---------|
|          |       | 3 σ     |        | 3 σ     |        |
|          |       | 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 | 0.06 |
| 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 |

| Barcode | Plate | UZH 2 σ | UZH 2 σ | EPFL 2 σ | EPFL 2 σ |
|---------|-------|---------|---------|---------|---------|
|          |       | 2 σ     |        | 2 σ     |        |
|          |       | 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 |
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 obtained by independent analysis at UZH and EPFL were calculated according to Equation (1) for 3σ.

| Barcode   | Plate | UZH       | EPFL       |
|-----------|-------|-----------|------------|
|           |       | 3 sigma   | 3 sigma    |
|           |       | 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-100 | Nocodazole               | 0.75  | 0.08    | yes   |
| Prestw-1020 | Rimenoxone               | 0.39  | 0.00    | yes   |
| Prestw-1040 | Pyrimidimine             | 0.04  | 0.00    | yes   |
| Prestw-1044 | Predniscarbate           | 0.40  | 0.00    | yes   |
| Prestw-1014 | Prenoxin Lysinate        | 0.22  | 0.00    | yes   |
| Prestw-1110 | Parbendazole            | 0.40  | 0.02    | yes   |
| Prestw-1119 | Clofoglane acetate       | 0.53  | 0.02    | yes   |
| Prestw-1134 | Daeticine                | 0.91  | 0.00    | yes   |
| Prestw-1159 | Sulfamidin HCl           | 0.74  | 0.06    | yes   |
| Prestw-1118 | Nabuglubine hydrochloride | 0.87  | 0.00    | yes   |
| Prestw-1160 | Sporicidaline            | 0.86  | 0.03    | yes   |
| Prestw-1196 | TTopotecan               | 0.62  | 0.04    | yes   |
| Prestw-1198 | Tranilast               | 0.50  | 0.02    | yes   |
| Prestw-1272 | Zopiclone acetate       | 0.34  | 0.05    | yes   |
| Prestw-1274 | Mibrodostron            | 0.54  | 0.05    | yes   |
| Prestw-1247 | Aminodine               | 0.62  | 0.02    | yes   |
| Prestw-1248 | Claudimine              | 0.72  | 0.03    | yes   |
| Prestw-1290 | Carboxane acetate       | 0.38  | 0.08    | yes   |
| Prestw-1509 | Deflazocort             | 0.56  | 0.01    | yes   |
| Prestw-1565 | Paclitaxel              | 0.88  | 0.02    | yes   |
| Prestw-1754 | Desonide                | 0.48  | 0.06    | yes   |
| Prestw-1730 | Mefloquine pivalate      | 0.60  | 0.02    | yes   |
| Prestw-1715 | Algestone acetophenide  | 0.11  | 0.00    | yes   |
| Prestw-1722 | Azatadine maleate       | 0.28  | 0.13    | yes   |
| Prestw-1739 | Buprenorcin hydrochloride | 0.36  | 0.09    | yes   |
| Prestw-1741 | Lopetredol etbonate     | 0.46  | 0.05    | yes   |
| Prestw-1752 | E questions acetate     | 0.53  | 0.06    | yes   |
| Prestw-1761 | Ritrapiram benzate      | 0.43  | 0.00    | yes   |
| Prestw-1801 | Ciclesonide             | 0.55  | 0.03    | yes   |
| Prestw-1802 | Darunazol                | 0.43  | 0.06    | yes   |
| Prestw-1812 | Mefloquine pivalate      | 0.60  | 0.02    | yes   |
| Prestw-20 | Miconidil                | 0.06  | 0.01    | yes   |
| Prestw-200 | Camptothecine (S+)      | 0.69  | 0.02    | yes   |
| Prestw-217 | Mebendazole             | 0.36  | 0.02    | yes   |
| Prestw-217 | Mebendazole             | 0.36  | 0.02    | yes   |
| Prestw-222 | Antimycin A             | 0.53  | 0.08    | yes   |
| Prestw-223 | Viletromidin acetate     | 0.22  | 0.09    | yes   |
| Prestw-226 | Griserudin               | 0.37  | 0.07    | yes   |
| Prestw-244 | Glutethimide, para-amo  | 0.59  | 0.00    | yes   |
| Prestw-260 | Praziquintel            | 0.57  | 0.05    | yes   |
| Prestw-268 | Vinpocetine              | 0.41  | 0.01    | yes   |
| Prestw-271 | Vincamycin              | 0.25  | 0.00    | yes   |
| Prestw-272 | Indomethacin            | 0.41  | 0.00    | yes   |
| Prestw-273 | Cortisone               | 0.57  | 0.01    | yes   |
| Prestw-274 | Prednisolone            | 0.61  | 0.00    | yes   |
| Prestw-275 | Fenofibrate             | 0.15  | 0.01    | yes   |
| Prestw-279 | Methyldiprinodol, 6-alpha | 0.61  | 0.00    | yes   |
| Prestw-299 | Metformin               | 0.12  | 0.01    | yes   |
| Prestw-318 | Quinacrine acetophenide | 0.11  | 0.03    | yes   |
| Prestw-337 | Procarcumid hydrochloride | 0.14  | 0.01    | yes   |
| Prestw-339 | Guantacrine acetate     | 0.19  | 0.01    | yes   |
| Prestw-34 | Traitembene            | 0.14  | 0.00    | yes   |

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

1. The Image Data Resource (IDR). The Image Data Resource (IDR) at <https://idr.openmicroscopy.org/>
2. Krilov, L. R. Adenovirus infections in the immunocompromised host. Pediatr. Infect. Dis. J. 24, 555–566 (2005).
3. Greber, U. F., Arnberg, N., Wadell, G., Benkó, M. & Kremer, E. J. Adenoviruses - from pathogens to therapeutics: a report on the 10th International Adenovirus Meeting. Cell Microbiol. 15, 16–23 (2013).
4. Tunkel, A. R., Baron, E. L., Buch, K. A., Marty, F. M. & Martinez-Lage, M. Case 31-2019: A 45-Year-Old Woman with Headache and Somnolence. N. Engl. J. Med. 381, 1459–1470 (2019).
5. Gray, G. C. et al. Genotype prevalence and risk factors for severe clinical adenovirus infection, United States 2004-2006. Clin. Infect. Dis. 45, 1120–1131 (2007).
6. Metzgar, D. et al. Abrupt emergence of diverse species B adenoviruses at US military recruit training centers. J. Infect. Dis. 196, 1465–1473 (2007).
7. Lynch, J. P. & Kajon, A. E. Adenovirus: epidemiology, global spread of novel serotypes, and advances in treatment and prevention. Semin Respir Crit Care Med 37, 586–602 (2016).
8. Haque, E., Banik, U., Monowar, T., Anthony, L. & Adhikary, A. K. Worldwide increased prevalence of human adenovirus type 3 (HAdV-3) respiratory infections is well correlated with heterogeneous hypervariable regions (HVRs) of hexon. PLoS One 13, e0194516 (2018).
9. Ginn, S. L., Amaya, A. K., Alexander, I. E., Edelstein, M. & Abedi, M. R. Gene therapy clinical trials worldwide to 2017: An update. J Gene Med 20, e3015 (2018).
10. Jiang, H. et al. Oncolytic adenovirus research evolution: from cell-cycle checkpoints to immune checkpoints. Curr Opin Virol 13, 33–39 (2015).
11. Lawler, S. E., Speranza, M.-C., Cho, C.-F. & Chiocca, E. A. Oncolytic viruses in cancer treatment: A review. JAMA Oncol. 3, 841–849 (2017).
12. Mennechet, F. J. D. et al. A review of 65 years of human adenovirus seroprevalence. Expert Rev. Vaccines 18, 597–613 (2019).
13. Lion, T. Adenovirus persistence, reactivation, and clinical management. FEBS Lett. (2019). doi:10.1002/1873-3468.13576
14. Ismail, A. M. et al. Genomic foundations of evolution and ocular pathogenesis in human adenovirus species D. FEBS Lett. 593, 3583–3608 (2019).
15. Harrach, B., Tarján, Z. L. & Benkó, M. Adenoviruses across the animal kingdom: a walk in the zoo. FEBS Lett. (2019). doi:10.1002/1873-3468.13687
16. Reddy, V. S., Natchiar, S. K., Stewart, P. L. & Nemerow, G. R. Crystal structure of human adenovirus at 3.5 Å resolution. Science 329, 1071–1075 (2010).
17. Benevento, M. et al. Adenovirus composition, proteolysis, and disassembly studied by in-depth qualitative and quantitative proteomics. J. Biol. Chem. 289, 11421–11430 (2014).
18. Greber, U. F. & Flatt, J. W. Adenovirus entry: from infection to immunity. Annu. Rev. Virol. 6, 177–194 (2019).
19. Bauer, M. et al. The e3 ubiquitin ligase mind bomb 1 controls adenovirus genome release at the nuclear pore complex. Cell Rep. 29, 3785–3795.e8 (2019).
20. Prasad, V. et al. The UPR sensor IRE1α and the adenovirus E3-19Kglycoprotein sustain persistent and lytic infections. Nat. Commun. (2020).
21. Yakimovich, A. et al. Cell-free transmission of human adenovirus by passive mass transfer in cell culture simulated in a computer model. J. Virol. 86, 10123–10137 (2012).
22. Tollefson, A. E. et al. The adenovirus death protein (E3-11.6K) is required at very late stages of infection for efficient cell lysis and release of adenovirus from infected cells. J. Virol. 70, 2296–2306 (1996).
23. Doronin, K. et al. Overexpression of the ADP (E3-11.6K) protein increases cell lysis and spread of adenovirus. Virology 305, 378–387 (2003).
24. Lenaerts, L. & Naesens, L. Antiviral therapy for adenovirus infections. *Antiviral Res.* **71**, 172–180 (2006).

25. Wold, W. S. M., Tollefson, A. E., Ying, B., Spencer, J. F. & Toth, K. Drug development against human adenoviruses and its advancement by Syrian hamster models. *FEMS Microbiol. Rev.* **43**, 380–388 (2019).

26. Wall, G. *et al.* Screening a Repurposing Library for Inhibitors of Multidrug-Resistant Candida auris Identifies Ebselen as a Repositionable Candidate for Antifungal Drug Development. *Antimicrob. Agents Chemother.* **62**, (2018).

27. Chauvin, C. *et al.* High-Throughput Drug Screening Identifies Pazopanib and Clofilium Tosylate as Promising Treatments for Malignant Rhabdoid Tumors. *Cell Rep.* **21**, 1737–1745 (2017).

28. Prestwick Chemical publications. *Prestwick Chemical publications* at <http://www.prestwickchemical.com/libraries-publications.html>

29. Yakimovich, A. *et al.* Plaque2.0-A High-Throughput Analysis Framework to Score Virus-Cell Transmission and Clonal Cell Expansion. *PLoS One* **10**, e0138760 (2015).

30. Greber, U. F., Willetts, M., Webster, P. & Helenius, A. Stepwise dismantling of adenovirus 2 during entry into cells. *Cell* **75**, 477–486 (1993).

31. R Core Team. *R: A Language and Environment for Statistical Computing.* (R Foundation for Statistical Computing, 2018).

32. Berthold, M. R. *et al.* KNIME - the Konstanz information miner. *SIGKDD Explor. Newsl.* **11**, 26 (2009).
| Barcode   | Plate  | numberOf Nuclei | numberOf Infected Nuclei | infection Index | numberOf Plaques | total Virus Intensity | numberOf Nuclei | numberOf Infected Nuclei | infection Index | numberOf Plaques | total Virus Intensity |
|-----------|--------|-----------------|--------------------------|-----------------|------------------|----------------------|-----------------|--------------------------|-----------------|------------------|----------------------|
| BSF018104 | Za     | -1.11           | 0.50                     | 0.57            | 0.07             | -1.20                | 0.36            | 0.47                     | 0.52            | 0.08             |                      |
| BSF018105 | Zb     | -8.10           | 0.30                     | 0.45            | -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                 |

| Barcode   | Plate  | numberOf Nuclei | numberOf Infected Nuclei | infection Index | numberOf Plaques | total Virus Intensity | numberOf Nuclei | numberOf Infected Nuclei | infection Index | numberOf Plaques | total Virus 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                 |
| Barcode     | Plate     | NumberOf Nuclei | NumberOf Infected Nuclei | Infection Index | NumberOf Plaques | Total Virus Intensity | NumberOf Nuclei | NumberOf Infected Nuclei | Infection Index | NumberOf Plaques | Total Virus 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 | yes | | |
| Prestw-1000| Lymecycline no | no | | |
| Prestw-1001| Alfadolone acetate no | no | | |
| Prestw-1002| Alfaxalone no | no | | |
| Prestw-1003| Azapropazone no | no | | |
| Prestw-1004| Meptazinol hydrochloride no | no | | |
| Prestw-1005| Apramycin no | no | | |
| Prestw-1007| Pursultiamine Hydrochloride no | no | | |
| Prestw-1008| Gabexate mesilate no | no | | |
| Prestw-1009| Pivampicillin no | no | | |
| Prestw-101| R(-) Apomorphine hydrochloride hemihydrate no | no | | |
| Prestw-1011| Flucloxacillin sodium no | no | | |
| Prestw-1012| Trapidil no | no | | |
| Prestw-1013| Deptropine citrate no | no | | |
| Prestw-1014| Sertraline no | no | | |
| Prestw-1015| Ethamsylate no | no | | |
| Prestw-1016| Moxonidine no | no | | |
| Prestw-1017| Etilefrine hydrochloride no | no | | |
| Prestw-1018| Alprostadil no | no | | |
| Prestw-1019| Tribenoside no | no | | |
| Prestw-102| Amoxapine no | no | | |
| Prestw-1020| Rimexolone 0.392103742 0.075804134 yes | yes | | |
| Prestw-1021| Isradipine no | no | | |
| Prestw-1022| Isometheptene mucate no | no | | |
| Prestw-1024| Nifurtimox no | no | | |
| Prestw-1025| Letrozole no | no | | |
| Prestw-1026| Arbutin no | no | | |
| Prestw-1027| Tocainide hydrochloride no | no | | |
| Prestw-1028| Benzathine benzylpenicillin no | no | | |
| Prestw-1029| Risperidone no | no | | |
| Prestw-103| Cyproheptadine hydrochloride no | no | | |
| Prestw-1030| Torsemide no | no | | |
| Code     | Name                              | Status |
|----------|-----------------------------------|--------|
| 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 | Metyldopate hydrochloride        | no     |
| Prestw-1039 | Levocabastine hydrochloride      | no     |
| Prestw-104  | Famotidine                       | no     |
| Prestw-1040 | Pyrvinium pamoate                | yes    |
| Prestw-1041 | Etomidate                        | no     |
| Prestw-1042 | Tridihexethyl chloride           | no     |
| Prestw-1043 | Penbutolol sulfate               | no     |
| Prestw-1044 | Prednicarbate                    | 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 | Methiazone | 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 Nalidixic acid  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
| Code       | Name                        | Concentration | Stability | Result |
|------------|-----------------------------|---------------|-----------|--------|
| Prestw-1134 | Cytarabine                 | 0.905540871   | 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   | 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   | yes       |
| Prestw-1180 | Docetaxel                   | 0.856343595   | 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            |           |
| Code       | Name                           | Action | Concentration | Confirmed |
|------------|--------------------------------|--------|---------------|-----------|
| Prestw-119 | Picotamide monohydrate         | no     |               |           |
| Prestw-1190| Olmesartan                     | no     |               |           |
| Prestw-1192| Oxandrolone                    | no     |               |           |
| Prestw-1195| Toltrazuril                    | no     |               |           |
| Prestw-1196| Topotecan                      | yes    | 0.61923066    | 0.043792234 |
| Prestw-1197| Toremifene                     | no     |               |           |
| Prestw-1198| Tranilast                      | yes    | 0.502083509   | 0.024539976 |
| Prestw-1199| Tripeleennamine hydrochloride  | no     |               |           |
| Prestw-12  | Benzonatate                    | yes    | 0.853668407   | 0.055294598 |
| Prestw-120 | Triamcinolone                  | yes    | 0.600492086   | 0.025733241 |
| 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| Benztrpine mesylate           | no     |               |           |
| Prestw-1239| Bicalutamide                  | no     |               |           |
| Prestw-1241| Bifonazole                    | no     |               |           |
| Code   | Name                            | Action |
|--------|---------------------------------|--------|
| Prestw-1242 | Erlotinib                      | no     |
| Prestw-1244 | Bosentan                      | no     |
| Prestw-1246 | Bromhexine hydrochloride      | no     |
| Prestw-1249 | Famiclovir                     | no     |
| Prestw-125  | Perphenazine                   | no     |
| Prestw-1251 | Butalbital                     | no     |
| Prestw-1252 | Butenafine Hydrochloride      | no     |
| Prestw-1253 | Butylscopolammonium (n-) bromide | no |
| Prestw-1254 | Pentiazac                      | 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                    | yes    |
| Prestw-1267 | Gestrinone                     | no     |
| Prestw-1268 | Guaiacol                       | no     |
| Prestw-1269 | Haloprogin                     | no     |
| Prestw-127  | Isoniazole                     | 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 | Hydroxycholoroquine 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     |
| Code     | Name                              | Value   | Available |
|----------|-----------------------------------|---------|-----------|
| 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 Nyldrin 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 Penipentol | 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 |
| Code         | Name                              | Yes/No  |
|--------------|-----------------------------------|---------|
| Prestw-1709  | Estramustine                       | no      |
| Prestw-171   | Tranexamic acid                    | no      |
| Prestw-1710  | Ethoxzolamide                      | no      |
| Prestw-1711  | Felbamate                          | no      |
| Prestw-1712  | Flumethasone pivalate              | yes     |
| Prestw-1713  | Fenoldopam                         | no      |
| Prestw-1714  | Adapalene                          | no      |
| Prestw-1715  | Algestone acetophenide             | yes     |
| Prestw-1716  | Altenogest                         | 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                  | yes     |
| Prestw-1723  | Benzoxiquine                       | no      |
| Prestw-1726  | Cefpiramid                         | no      |
| Prestw-1727  | Cefpodoxime proxetil               | no      |
| Prestw-1728  | Cefprozil                          | no      |
| Prestw-1729  | Ceftibuten                         | no      |
| Prestw-173   | Tranycypromine 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         | yes     |
| Prestw-1741  | Loteprednol etabonate              | 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
| Code   | Compound                      | Result |
|--------|-------------------------------|--------|
| 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 | Tirastricol, 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 | Penspiride 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 |
| Product Code | Product Name                  | Test Result |
|-------------|-------------------------------|-------------|
| 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                  | 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                   | yes         |
| Prestw-269  | Clomipramine hydrochloride    | no          |
| Prestw-27   | Doxylamine succinate          | no          |
| Prestw-270  | Pendiline hydrochloride       | no          |
| Prestw-271  | Vincamine                     | yes         |
| Prestw-272  | Indomethacin                  | yes         |
| Prestw-273  | Cortisone                     | yes         |
| Prestw-274  | Prednisolone                  | yes         |
| Prestw-275  | Fenofibrate                   | 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 | Acetzolamide | 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 |
| Prestw-319 | Clofilium tosylate | yes |
| 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 |
| Name                        | Code       | Value       | Yes/No   |
|-----------------------------|------------|-------------|----------|
| Zoxazolamine                | Prestw-328 | no          |          |
| Tacrine hydrochloride       | Prestw-329 | no          |          |
| Diprophylline               | Prestw-33  | no          |          |
| Bisoprolol fumarate         | Prestw-330 | no          |          |
| Tremorine dihydrochloride   | Prestw-331 | no          |          |
| Practolol                   | Prestw-332 | no          |          |
| Zidovudine, AZT             | Prestw-333 | no          |          |
| Sulfisoxazole               | Prestw-334 | no          |          |
| Zaprinast                   | Prestw-335 | no          |          |
| Chlormezanone               | Prestw-336 | no          |          |
| Procainamide hydrochloride  | Prestw-337 | 0.137586477 | yes      |
| N6-methyladenosine          | Prestw-338 | no          |          |
| Guanfacine hydrochloride    | Prestw-339 | 0.187986194 | yes      |
| Triamterene                 | Prestw-34  | 0.141584474 | yes      |
| Domperidone                 | Prestw-340 | no          |          |
| Furosemide                  | Prestw-341 | no          |          |
| Methapyrilene hydrochloride | Prestw-342 | no          |          |
| Desipramine hydrochloride   | Prestw-343 | no          |          |
| Clorgyline hydrochloride    | Prestw-344 | no          |          |
| Clenbuterol hydrochloride   | Prestw-345 | no          |          |
| Maprotiline hydrochloride   | Prestw-346 | no          |          |
| Thioguanosine               | Prestw-347 | 0.179913987 | yes      |
| Chlorprothixene hydrochloride | Prestw-348 | no          |          |
| Ritodrine hydrochloride     | Prestw-349 | no          |          |
| Dapsone                     | Prestw-35  | no          |          |
| Clozapine                   | Prestw-350 | no          |          |
| Chlorthalidone              | Prestw-351 | no          |          |
| Dobutamine hydrochloride    | Prestw-352 | no          |          |
| Moclobemide                 | Prestw-353 | 0.142220859 | yes      |
| Hycanthone                  | Prestw-355 | 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 | Benz bromarone | 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
| Code  | Compound                        | Availability |
|-------|---------------------------------|--------------|
| Prestw-42 | Moxisylyte hydrochloride       | 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           |
| Code   | Name                                           | Molecular Weight | Molar Extinction Coefficient | Result |
|--------|------------------------------------------------|------------------|-------------------------------|--------|
| Prestw-455 | Mehydroline 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-459 | Naphazoline hydrochloride                     | no               |                               |        |
| Prestw-460 | Dinoprost trometamol                          | no               |                               |        |
| Prestw-461 | Tropisetron HCl                               | no               |                               |        |
| Prestw-462 | Cefixime                                       | no               |                               |        |
| Prestw-463 | Metrizamide                                    | no               |                               |        |
| Prestw-464 | Neostigmine bromide                           | no               |                               |        |
| Prestw-465 | Niridazole                                     | no               |                               |        |
| Prestw-466 | Ticlopidine hydrochloride                     | no               |                               |        |
| Prestw-467 | Ceforanide                                     | no               |                               |        |
| Prestw-468 | Cefotetan                                      | no               |                               |        |
| Prestw-469 | Brompheniramine maleate                       | no               |                               |        |
| Prestw-470 | Primaquine diphosphate                        | 0.161620847      | 0.011225059                   | yes    |
| Prestw-471 | Progesterone                                   | no               |                               |        |
| Prestw-472 | Felodipine                                     | 0.156799322      | 0.007799217                   | yes    |
| Prestw-473 | Dicyclomine hydrochloride                     | 0.132347475      | 0.02511396                    | yes    |
| Prestw-474 | Serotonin hydrochloride                       | 0.132305018      | 0.005810307                   | yes    |
| Prestw-475 | Cefotam hydrochloride                          | no               |                               |        |
| Prestw-476 | Benperidol                                     | no               |                               |        |
| Prestw-477 | Cefaclor hydrate                              | no               |                               |        |
| Prestw-478 | Colistin sulfate                               | no               |                               |        |
| Prestw-479 | Daunorubicin hydrochloride                    | 1.002834608      | 0.00290379                    | yes    |
| Prestw-480 | Dosulepin hydrochloride                       | no               |                               |        |
| Prestw-481 | Ceftazidime pentahydrate                      | no               |                               |        |
| Prestw-482 | Amyleine hydrochloride                        | no               |                               |        |
| Prestw-483 | Iobenguane sulfate                            | no               |                               |        |
| Prestw-484 | Metixene hydrochloride                        | no               |                               |        |
Prestw-492 Nitrofurazone   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             |
| Code   | Name                                           | Status |
|--------|------------------------------------------------|--------|
| 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 | Tetracaine hydrochloride                        | no     |
| Prestw-572 | Mometasone furoate                              | 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 | Isofupredone acetate                            | 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                           | 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     |
| Code    | Compound                                | Activity |
|---------|-----------------------------------------|----------|
| 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 | yes |
| Prestw-719 | Cephalothin sodium salt | no |
| Prestw-72 | Imipramine hydrochloride | 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 Mephenetermine hemisulfate no
Prestw-728 Sulfadimethoxine no
Prestw-729 Sulfanilamide no
Prestw-73 Sulindac no
Prestw-730 Balsalazide Sodium no
Prestw-731 Sulfadinoxaline 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 | Sulfamer | 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 | Clofibrate 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 maleate 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 |
| Code       | Chemical Name                      | Presence |
|------------|------------------------------------|----------|
| 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 Phthalysulfathiazole no
| Code   | Name                        | Result |
|--------|-----------------------------|--------|
| 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 Loroglumide 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 Benzerazide 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 | Tyloxoapol | 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 |
|        | Name                              |      |      |        |
|--------|-----------------------------------|------|------|--------|
| 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 | Cyclopentiazide                  |      |      | 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     |
| PCL_ID      | compoundIdentifier | Analysis | Nuclei Infected nuclei | Infection index | Plaques | Virus intensity [AU] | Hit |
|-------------|--------------------|----------|------------------------|-----------------|---------|----------------------|-----|
| 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    | -                    | -   |
|             | EPFL               | 29'749   | 15'156                 | 0.51            | 21.11   |
| 5.02E+09    | 1.00               | 1.00     | 1.00                   | 1.00            | 1.00    | -                    | -   |
| DFT         | DFT                | pos. ctr. | no                     | UZH             | 30'204  | 3'595                | 0.12|
| 2.90E+09    | 0.83               | 0.13     | 0.15                   | 0.00            | 0.30    | -                    | -   |
|             | EPFL               | 20'745   | 1'776                  | 0.98            | 0.03    |
| 1.62E+09    | 0.70               | 0.15     | 0.00                   | 0.32            |
| Prestw-1764 | Nelfinavir mesylate| PCL      | no                     | UZH             | 30'908  |
| 497         | Prestw-388         | Dequalinium dichloride | yes | UZH | 28'763 |
| Prestw-1717 | Aminacrine        | Prestw-925 | Thonzonium bromide   | no | UZH | 30'644 |
| 1764        | Prestw-925        | 452      | 1214                   | 1375            |
| 497         | Prestw-1717       | 452      | 1214                   | 1375            |
| 497         | Prestw-925        | 452      | 1214                   | 1375            |
