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Mitigation of NADPH Oxidase 2 Activity as a Strategy to Inhibit Peroxynitrite Formation*[S]

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Using high throughput screening-compatible assays for superoxide and hydrogen peroxide, we identified potential inhibitors of the NADPH oxidase (Nox2) isoform from a small library of bioactive compounds. By using multiple probes (hydroethidine, hydropropidine, Amplex Red, and coumarin boronate) with well defined redox chemistry that form highly diagnostic marker products upon reaction with superoxide ($O_2^{\cdot-}$), hydrogen peroxide (H_2O_2), and peroxynitrite ($ONOO^-$), the number of false positives was greatly decreased. Selected hits for Nox2 were further screened for their ability to inhibit $ONOO^-$ formation in activated macrophages. A new diagnostic marker product for $ONOO^-$ is reported. We conclude that the newly developed high throughput screening/reactive oxygen species assays could also be used to identify potential inhibitors of $ONOO^-$ formed from Nox2-derived $O_2^{\cdot-}$ and nitric oxide synthase-derived nitric oxide.

NADPH oxidase (Nox)[4] enzymes (Nox1–5 and Duox1/2) have been proposed as potential therapeutic targets in the treatment of a variety of inflammatory and fibrotic diseases, including cancer (1–3). Unlike other redox-active enzymes for which generation of reactive oxygen species (ROS) is an "accidental" by-product of their primary catalytic function, the only known function of Nox enzymes is generation of ROS (*e.g.* $O_2^{\cdot-}$ and H_2O_2) (Fig. 1) (4, 5). Several Nox isoforms, including Nox2, form both $O_2^{\cdot-}$ and H_2O_2 (via dismutation of $O_2^{\cdot-}$), with the exception of Nox4, which generates primarily H_2O_2 with little or no detectable $O_2^{\cdot-}$ (4, 5). A major impediment to advancing Nox research is the paucity of selective inhibitors of Nox isoforms, including Nox1 and -2 (6). This is due in part to the lack of reliable and high throughput-compatible detection probes and assays that are specific for $O_2^{\cdot-}$ and H_2O_2. With the recent discovery of new probes with well defined redox chemistry that form highly diagnostic marker products upon reaction with ROS/RNS both under *in vitro* and *in vivo* conditions and high throughput global profiling assays (Table 1) (7), we can now screen a small library of bioactive compounds. One of the objectives of this study is to identify small molecule inhibitors of the Nox2 isoform using the high throughput screening (HTS)/ROS-based assay(s) that largely eliminate false positives. Previously, we reported the power of our newly developed HTS/ROS assays in identifying true "hits" for Nox2 inhibition and eliminating false positives at the outset (8). Typically, the chemiluminescent probe, L-012, has been used in Nox assay (9). Comparison between L-012 assay and our HTS/ROS assay revealed that L-012 increased false positives by at least a factor of 4 and that this increase is due to inhibition of peroxidase enzyme used in the L-012/Nox assay (10). A related objective of this study is to also identify new small molecule inhibitors of RNS (*e.g.* peroxynitrite). Peroxynitrite ($ONOO^-$) is a potent oxidizing and nitrating species formed from a diffusion-controlled reaction between $O_2^{\cdot-}$ and nitric oxide ('NO) (Fig. 1) (11, 12) and has been implicated in various neurodegenerative and cardiovascular diseases (13–15). Although ongoing efforts focus on antinitration strategies mostly through direct scavenging of $ONOO^-$ and/or related species (16), a better approach is to suppress the sources of generation of $O_2^{\cdot-}$ (Nox) and/or inhibition of nitric-oxide synthase, particularly inducible NOS (Fig. 1) (17, 18). In this study, we identified several candidate Nox2 inhibitors through HTS-based ROS assays from testing a library of >2,000 bioactive compounds at Broad Institute. Selected hits for Nox2 inhibition were further tested for inhibition of $ONOO^-$ formation in activated macrophages. Results suggest that the HTS/ROS strategy developed herein could be used to

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[S] This article contains supplemental Table S1.

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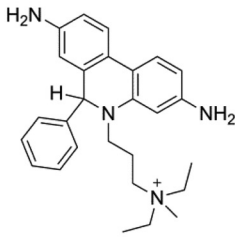
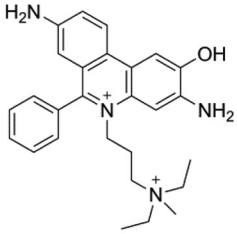
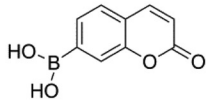
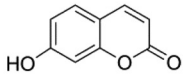
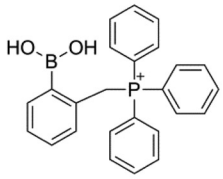
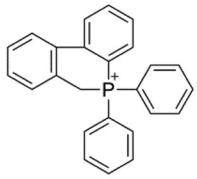
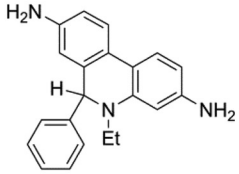
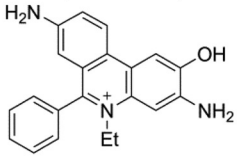
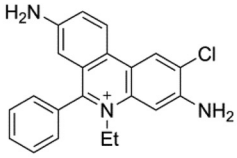
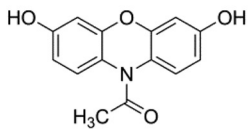
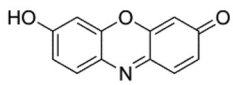
[4] The abbreviations used are: Nox, NADPH oxidase; HTS, high throughput screening; ROS, reactive oxygen species; RNS, reactive nitrogen species; HE, hydroethidine; SOD, superoxide dismutase; CBA, coumarin boronic acid; HPr^+, hydropropidine; 2-OH-Pr^{2+}, 2-hydroxypropidium; 2-OH-E^+, 2-hydroxyethidium; PMA, phorbol myristate acetate; cyclo-*o*-MitoPh, 9,10-dihydro-9,9-diphenyl-9-phosphoniaphenanthrene bromide; COH, 7-hydroxycoumarin; *d*HL60, differentiated HL60; MPO, myeloperoxidase; HBSS, Hanks' balanced saline solution; DEPMPO, 5-(diethoxyphosphoryl)-5-methyl-1-pyrroline-*N*-oxide; DPI, diphenyleneiodonium; dtpa, diethylenetriaminepentaacetate.

TABLE 1
Structures of ROS/RNS-specific probes, their reaction products and detection methods

Probe	Diagnostic product(s)	ROS/RNS species	Detection technique(s)
Hydropropidine (HPr^+) 	2-Hydroxypropidium (2-OH-Pr^{++}) 	$O_2^{\bullet-}$-specific product	• HPLC with fluorescence detection • LC-MS • Fluorimetry of the complex of 2-OH-Pr^{++} with DNA
Coumarin boronic acid (CBA) 	7-Hydroxycoumarin (COH) 	H_2O_2 (catalase-sensitive) $ONOO^-$ (catalase-insensitive) HOCl (catalase-sensitive, MPO inhibitor-sensitive)	• HPLC with fluorescence detection • LC-MS • Fluorimetry
ortho-MitoPhB$(OH)_2$ 	*cyclo-o*-MitoPh 	$ONOO^-$-specific product	• LC-MS
Hydroethidine (HE) 	2-Hydroxyethidium (2-OH-E^+) 	$O_2^{\bullet-}$-specific product	• HPLC with fluorescence detection • LC-MS • Fluorimetry of the complex of 2-OH-E^+ with DNA
	2-Chloroethidium (2-Cl-E^+) 	HOCl-specific product	• LC-MS
Amplex Red 	Resorufin 	H_2O_2 (HRP-dependent, catalase-sensitive)	• HPLC with fluorescence detection • Fluorimetry

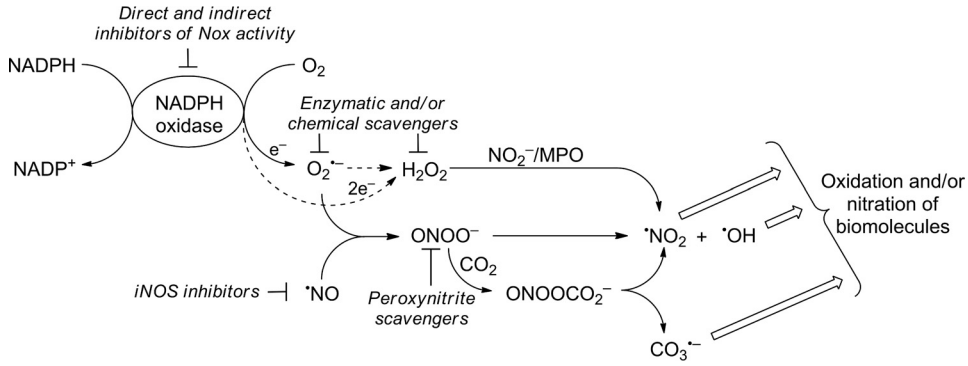


FIGURE 1. **Generation of reactive oxygen and reactive nitrogen species from NADPH oxidase and nitric-oxide synthase, and their abrogation by Nox inhibitors and ROS/RNS scavengers.**

identify Nox2 inhibitors that inhibit $ONOO^-$ formation. In this study we also discovered a new diagnostic marker product for specific detection and quantitation of peroxynitrite in biological systems. One of the objectives of this study is to also use these candidate inhibitors of Nox2 as potential inhibitors of $ONOO^-$ generated via Nox2 intermediacy.

Experimental Procedures

Materials—All compounds in the HTS library were routinely dissolved in DMSO and stored at −20 °C. DMSO concentration (<1%) was kept the same in both control and treatment conditions. In confirmatory studies, stock solutions were prepared at higher concentrations (typically 10 mM or higher), such that the final concentration of the solvent vehicle was kept minimal (<0.3% v/v) upon dilution. Hydropropidine (HPr^+), coumarin boronic acid (CBA), and *ortho*-mito-phenylboronic acid (*o*-MitoPhB$(OH)_2$) were synthesized according to published procedures (19–22). Deuterated (d_{15}) analogs of *o*-MitoPhB$(OH)_2$ and *o*-Mito$PhNO_2$ were synthesized in the analogous protocol to *o*-MitoPhB$(OH)_2$ but using deuterated triphenylphosphine (d_{15}-PPh_3), whereas d_{15}-*o*-MitoPhOH was synthesized by oxidation of d_{15}-*o*-MitoPhB$(OH)_2$ by excess H_2O_2. Amplex Red (10-acetyl-3,7-dihydroxyphenoxazine), resorufin, and 7-hydroxycoumarin were purchased from Cayman and Sigma. Hydroethidine (HE) was from Invitrogen. Authentic standards of 2-hydroxyethidium (2-OH-E^+) and 2-hydroxypropidium (2-OH-Pr^{2+}) were synthesized as described previously (19, 23, 24). Stock solutions of CBA, HE, and Amplex Red were prepared at 20–100 mM concentration in DMSO and stored at −80 °C. For experiments involving HOCl, DMSO was replaced with ethanol. Horseradish peroxidase (HRP, type VI), superoxide dismutase (SOD), catalase and all other reagents were obtained from Sigma.

For organic synthesis, THF was distilled under dry argon atmosphere in the presence of sodium and benzophenone. All reagents were used as received without further purification. The reactions were monitored by TLC on silica gel (Merck 60F254). Crude materials were purified by flash chromatography on Merck silica gel 60 (0.040–0.063 mm). ^{31}P NMR, ^1H NMR, and ^{13}C NMR spectra were recorded with Bruker DPX 300 or 400 spectrometers at 121.49, 300.13, and 75.54 MHz, respectively. ^{31}P NMR measurements were carried out in $CDCl_3$ using 85% H_3PO_4 as an external standard with broad band ^1H decoupling. ^1H NMR and ^{13}C NMR measurements were carried out in $CDCl_3$ using TMS or $CDCl_3$ as internal reference, respectively. Chemical shifts (δ) are reported in parts/million and coupling constant *J* values in hertz. Mass spectrometry analyses were performed at the University of Aix-Marseille (Spectropole).

HTS-compatible Cellular Models of Nox2—Human promyelocytic leukemia HL60 cells (Sigma) differentiated into neutrophil-like cells by all-*trans*-retinoic acid were used as the HTS-compatible source of Nox2 model system for screening Nox2 inhibitors (25, 26). HL60 cells were incubated with all-*trans*-retinoic acid (1 μM) for 4–5 days for converting nondifferentiated cells into differentiated cells. Nox2 activation was achieved by treating differentiated HL60 (*d*HL60) cells with phorbol myristate acetate (PMA, 1 μM) (8).

High Throughput Screening of the Small Library of Bioactive Compounds at Broad Institute—To test the inhibitory effects of the compounds included in the library of the bioactive compounds, we preincubated *d*HL60 cells with the potential inhibitors for 30 min, followed by addition of PMA and the appropriate probe, as shown in Table 2. After 90 min of incubation at 37 °C in a CO_2-free incubator, the extent of oxidation of the probes was measured with PerkinElmer Life Sciences Envision plate reader (PerkinElmer Life Sciences) using the following excitation/emission filter sets: 485/590 nm, 355/460 nm, and 531/595 nm, for hydropropidine + DNA, coumarin boronic acid, and Amplex Red + HRP, respectively.

Signal Optimization, HTS Statistics, and Z′ Values—We used the Z′ factor method as a measure of the assay quality or performance. As positive control (control+ signal), *d*HL60 cells were incubated with PMA in the presence of DMSO. The negative control (control− signal) included cells in the presence of phenylarsine oxide (1 μM) used as Nox2 inhibitor. The dynamic range was established by the difference between averaged maximal (control+) and minimal (control−) signals. The Z′ factor was calculated using Equation 1 (27),

$$Z' = 1 - \frac{3SD_{control+} + 3SD_{control-}}{|mean_{control+} - mean_{control-}|} \qquad \text{(Eq. 1)}$$

where control+ and control− correspond to PMA-stimulated cells in the presence of DMSO only or 1 μM phenylarsine oxide, respectively, and S.D. values are the corresponding standard deviations.

The calculated Z′ values determined at Broad Institute in 384-well plates for all three HTS assays (hydropropidine + DNA, coumarin boronic acid, and Amplex Red + HRP) were 0.45, 0.64, and 0.79, respectively. Assuming the inhibitor identification threshold of 3× S.D. deviation of the neutral (negative) control (DMSO), we can determine positive hits with a 42, 28, and 15% inhibition for hydropropidine + DNA, coumarin boronic acid, and Amplex Red + HRP, respectively.

Oxygen Consumption Experiments—Nox activity was determined by measuring rates of oxygen consumption in PMA-activated differentiated HL60 cells using a Seahorse XF96 extracellular flux analyzer (8, 28). Cell suspensions were prepared in phenol red-free RPMI 1640 medium (without bicarbonate) and aliquoted (80 μl per well) into 96-well plates to obtain a final cell count of 2×10^4 cells per well. After spinning down the cells, additional RPMI 1640 medium (100 μl per well) was added. Oxygen measurements were initiated, and at the specified time points, inhibitors of Nox were added, followed by injection of PMA. Alternatively, cells were pre-incubated with Nox2 inhibitors and transferred into measurement plates, and the response to PMA was tested. We used rotenone (1 μM) and antimycin (10 μM) to dissect out the contribution of mitochondrial respiration to the total oxygen consumption rate. This also enables one to monitor the effects of Nox2 inhibitors on mitochondrial respiration (8).

Synthesis of 9,10-Dihydro-9,9-diphenyl-9-phosphoniaphenanthrene bromide (cyclo-o-MitoPh)—cyclo-*o*-MitoPh was obtained by adapting the procedures described in the literature (29–31). The scheme for synthesis of cyclo-*o*-MitoPh is shown in Fig. 9*a*. Briefly, after formulation of compound **1** in the presence of *n*-butyl lithium and *N*,*N*-dimethylformamide, compound **2** was reduced by sodium borohydride to obtain compound **3**. Bromation of compound **3** by PBr_3 afforded compound **4** (29). A solution of 2′-bromo-2-bromomethylbiphenyl **4** (3.3 g, 10 mmol) in methanol (100 ml) was heated under reflux for 24 h. After solvent removal, the light yellow liquid compound was distillated from the reaction mixture to obtain 2′-bromo-2-methoxymethylbiphenyl **5** (2.5 g, 90%) with the following parameters: ^{1}H NMR (400 MHz): δ 7,66–7.64 (1H, d, J = 8.2), 7.55–7.54 (1H, d, J = 7.2), 7.44–7.40 (1H, t), 7.37–7.34 (2H, m), 7.27–7.21 (2H, m), 7.16–7.14 (1H, d, J = 6.5), 4.29–4.26 (1H, d, J = 12.3), 4.17–4.14 (1H, d, J = 12.3), 3.25 (3H, s); and ^{13}C NMR (300 MHz): δ 141.8–141.4 (d), 140.8–140.2 (d), 136.1 (s), 135.4 (s), 132.5 (s), 131.1 (s), 130.0 (s), 129.6–129.0 (m), 128.1–128.1 (d), 127.9–127-2 (m), 127.1–127.0 (d), 123.6 (s), 72.4–72.0 (d), 58.2–58.1 (d). MS calculated for $C_{14}H_{13}BrO$ was 277.1 and found was 277.1.

The Grignard reagent was prepared from 2′-bromo-2-methoxymethylbiphenyl **5** (1.6 g, 5.8 mmol), magnesium turnings (0.4 g), and trace amount of iodine in THF (20 ml). Then diphenylphosphinous chloride (1.91 g, 8.6 mmol) in THF (20 ml) was added under argon. The mixture was heated under reflux for 3 h. After addition of diluted HCl, the compound was extracted with diethyl ether from aqueous solution. The ether phase was dried with Na_2SO_4 and solvent, and some volatile part of residue was distilled. 2′-Diphenylphosphino-2-methoxymethylbiphenyl **6** was recrystallized from ethanol (380 mg, 15%).

The NMR parameters of compound **6** are as follows: ^{31}P NMR (121.49 MHz), δ −13.76; ^{1}H NMR (400 MHz), δ 7,37–7.44 (1H, d, J = 7.70), 7.26–6.92 (16H, m), 6.75–6.72 (1H, d, J = 7.52), 4.02 (2H, s), 3.09 (3H, s). 2′-Diphenylphosphino-2-methoxymethylbiphenyl **6** (380 mg, 0.88 mmol) was dissolved in 10 ml of HBr in glacial acetic acid and heated under reflux for 3 h. The solvent was removed, and the cyclo-*o*-MitoPh was recrystallized from ethyl acetate/ethanol (290 mg, 93%). The parameters for cyclo-*o*-MitoPh are as follows: ^{31}P NMR (121.49 MHz), δ 12.68; ^{1}H NMR (300.13 MHz), δ 8.10–8.03 (2H, m), 7.93–7.80 (5H, m), 7.75–7.66 (3H, m), 7.64–7.52 (5H, m), 7.40–7.29 (3H, m); 5.25 (2H, d, J = 14.2); and ^{13}C NMR (300 MHz), δ 149.9 (s), 141.87 (s), 136.2 (d), 135.2 (d), 134.2 (s), 134.0 (s), 133.0 (s), 132.9 (s), 132.8 (s), 132.5 (s), 132.3 (s), 130.7 (s), 130.4 (s), 130.3 (s), 129.6 (s), 128.9 (s), 128.8 (s), 127.8 (s), 127.7 (s), 126.8–126.7 (d), 125.0 (s), 124.9 (s), 116.5 (s), 115.4 (s), 25.7 (s). MS calculated for $C_{25}H_{20}P^+$ was 351.1 and found was 351.1.

HPLC Analyses of the Specific Products Formed from Oxidation of Probes—HPLC-based analyses of the products of oxidation of HE and CBA probes were carried out using Agilent 1100 system equipped with absorption and fluorescence detectors, as described elsewhere (7, 8). Rapid simultaneous monitoring of superoxide and hydrogen peroxide was carried out as reported previously (8), but the Supelco Ascentis Express phenyl-hexyl column (5 cm × 4.6 mm, 2.7 μm) was used. The compounds were eluted isocratically using mobile phase consisting of water (65%), acetonitrile (35%), and trifluoroacetic acid (0.1%) at a flow rate of 2 ml/min. The column temperature was set at 30 °C. Under these conditions the following probes and products were monitored: HE (0.30 min), 2-OH-E^+ (0.60 min), E^+ (0.67 min), E^+-E^+ (1.30 min), CBA (0.35 min), and COH (0.42 min). This method was also used in the rapid quantitative analyses of 2-OH-E^+ or COH formation from HE or CBA in RAW 264.7 cells generating $O_2^{\cdot-}$ or $ONOO^-$.

LC-MS/MS Analyses of o-MitoPhB(OH)$_2$-derived Products—Analyses of *o*-MitoPhB$(OH)_2$ and its oxidation/nitration products were performed as described recently (21, 32). The method was modified for newly characterized products, including cyclo-*o*-MitoPh, and deuterated analogs were used as internal standards for quantitative analyses.

Dose-Response Analyses—For determination of the apparent IC_{50} values, the dose-response fitting application was used, as implemented in OriginPro 9.1.0 program (OriginLab Corp.). Equation 2 used for the fitting is as follows:

$$y = A_1 + \frac{A_2 - A_1}{1 + 10^{(\log IC_{50} - \log c)p}} \qquad \text{(Eq. 2)}$$

where y is the measured quantity (proportional to Nox2 enzyme activity); A_1 and A_2 correspond to bottom and top asymptotes, p to the Hill slope, and c is the concentration of the compound.

Results

Overview of HTS/ROS Assays Used in the Identification of Nox Inhibitors—To reliably identify inhibitors of Nox isoforms, we developed the following primary and secondary assays for HTS/ROS analysis (Fig. 2), as described recently (8). Hydropro-

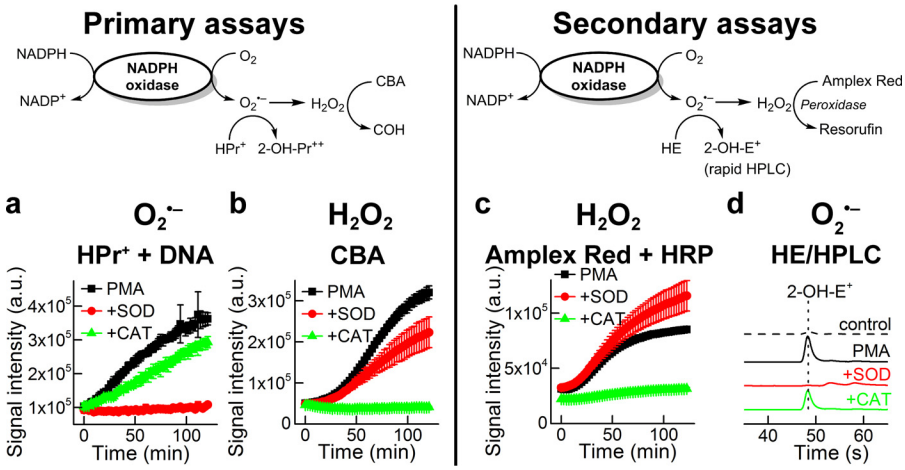


FIGURE 2. **Detection of superoxide and hydrogen peroxide generated from Nox2.** Primary and secondary assays are shown. *a*, increase in fluorescence intensity due to formation of the superoxide-specific product, 2-OH-Pr^{2+}, in *d*HL60 cells activated by PMA. *b*, increase in fluorescence intensity due to catalase-sensitive H_2O_2 oxidation product, COH, in *d*HL60 cells and PMA. *c*, increase in fluorescence intensity due to formation of resorufin. *d*, HPLC of 2-OH-E^+, the specific product of HE and $O_2^{\cdot-}$, in control and PMA-activated *d*HL60 cells in the presence of SOD and catalase (adapted from Ref. 8).

TABLE 2

Step-by-step protocol applied to screen the library of bioactive compounds at The Broad Institute

(i) Cell culture and differentiation of HL60 cells
1) Grow HL60 cells in RMPI 1640 medium containing 10% FBS and antibiotics
2) To a new flask add HL60 cells (10^5 cells/ml) and add all-*trans*-retinoic acid (final concentration, 1 μM)
3) Incubate the cells for 4 days
(ii) Preparation of cell suspension
1) Transfer cell suspension into centrifuge tubes and spin down the cells
2) Remove the medium (supernatant) and resuspend the cells in HBSS containing 25 mM HEPES buffer (pH 7.4) and 0.1 mM dtpa
3) Count the cells and prepare the cell suspension in HBSS containing 25 mM HEPES buffer (pH 7.4) and 0.1 mM dtpa at a density of 10^5 cells/ml
(iii) Cell inhibition
1) Aliquot the cell suspension into black 384-well plates using Thermo Multidrop Combi instrument under sterile conditions
2) Add 100 nl of compound solutions (5–10 mM in DMSO) using a CyBi®-Well (CyBio) equipped with a 100-nl pin tool
3) Incubate the cells with inhibitors for 30 min at 37 °C in a CO_2-free incubator
(iv) Plate reader-based 384-well plate-based assays
1) Add 10 μl/well probes (5× solutions in HBSS containing 25 mM HEPES buffer (pH 7.4), 0.1 mM dtpa, and 0.1 mg/ml BSA) to the 384-well plates containing cells with inhibitors using a Thermo Multidrop Combi instrument. From this point minimize the exposure of plates to light
2) Add 10 μl/well PMA (5× solutions in HBSS containing 25 mM HEPES buffer (pH 7.4), 0.1 mM dtpa and 0.1 mg/ml BSA) to the 384-well plates containing cells with compounds and probes using another Thermo Multidrop Combi instrument
3) Incubate the activated cells with probes for 90 min at 37 °C in a CO_2-free incubator
4) Read the fluorescence intensity in the 384-well plates using an Envision (PerkinElmer Life Sciences) plate reader

pidine (HPr^+) was used as a primary probe for extracellular $O_2^{\cdot-}$ measurement (19). HPr^+ reacts with $O_2^{\cdot-}$ ($k = 1.2 \times 10^4\ M^{-1}\ s^{-1}$) to form a specific and diagnostic marker product, 2-hydroxypropidium (2-OH-Pr^{2+}) (19). 2-OH-Pr^{2+} fluorescence quantum yield is enhanced >10-fold in the presence of added DNA. Coumarin-7-boronic acid (CBA) was used as another primary assay probe for measuring H_2O_2. CBA reacts with H_2O_2 (catalase-sensitive) considerably slower ($k = 1.5\ M^{-1}s^{-1}$), as compared with its catalase-insensitive reaction with $ONOO^-$ ($k = 1.1 \times 10^6\ M^{-1}\ s^{-1}$), to form a highly fluorescent product, COH (33). Over the duration of the reaction between CBA and H_2O_2, there was significantly less spontaneous decomposition of CBA as compared with other boronate probes (33, 34).

The addition of PMA (activator of PKC signaling pathway) to differentiated HL60 cells (overexpressing Nox2) in the presence of HPr^+ and DNA causes a linear increase in 2-OH-Pr^{2+} fluorescence ($O_2^{\cdot-}$ reaction) that was inhibited by SOD and not by catalase (Fig. 2). Concomitantly, there is an increase in COH fluorescence (H_2O_2 reaction with CBA) that is inhibited by catalase and not by SOD (Fig. 2).

In the secondary assay, we used the probe hydroethidine (HE) and detected 2-hydroxyethidium (2-OH-E^+) (specific product of HE reaction with $O_2^{\cdot-}$) using ultra-HPLC (Fig. 2). For measuring H_2O_2, the probe Amplex Red was used in the presence of HRP to monitor resorufin (formed from Amplex Red oxidation with H_2O_2/HRP) using a plate reader. The addition of PMA to differentiated HL60 cells in the presence of Amplex Red and HRP causes an increase in the fluorescence intensity of resorufin that is abrogated by catalase but not by SOD (Fig. 2). Under these conditions, $O_2^{\cdot-}$ is detected by measuring 2-OH-E^+ (by HPLC) that was inhibited by SOD and not by catalase (Fig. 2). These assays provide the foundation for rigorous measurements of $O_2^{\cdot-}$ and H_2O_2 using three different probes for high throughput screening studies (8).

Screening the Library of Bioactive Compounds, Identification of Potential Nox2 Inhibitors—We applied the ROS/HTS assays, as discussed above, to screen a subset library of bioactive drugs as Nox2 inhibitors at Broad Institute Probe Development Center. First, we fulfilled the HTS assay "readiness" criteria for the primary and secondary assay probes (HPr^+, CBA, and Amplex Red).

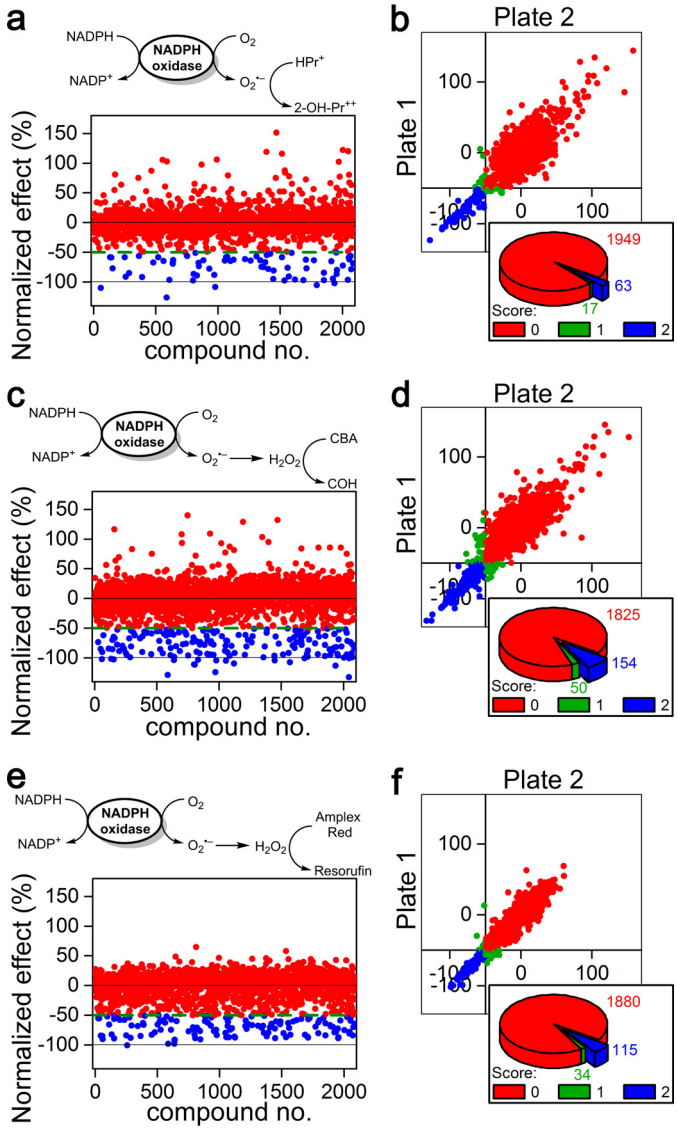


FIGURE 3. **Results of screening of a library of bioactive compounds (≈2,000) using the following three probes: hydropropidine (50 μM) in the presence of DNA (0. 1 mg/ml) as a probe for $O_2^{\cdot-}$ (*a* and *b*), and coumarin boronic acid (100 μM, *c* and *d*) or Amplex Red (50 μM) in the presence of HRP (0.1 units/ml, *e* and *f*) as probes for H_2O_2.** *d*HL60 cells were stimulated with PMA (1 μM) to induce Nox2 activity in HBSS supplemented with HEPES buffer (25 mM) and dtpa, 0.1 mM. *a, c,* and *e,* schemes of oxidation of the probes and the results of screening after normalization. *b, d,* and *f,* plate-to-plate reproducibility data and number of negative/inconclusive/positive hits for each assay. Score *0* (*red color*) corresponds to negative; *1* (*green color*) to inconclusive, and *2* (*blue color*) to positive hits.

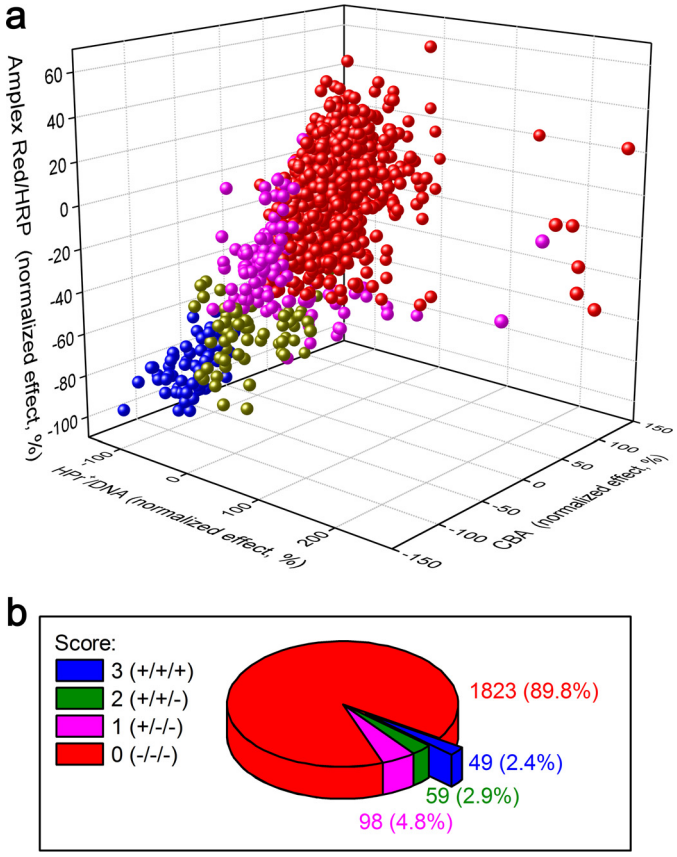


FIGURE 4. **Results of screening of a library of bioactive compounds (≈2,000) using the following three probes: hydropropidine (50 μM) in the presence of DNA (0. 1 mg/ml) as a probe for $O_2^{\cdot-}$, and coumarin boronic acid (100 μM) or Amplex Red (50 μM) in the presence of HRP (0.1 units/ml) as probes for H_2O_2.** *a,* correlation of the results of the three assays for Nox2 activity. *b,* results of screening as a percentage of positive hits in one, two, or all three assays. All experimental conditions are as described in Fig. 3.

The list of 2,029 compounds, together with the results of screening of their normalized effects on Nox2 activity using HPr^+, CBA, and Amplex Red probes, are shown in supplemental Table 1. The stepwise protocol used in the HTS/ROS studies at Broad Institute is shown in Table 2. The effects of 2,029 compounds on $O_2^{\cdot-}$ formation by monitoring the formation of 2-OH-Pr^{2+} in PMA-activated differentiated HL60 cells are shown in Fig. 3. 2-OH-Pr^{2+} formation in the presence of DMSO and phenylarsine oxide (1 μM) was normalized to 0% (no effect) and −100% (complete inhibition) (Fig. 3*a*). We set a 50% inhibition (Fig. 3*a, green dashed line*) as a threshold criterion for a "hit." *Blue dots* in Fig. 3*a* indicate compounds inhibiting 2-OH-Pr^{2+} formation by >50%, and *red dots* indicate compounds exhibiting <50% inhibition (Fig. 3*a*). Fig. 3*b* shows the plate-to-plate comparison showing the reproducibility of data for each compound, and the *pie chart* (*inset* in Fig. 3*b*) shows 63 out of 2,029 compounds exhibit >50% inhibition of 2-OH-Pr^{2+} formation (*blue chart* with positive >50% inhibition in both plates). Fig. 3, *c* and *d,* shows similar results for COH formation from CBA. One hundred fifty four compounds from the screened library inhibited COH formation by >50% in both plates (Fig. 3*d*, *inset*). Corresponding results obtained using the Amplex Red probe measuring H_2O_2 are shown in Fig. 3, *e* and *f*.

The three-dimensional hit correlation plot for all three assay probes, HPr^+, CBA, and Amplex Red, is shown in Fig. 4*a*. Of the 2,029 compounds tested, 49 compounds (2.4%, *blue pie chart* in Fig. 4*b*) were identified as hits with all three probes (Table 3), using 50% inhibition threshold. The *red color* in Fig. 4*b* corresponds to negative result for all three probes (−/−/−); *magenta* is used for compounds that scored a positive result for a single probe (+/−/−); *green* is used for compounds that scored positively with two probes (+/+/−); and *blue* is used for positive results for all three probes (+/+/+). The list of "positive hits" shown in *blue* in Fig. 4*b*, together with the average extent of inhibition at ~30 μM concentration is shown (Table

TABLE 3

Positive hits obtained during screening of the library of bioactive compounds using three probes as follows: hydropropidine (50 μM) in the presence of DNA (0.1 mg/ml) as a probe for $O_2^{\cdot-}$, and coumarin boronic acid (100 μM) or Amplex Red (50 μM) in the presence of HRP (0.1 units/ml) as probes for H_2O_2

Differentiated HL60 cells were stimulated with PMA (1 μM) to induce Nox2 activity in HBSS supplemented with HEPES buffer (25 mM) and dtpa (0.1 mM).

No.	Compound name	HPr^+ + DNA	CBA	Amplex Red + HRP
		Normalized score		
1	Miconazole nitrate	−125.8	−128.7	−97.9
2	Methiothepin maleate[a]	−109.5	−101.8	−84.8
3	Mitoxantrone·HCl[a]	−108.1	−104.0	−83.1
4	NNC 55-0396·2HCl	−105.2	−93.9	−80.2
5	Nonoxynol-9	−101.7	−112.9	−77.2
6	5-Nonyloxytryptamine oxalate	−97.0	−111.0	−82.9
7	10-DEBC·HCl[a]	−96.8	−100.4	−82.6
8	Thioridazine·HCl	−96.4	−94.9	−74.2
9	GW7647	−96.2	−132.0	−80.6
10	Diphenyleneiodonium chloride	−95.6	−73.6	−58.4
11	nTZDpa	−94.7	−96.3	−72.1
12	Cetylpyridinium chloride	−93.9	−82.9	−78.3
13	Suloctidil	−91.2	−94.5	−100.3
14	Lylamine·HCl	−90.5	−107.4	−82.8
15	Perphenazine	−88.8	−102.8	−74.1
16	RS 39604·HCl	−88.1	−123.7	−74.1
17	Trifluoperazine·HCl	−86.4	−94.4	−88.6
18	NNC 26-9100	−86.1	−111.4	−88.3
19	Gambogic acid	−84.7	−98.8	−87.8
20	Ginkgolic acid	−84.0	−77.8	−63.4
21	Fluphenazine·HCl	−80.4	−104.1	−88.6
22	Chlorpromazine	−79.7	−95.8	−86.9
23	Amsacrine	−78.8	−99.1	−83.8
24	Amiodarone·HCl	−77.5	−94.3	−67.7
25	SNAP 5089	−76.9	−102.4	−88.8
26	Benzethonium chloride	−76.9	−97.7	−87.3
27	Thimerosal	−76.1	−91.3	−71.2
28	GR 127935·HCl	−73.3	−77.5	−90.6
29	Hexachlorophene	−68.3	−83.6	−64.5
30	Benzbromarone	−67.3	−92.1	−76.4
31	Embelin[a]	−65.0	−87.3	−69.4
32	CGP 71683·HCl	−64.7	−79.8	−71.9
33	Tamoxifen citrate	−63.9	−73.6	−66.6
34	Demethylasterriquinone B1[a]	−63.7	−104.4	−86.9
35	RS 17053·HCl	−63.4	−75.6	−69.1
36	IKK 16	−63.2	−77.9	−59.7
37	Mefloquine	−62.7	−98.5	−90.8
38	GW 3965·HCl	−62.4	−91.7	−87.4
39	Dyclonine·HCl	−62.4	−92.9	−85.7
40	Thiothixene[a]	−61.9	−73.0	−52.6
41	Chlorprothixene·HCl[a]	−58.4	−94.3	−80.2
42	Sulconazole nitrate	−58.2	−71.3	−60.0
43	Trimipramine maleate	−57.9	−101.5	−82.4
44	Tioconazole	−57.9	−91.6	−83.8
45	Trimeprazine tartrate[a]	−56.2	−67.2	−84.8
46	A-7·HCl	−56.1	−95.9	−76.8
47	Mibefradil·2HCl	−51.0	−89.3	−70.5
48	Triflupromazine·HCl	−50.9	−79.0	−60.1
49	L655240[a]	−50.2	−93.3	−72.1

[a] These were identified as pan assay interference compound (38).

3). This list contains Food and Drug Administration-approved drugs that include dopamine receptor blockers and drugs used in the treatment of schizophrenia and antimalarial and antifungal agents. Some of these drugs have been previously used or identified as inhibitors of Nox isoforms (35, 36). Interestingly, the compound, mitoxantrone, identified as the most potent inhibitor of Nox2 activity in *d*HL60 cells (Table 2) strongly inhibited pancreatic ductal adenocarcinoma survival (37). The positive hits were further evaluated to filter out pan assay interference compounds (38, 39). Of the 49 hits, nine were tested positive when screened against the library of the pan assay interference compounds, as defined in Ref. 38 and shown in Table 3.

Confirmatory Assays, Dose Response, and Oxygen Consumption Measurements—We confirmed the inhibitory effect of compounds selected from positive hits (Table 3) on Nox2 activity by determining their dose response. We screened over 20 commercially available compounds selected from Table 3 for the confirmatory assays. The apparent IC_{50} values for inhibition of Nox2 activity in the *d*HL60 model determined with a fluorescence plate reader using the CBA-based assay are shown in Table 4. Next, the effect of selected compounds on Nox2 activity was tested by HPLC-based simultaneous monitoring of $O_2^{\cdot-}$ and H_2O_2 (Fig. 5, *a* and *b*), by measuring oxygen consumption stimulated by Nox2 activation using the 96-well plate-based extracellular flux analyzer (Seahorse XF96, Fig. 5, *c* and *d*) and by monitoring the inhibitory effect on spin-trapped superoxide adduct using DEPMPO (data not shown). Fig. 5*a* shows the results of the confirmatory assays for selected compounds, sulconazole, mefloquine, cetylpyridinium cation, and DPI, on formation of 2-hydroxyethidium, the specific marker product for $O_2^{\cdot-}$. Similarly, Fig. 5*b* shows the effect of these compounds

TABLE 4

IC_{50} values for selected positive hits, determined by monitoring the effect of the compounds on the rate of oxidation of coumarin boronic acid (100 μM) as a probe for H_2O_2

Differentiated HL60 cells were stimulated with PMA (1 μM) to induce Nox2 activity in HBSS supplemented with HEPES buffer (25 mM) and dtpa (0.1 mM) and the extent of probe oxidation was monitored in 384-well plates using fluorescence plate reader.

No.	Compound	IC_{50} (μM)	
		Mean	S.D.
1	Amiodarone·HCl	11	2
2	Amoxapine	16	4
3	Benzbromarone	13	1.5
4	Benzethonium chloride	23	0.7
5	Cetylpyridinium chloride	2.3	0.3
6	Chlorpromazine·HCl	13	0.6
7	Clotrimazole	59	25
8	Diphenyleneiodonium	0.08	0.07
9	Dyclonine	39	16
10	Econazole nitrate	22	1.1
11	Hexachlorophene	2.2	0.4
12	Mefloquine·HCl	16	0.4
13	Miconazole	15	6.5
14	Mitoxantrone	18	12
15	Phenylarsine oxide	0.2	0.04
16	Promazine·HCl	31	1.6
17	Sulconazole nitrate	19	2.6
18	Suloctidil	7.7	3.5
19	Tamoxifen citrate	18	0.5
20	Thimerosal	2.2	0.6
21	Thioridazine	9.3	2.1
22	Tioconazole	9.2	0
23	Trifluoperazine	9	2.2
24	Triflupromazine·HCl	12	2.6

on COH, the product of the reaction of CBA probe with H_2O_2. The IC_{50} values for these compounds to inhibit $O_2^{\cdot-}$ and H_2O_2 production also compare favorably with those measured using Nox2-mediated oxygen consumption. We next verified that at these concentrations sulconazole, mefloquine, and cetylpyridinium cations inhibited formation of the DEPMPO-superoxide adduct. All three compounds completely blocked formation of DEPMPO-$^{\cdot}$OOH adduct, when used at 100 μM for sulconazole and mefloquine or 10 μM for cetylpyridinium and DPI cations (data not shown).

Inhibition of Nox2 in Activated RAW 264.7 Macrophages—Following the experiments on *d*HL60 cells, we tested whether the selected hits can also inhibit Nox2 activity in a different cellular model for Nox2 activity, namely PMA-stimulated RAW 264.7 cells. Activation of RAW 264.7 cells in the presence of the hydroethidine probe led to a significant increase in the HPLC peak of 2-hydroxyethidium (monitored with a fluorescence detector) (Fig. 6*a*), as reported earlier (7). We measured the yield of 2-OH-E^+ upon PMA-induced Nox2 activation in the presence of several compounds identified as apparent Nox2 inhibitors in *d*HL60 cells, with DPI used as a positive control for Nox2 inhibition. At these concentrations, all of the compounds tested decreased the intensity of the peak of 2-OH-E^+ (Fig. 6*a*, fluorescence mode), confirming the ability of these compounds to inhibit Nox2 activity in intact cells. Quantitative analysis of the HPLC data (Fig. 6*b*) based on the use of authentic standards for 2-OH-E^+, E^+, and E^+-E^+ shows that the compounds inhibit the yield of 2-OH-E^+, while having no effect on ethidium (E^+), the nonspecific oxidation product (with the exception of benzethonium cation), and variable effects on the one-electron oxidation dimeric product (diethidium, E^+-E^+). These results confirm that the HTS hits for Nox2 identified using the differentiated HL60 cells also inhibit $O_2^{\cdot-}$ formation from Nox2 in RAW 264.7 cells.

Do Nox2 Inhibitors Also Inhibit Generation of Peroxynitrite?—Next, we tested whether the compounds listed in Table 4 that inhibit Nox2 activity in PMA-stimulated RAW 264.7 cells could also inhibit generation of peroxynitrite formed from $O_2^{\cdot-}$ and $^{\cdot}$NO reaction in the same cellular model. RAW macrophages were stimulated to co-generate both $^{\cdot}$NO and $O_2^{\cdot-}$ via activation of inducible NOS and Nox2 (using LPS, interferon-γ, and phorbol ester), as reported earlier (7). CBA was used to monitor $ONOO^-$ in cell-free systems and from activated macrophages by monitoring COH (catalase-insensitive) generation (7, 20, 33). Results show that several but not all Nox2 inhibitors identified from the screen of the bioactive library using the *d*HL60 model inhibited $ONOO^-$-dependent COH formed from CBA. Of note, the compounds inhibiting $ONOO^-$ formation in RAW 264.7 cells also inhibited Nox2 activity in these cells, as demonstrated in Fig. 6. Fig. 7*b* shows the dose-dependent inhibition of $ONOO^-$ formed from activated macrophages in the presence of selected hits for Nox2 inhibition (*e.g.* DPI, sulconazole, mefloquine, and cetylpyridinium). As shown, DPI potently inhibits $ONOO^-$ formation with an IC_{50} of 0.4 μM. However, DPI being a non-selective inhibitor of flavoproteins may also block $^{\cdot}$NO production by inhibition of inducible NOS. The IC_{50} values for sulconazole, mefloquine and cetylpyridinium cation to inhibit $ONOO^-$ formation were determined to be 33, 36, and 4 μM, respectively. These values compare favorably with their IC_{50} values to inhibit $O_2^{\cdot-}$ generation in PMA-stimulated RAW 264.7 cells (Fig. 7*a*) and the *d*HL60 Nox2 model (Table 4). These results suggest that the HTS/ROS assay with CBA can be used to identify novel inhibitors of $ONOO^-$ formation as well.

Specific Detection of a Cyclized Product during Peroxynitrite Reaction with Ortho-substituted Mitophenylboronic Acid—Recently, we developed a new probe, *o*-MitoPhB$(OH)_2$, that rapidly reacts with $ONOO^-$ forming a minor product, *o*-MitoPhNO_2, that is very specific for $ONOO^-$ (Fig. 8*a*) and is unaffected by glutathione or other biologically relevant reductants (21, 22). As this product is not fluorescent, we used HPLC with absorption detection for quantitative analyses, and we confirmed it is formed in RAW 264.7 cells in activated macrophages (22). However, using an LC-MS/MS method, we found that this product (*i.e.* *o*-MitoPhNO_2) was detected in a relatively low yield (21). Quantitative analysis of the LC-MS data revealed an additional minor product (m/z = 351) formed during the reaction between *o*-MitoPhB$(OH)_2$ and $ONOO^-$. The same product was detected in extracts from RAW 264.7 cells, when activated to produce $ONOO^-$ (see below). The structure of this product was assigned to cyclo-*o*-MitoPh (Fig. 8*a*, shown in *red*) formed by radical-induced intramolecular cyclization mechanism (Fig. 8*a*, minor radical pathway). This was supported by the observation that during the reaction of $ONOO^-$ with d_{15}-*o*-MitoPhB$(OH)_2$ (with all protons on triphenylphosphonium moiety substituted by deuterium), the product with m/z = 365 atomic mass units is formed, indicating the loss of one deuterium atom. The identity of this product was further verified by independent synthesis of cyclo-*o*-MitoPh (Fig. 9*a*), and the structure was confirmed by mass spectrometry, NMR, and

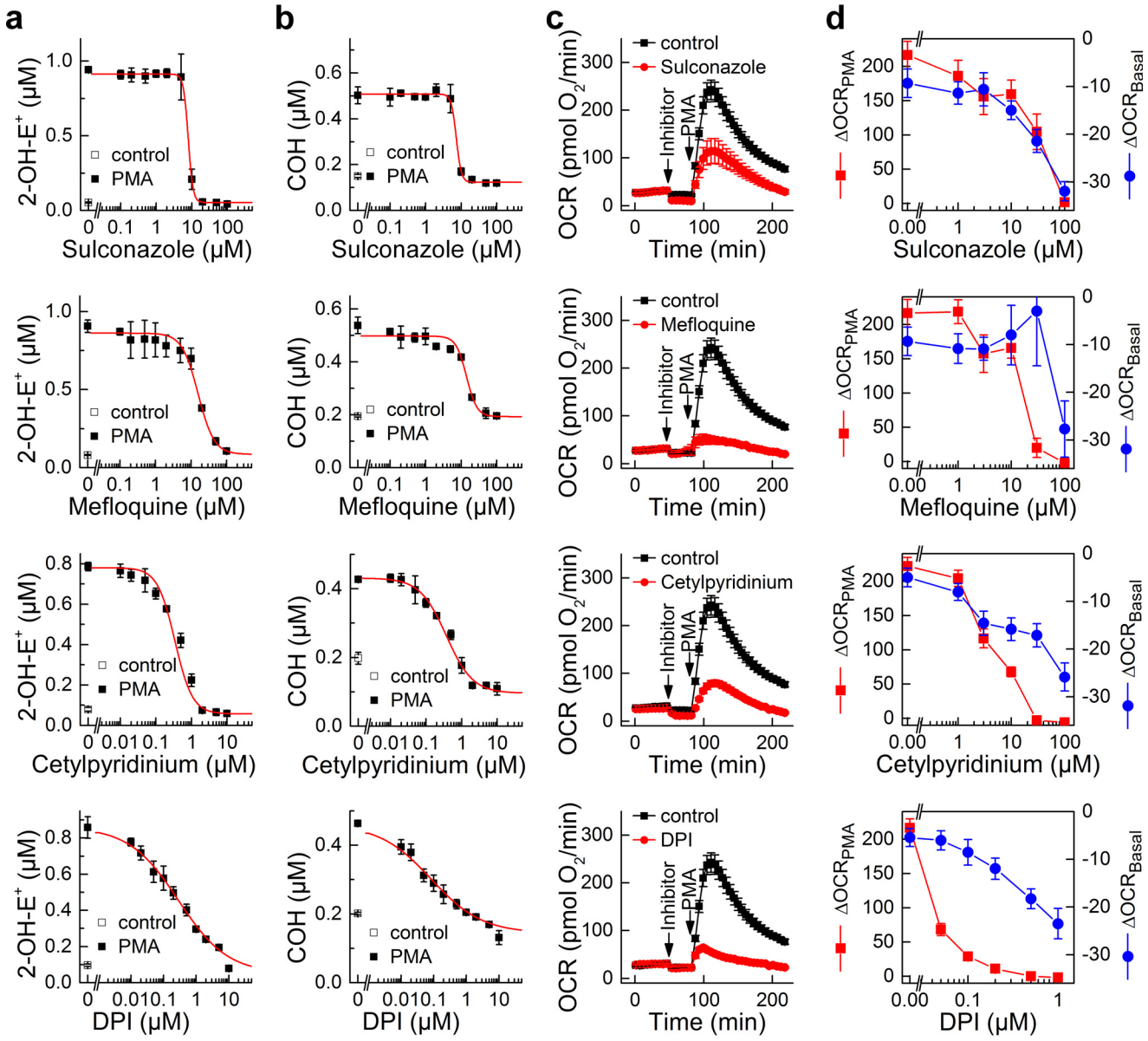


FIGURE 5. **Results of confirmatory assays for selected positive hits from Nox2 inhibitor screening.** Dose-response results of four selected inhibitors of Nox2 on 2-OH-E^+ (*a*) and COH (*b*) formation in PMA-activated *d*HL60 cells, using the HPLC-based assay for simultaneous monitoring of $O_2^{\cdot-}$ and H_2O_2. *c*, effect of the same four inhibitors on oxygen consumption (mitochondrial respiration and NADPH oxidase activation) measured using the Seahorse extracellular flux analyzer. Concentrations of inhibitors are as follows: DPI, 0.1 μM; sulconazole, 30 μM; mefloquine, 30 μM; cetylpyridinium chloride, 10 μM. *d*, dose-dependent response to the same four inhibitors on basal mitochondrial respiration (ΔOCR_{Basal}, shown in *blue*) and the NADPH oxidase activation by PMA injection (ΔOCR_{PMA}, shown in *red*).

x-ray crystallography (Fig. 9*b*). The LC-MS/MS parameters (retention time, *m*/*z* value, and MS/MS fragmentation pattern) of the minor product of *o*-MitoPhB$(OH)_2$ reaction with authentic $ONOO^-$ were identical to those of the authentic cyclo-*o*-MitoPh (Fig. 8, *a* and *c*). The specificity of this product was tested using other oxidants (H_2O_2 and HOCl), which are known to oxidize boronic compounds and comparing the product identities and distribution (Fig. 8, *b* and *c*). Consistently with our previous research on the chemical reactivity of boronic compounds (20, 32, 40), the reaction between *o*-MitoPhB$(OH)_2$ and H_2O_2 yielded a single phenolic product (*o*-MitoPhOH), although additional minor products were detected with HOCl and $ONOO^-$. In addition to cyclized (cyclo-*o*-MitoPh) and nitrated (*o*-Mito$PhNO_2$) products, the products of nitration of *o*-MitoPhOH were also formed in the presence of excess $ONOO^-$. These products showed up at the *m*/*z* value of 414 and were assigned to isomers of *o*-Mito$Ph(NO_2)OH$ (Fig. 8*a*) (22). In addition, a small amount of the protonated form of triphenylphosphonium oxide (TPP=O, *m*/*z* = 279) was also detected. With HOCl, the minor product observed (using excess of HOCl) is chlorinated phenol *o*-MitoPh(Cl)OH (Fig. 8*a*), showing up as a double peak attributed to two isomers. Interestingly, other oxidation products, including triphenylphosphine oxide and brominated phenolic product (*o*-MitoPh(Br)OH)were also formed (Fig. 8). Although triphenylphosphine oxide formation can be explained by a nucleophilic attack of ClO^- on the phosphorus atom of the triphenylphosphonium moiety, the

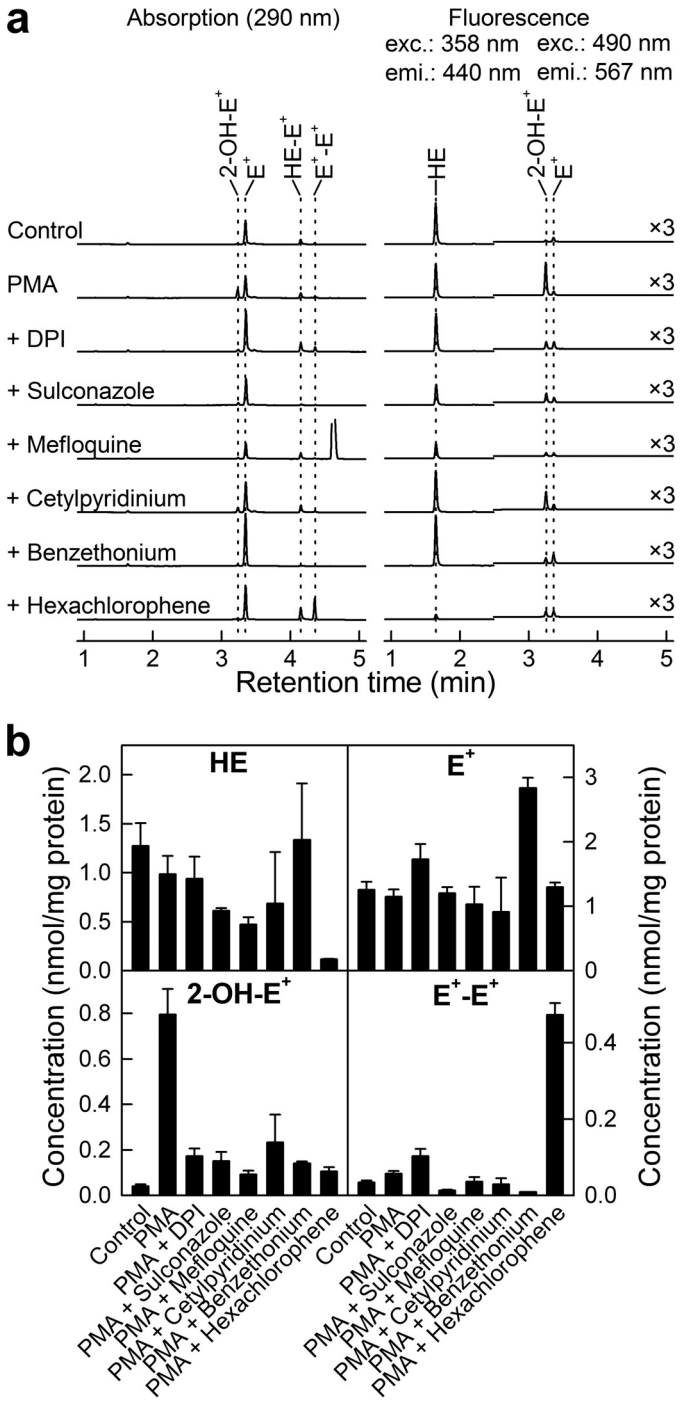


FIGURE 6. **Effect of selected hits on HE oxidation profiles in PMA-stimulated RAW 264.7 macrophages.** *a,* HPLCs at 290 nm (absorption detector) and the HPLC fluorescence traces (excitation/emission wavelengths, as shown). *b,* quantitative analyses of intracellular levels of HE and its oxidation products, after normalization to protein level. Concentrations of agents are as follows: PMA, 1 μM; DPI, 1 μM; sulconazole, 100 μM; mefloquine, 100 μM; cetylpyridinium chloride, 10 μM; benzethonium chloride, 100 μM; hexachlorophene, 100 μM.

brominated phenolic product indicates formation of HOBr via oxidation of the bromide anion (present as a counterion of *o*-MitoPhB$(OH)_2$ probe) by HOCl (41, 42). To test whether *o*-MitoPhB$(OH)_2$ can distinguish between peroxynitrite and myeloperoxidase (MPO)-mediated oxidation/nitration, we determined the products formed by MPO in the presence of hydrogen peroxide, with or without nitrite (Fig. 10*a*). The results indicate that both cyclo-*o*-MitoPh and *o*-MitoPhNO_2 products are specific for $ONOO^-$, although MPO in the presence of nitrite leads to nitration of the phenolic product, formed from oxidation of *o*-MitoPhB$(OH)_2$ by H_2O_2. The quantitative analysis of the oxidation/nitration of *o*-MitoPhB$(OH)_2$ by $ONOO^-$ indicates that yields of the minor specific products, cyclo-*o*-MitoPh and *o*-Mito-PhNO_2, are 10.5 ± 0.5 and 0.5 ± 0.1%, respectively (Fig. 10*b*). In the case of MPO-mediated oxidation in the presence of sodium nitrite, the major product seems to be nitrated phenols (*o*-MitoPh(NO_2)OH). The other product detected was triphenylphosphine oxide, formed by the MPO/H_2O_2 system both in the absence and presence of nitrite (data not shown). Next, we investigated the formation of peroxynitrite-specific products in activated macrophages and the effect of selected Nox2 inhibitors on the reaction products of *o*-MitoPhB$(OH)_2$ and $ONOO^-$ (Fig. 11). We have shown previously that stimulation of RAW 264.7 cells leads to formation of *o*-MitoPhOH and small amounts of *o*-Mito-PhNO_2 (21, 22). As shown in Fig. 11, the most exclusive minor product detected in cells was the cyclized product cyclo-*o*-MitoPh. In fact, the amount of *o*-Mito-PhNO_2 formed in cells is less than 5% of the yield of cyclo-*o*-MitoPh (Fig. 11*c*). The analysis of the effect of inhibitors on the yield of the major phenolic oxidation product of *o*-MitoPhB$(OH)_2$ gives mixed results, with mefloquine actually increasing the yield of this product. This suggests the possibility of multiple pathways of the formation and/or metabolism of the phenolic product inside the cells. In contrast, results show that selected candidate Nox2 inhibitors, including cetylpyridinium, sulconazole, mefloquine, and DPI, inhibit formation of cyclo-*o*-MitoPh and *o*-Mito-PhNO_2, the diagnostic products for $ONOO^-$ (Fig. 11*c*). This is consistent with the results of measurements of extracellular $ONOO^-$ (Fig. 7*b*) and further demonstrates the added value of determining the specific minor product(s) for $ONOO^-$ reaction with *o*-MitoPhB$(OH)_2$.

Discussion

Significance of Nox Inhibition—Nox enzyme-derived ROS/RNS are now recognized to play a central role in both inflammatory and fibrotic diseases (1, 2). The former includes both classical inflammatory conditions (*e.g.* arthritis and inflammatory bowel disease) and nonclassical conditions in which inflammation plays a central pathogenic role. For example, inflammatory lung diseases include acute respiratory distress syndrome, asthma, and chronic obstructive pulmonary disease, although other inflammatory conditions include Alzheimer and Parkinson diseases, ischemic stroke, and organ reperfusion injury during transplantation (43). Fibrotic diseases include liver fibrosis (*e.g.* following viral infection), idiopathic pulmonary fibrosis, and diabetic kidney disease. Nox2 has been implicated in inflammatory diseases and Nox4 in fibrotic diseases (1, 2). Existing therapies for both classes of diseases include steroids and other anti-inflammatory approaches, but they have proven to be ineffective. Therefore, there is a need for developing novel anti-inflammatory and antifibrotic agents based on other molecular targets. Nox enzymes are especially promising

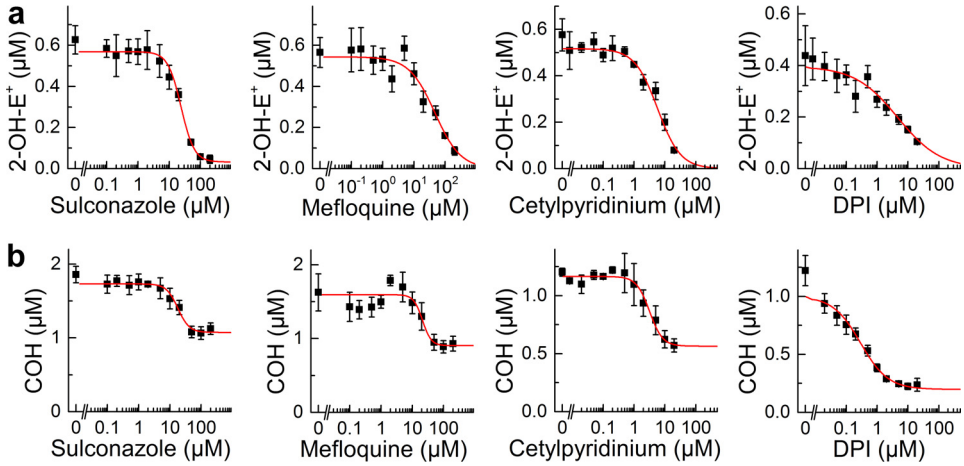


FIGURE 7. **Inhibition of O_2^- and $ONOO^-$ formation from activated RAW 264.7 cells by selected positive hits as follows: sulconazole, mefloquine, cetylpyridinium chloride, and DPI.** Cells were treated with inhibitors for 30 min in Dulbecco's PBS containing glucose and pyruvate followed by addition of PMA (1 μM) and the probe and incubated for 1 h at 37 °C. After incubation, the extracellular media were analyzed for 2-OH-E^+ or COH levels using a rapid HPLC method. *a*, RAW 264.7 cells were stimulated with PMA (1 μM) in the presence of HE (10 μM). *b*, RAW 264.7 cells were pretreated overnight with LPS (0.5 μg/ml) and IFNγ (50 units/ml) and stimulated with PMA (1 μM) in the presence of CBA (100 μM).

in this regard due to mounting evidence in humans and in other experimental models (44). Peroxynitrite, the product of diffusion-controlled reaction of nitric oxide and superoxide, has been implicated in several inflammatory diseases (15), including neurodegenerative diseases and chemotherapy-induced nephrotoxicity (45). Recent data also suggest the involvement of $ONOO^-$ in traumatic brain injury-induced neurodegeneration via activation of calpain in neurons (46, 47).

It has been proposed that Nox2-derived ROS/RNS from myeloid-derived suppressor cells in the tumor microenvironment are potentially responsible for decreased T cell reactivity and immunosuppressive effects (48). In this regard, small molecular weight compounds that inhibit Nox2 activity could play a vital role in providing additional mechanistic insight on the immune system in tumor microenvironments. The role of Nox/ROS in biology is paradoxical (49). High levels of O_2^- generated from Nox2 are essential for cell killing and host defense, whereas in other cells, low levels of ROS (O_2^- and H_2O_2 or both) generated from Nox are important for cell signaling (*e.g.* NF-κB activation). Nox inhibitors effectively abrogated proliferation of various cancer cell models (50). Preliminary results show that several compounds identified as potential Nox2 inhibitors (Table 4) significantly inhibit proliferation of human pancreatic cancer cells (data not shown). It is likely that follow-up studies will greatly improve the potency and selectivity of hit compounds using medicinal chemistry. Although this study is restricted to the Nox2 isoform, future investigations will broaden the scope of work to include other Nox isoforms using the appropriate HTS-compatible cell lines.

HTS/ROS/RNS Assay—ROS/RNS do not represent a single entity, but encompass a wide range of reactive species that exhibit oxidizing, nitrating, nitrosating, and halogenating properties (51, 52). To better understand the pathophysiological consequences of ROS/RNS, it is crucial to identify and characterize the species that are specifically responsible for a given "biologic and toxicologic" effect and to inhibit the specific sources of ROS/RNS generation (53). Doxorubicin, one of the most widely used chemotherapeutics, causes myocardial inflammation that is attributed to Nox-induced ROS/RNS formation in inflammatory cells (54–56). Genetic disruption of Nox2 mitigated doxorubicin-mediated contractile dysfunction, oxidative/nitrative stress, and inflammation (56). Thus, selective targeting of Nox2 may provide a novel therapeutic strategy for mitigation of ROS/RNS and cardiotoxic side effects, while maximizing its antitumor efficacy (56). To date, only a limited number of Nox isoform-selective inhibitors are available (57, 58). This is due in part to serious limitations of the existing ROS/RNS assays as described below.

Previous approaches have used sensitive but nonselective and artifact-prone ROS/RNS probes (59) for detecting Nox-derived oxidants, resulting in a high rate of false positives and potentially missing weaker but selective hits lost in the "noise." Many HTS-based H_2O_2 assays to detect Nox inhibitors included the enzyme HRP. The lack of probes' selectivity for specific oxidant and the susceptibility of the HTS assays to peroxidase substrates and inhibitors led to the controversy over the Nox-inhibitory potency of the positive hits selected, including apocynin, VAS2870, and 2-acetylphenothiazine (36, 60, 61). In fact, one of the authors recently reported a new myeloperoxidase inhibitor, identified during the HTS campaign for Nox2 inhibitors, using the L-012 probe as a Nox2 activity reporter (62). Using the present HTS/ROS approach, it is conceivable that false positives will be decreased by >75%, with the assay specificity allowing identification of weaker inhibitors that can later be improved through medicinal chemistry. In this work, we describe the use of ROS/RNS-specific probes whose redox chemistry is better understood with respect to reaction kinetics, stoichiometry and reaction products (63). Selective monitoring of specific ROS in the HTS assay is important. For example, these HTS assays can be extended to other cell types to gain new insight regarding enzymatic sources of ROS generation and subsequently unravel the role of ROS in disease-related biological processes. It is conceivable that a similar HTS/ROS assay may be used to identify inhibitors of other oxidants (*e.g.* hypochlorous acid) and their sources of generation using other fluorescent probes (Table 1).

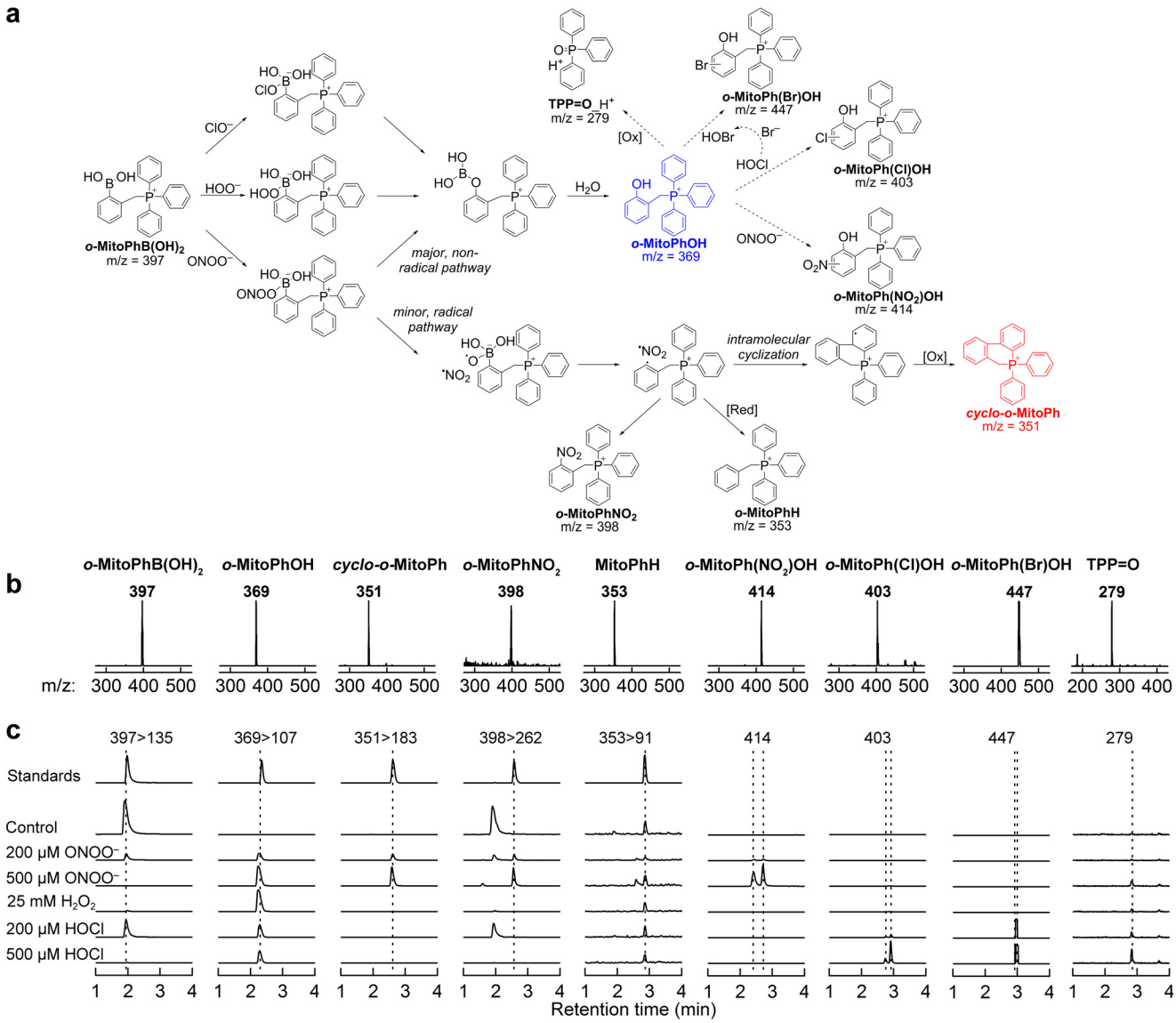


FIGURE 8. **Detection and characterization of specific products from the probe, *o*-MitoPhB(OH)$_2$.** *a,* proposed mechanism of oxidation of *o*-MitoPhB(OH)$_2$ by ONOO$^-$, H_2O_2, and HOCl. The major oxidation product, common for all oxidants, is shown in *blue*, and the peroxynitrite-specific cyclization product is shown in *red*. *Dashed arrows* indicate the possible subsequent oxidation/nitration/halogenation reactions of the major product, *o*-MitoPhOH. *b,* mass spectra of the products determined from the on-line spectra of the corresponding LC-MS peaks. *c,* LC-MS/MS traces (multiple reaction monitoring, indicated by parent ion > fragment ion pair) or LC-MS traces (single ion monitoring, indicated by the *m/z* value monitored) of the products detected during the reaction between *o*-MitoPhB(OH)$_2$ probe and the authentic ONOO$^-$, H_2O_2, and HOCl.

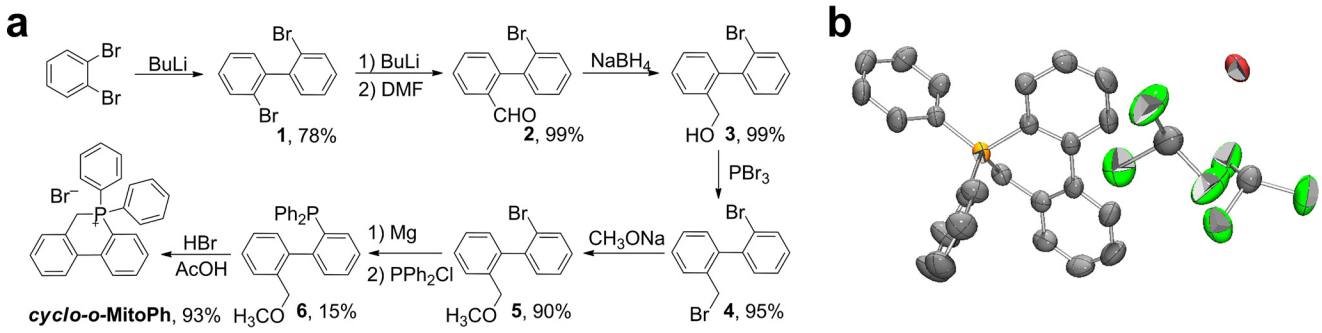


FIGURE 9. **Independent synthetic scheme for cyclo-*o*-MitoPh and structure determination by x-ray diffraction.** *a,* synthesis, and *b,* crystal structure of cyclo-*o*-MitoPh.

In this study, we identified new, oxidant-specific, products of the reaction of *o*-MitoPhB(OH)$_2$ with ONOO$^-$ and HOCl (Fig. 8). In the presence of the excess oxidant, the major phenolic product undergoes nitration or chlorination reaction, respectively, leading to isomeric nitro- or chloro-derivatives of MitoPhOH. Also, in the presence of HOBr, analogous products (*i.e.*

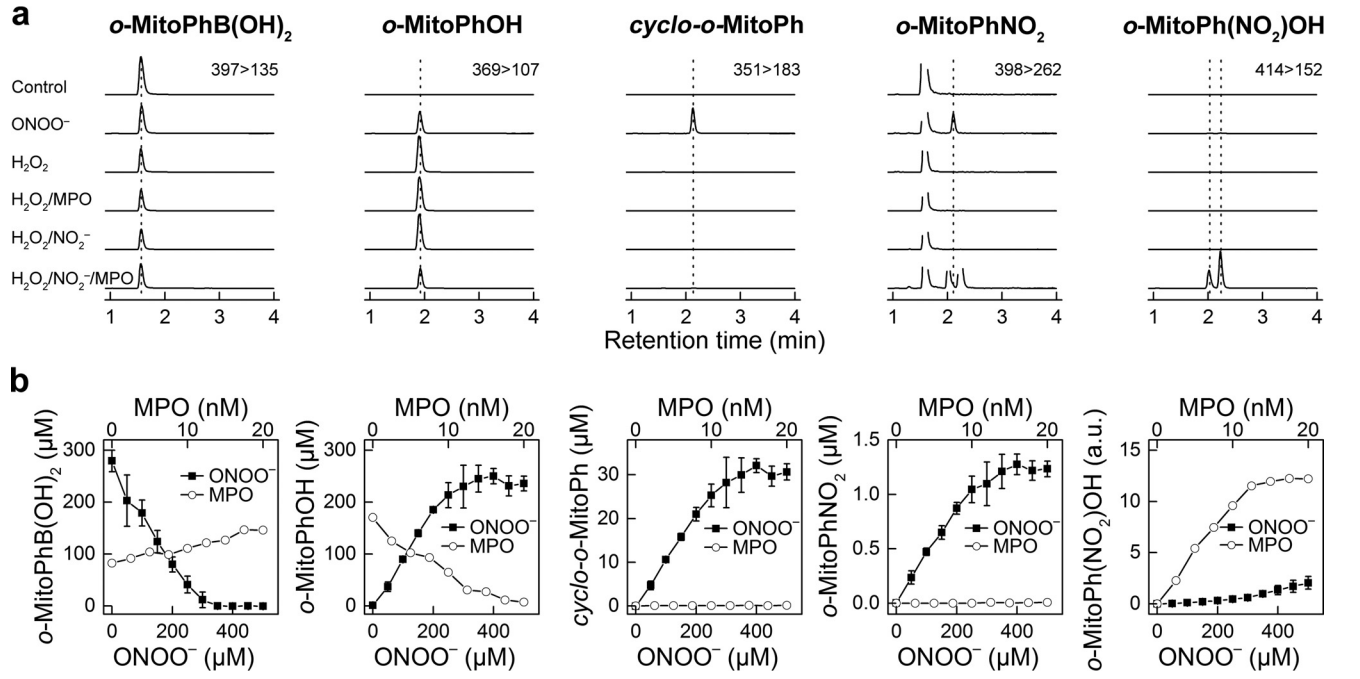


FIGURE 10. **Comparison of the products formed from oxidation of *o*-MitoPhB(OH)$_2$ by peroxynitrite and myeloperoxidase.** *a*, LC-MS/MS traces (multiple reaction monitoring, indicated by parent ion > fragment ion pair) of the products detected during the reaction between *o*-MitoPhB(OH)$_2$ probe (280 μM) and $ONOO^-$ (100 μM), H_2O_2 (1 mM), H_2O_2 (1 mM) + MPO (10 nM), H_2O_2 (1 mM) + $NaNO_2$ (10 mM), and H_2O_2 (1 mM) + $NaNO_2$ (10 mM) + MPO (10 nM). *b*, results of titration of *o*-MitoPhB(OH)$_2$ (280 μM) with $ONOO^-$ and MPO. *o*-MitoPhB(OH)$_2$ was incubated with MPO in the presence of H_2O_2 (1 mM) and $NaNO_2$ (10 mM) in 0.1 M phosphate buffer (pH 7.4) for 1 h at 25 °C.

MitoPh(Br)OH) are formed. With excess $ONOO^-$ or HOCl, the triphenylphosphine oxide was also formed (Fig. 8). Interestingly, with peroxynitrite, the most exclusive minor product, cyclo-*o*-MitoPh, was formed even when the probe was present in excess of the oxidant. The lack of effect of biologically relevant reductants (GSH and NADH) and the low efficiency of trapping of the phenyl radical (22) may be explained by rapid intramolecular cyclization due to addition of the phenyl radical to the benzene ring of the triphenylphosphonium moiety (Fig. 8*a*). As this product is not formed with any other oxidant or nitrating agent tested, it can serve as a specific diagnostic product of $ONOO^-$ and should be used as the ultimate proof of peroxynitrite intermediacy.

Inhibitory Mechanism of Nox2 Positive Hits on ROS Formation—Screening of the library of over 2,000 bioactive compounds generated a relatively high amount of positive hits, with the lowest yield (3.1%) using the hydropropidine-based assay. This was expected, as the compounds tested show a variety of biological activities and do not predominantly target NADPH oxidase. However, screening of a large, chemically diverse library of compounds will produce a significantly lower yield of active compounds. The HTS compatibility of the three assays (HPr^+, CBA, and Amplex Red-based) and the use of rapid HPLC analyses in the 384-well plate format will enable rapid orthogonal screenings to filter out false positives. Additionally, the use of chemical structure-based filters to remove pan assay interference compounds should further decrease the amount of compounds selected for post-screening studies/hit optimization process.

HL60 cells differentiated into a neutrophil-like phenotype by DMSO or all-*trans*-retinoic acid exhibited high expression of Nox2 as confirmed by Western blotting of both membrane-bound gp91^{phox} and cytosolic p47^{phox} subunits (8). The differentiated cells were compared with nondifferentiated cells in their response to PMA, an activator of protein kinase C, leading to the phosphorylation of the p47^{phox} cytosolic subunit, which, in turn, binds to p22^{phox} membrane protein. After the assembly of all cytosolic and membrane components, NADPH is oxidized, and its electrons are transferred to oxygen, generating $O_2^{\cdot-}$. Small molecules can inhibit $O_2^{\cdot-}$ and H_2O_2 by targeting specific steps of Nox activation as follows: Nox expression, ligand receptor binding, trafficking of Nox components to cell membrane, activation and assembly of Nox complex, NADPH binding, and electron transfer from the active site of the enzyme (64). To identify target of inhibition of Nox2, it is essential to perform a comprehensive analysis of phosphorylation of proteins of the regulatory subunits and the effect of inhibitors on phosphorylation and translocation of the cytosolic subunits to the membrane. These aspects will be a part of our future research. Some of the Nox2 inhibitors (*e.g.* promazines) identified in this work have previously been shown to block Nox2 activity in cell-free assays (36). Of added significance is the fact that selected hits also affect basal mitochondrial respiration in *d*HL60 cells (Fig. 5, *c* and *d*). Whereas sulconazole inhibits PMA response (Nox2 activation) and basal respiration similarly, other compounds are more selective in their inhibition of Nox2 activity, with little or less pronounced inhibition of mitochondrial function at selected concentrations. Although the inhibition of basal mitochondrial respiration and Nox2 activity may be linked, the inhibition of mitochondrial respiration *per se* is unlikely to block Nox2 activity. In fact, we have previously shown that rotenone, an inhibitor of mitochondrial complex I,

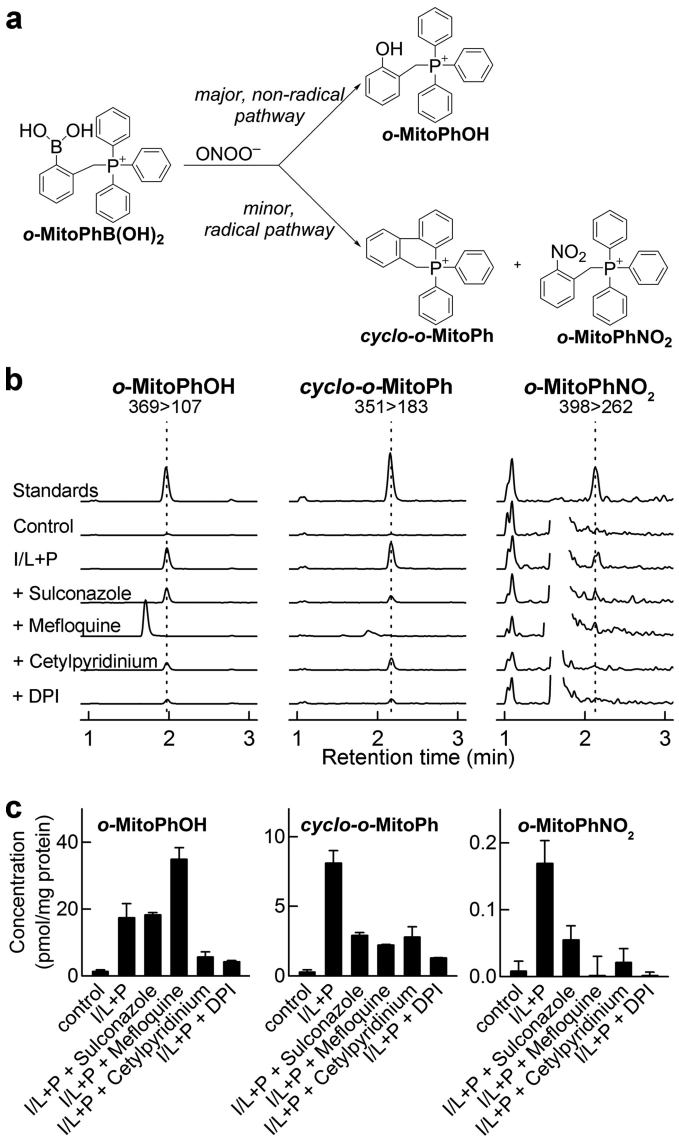


FIGURE 11. **Effect of selected positive hits for Nox2 inhibition on formation of *o*-MitoPhB(OH)$_2$ oxidation/nitration products, *o*-MitoPhOH, cyclo-*o*-MitoPh, and *o*-MitoPhNO$_2$.** *a,* scheme showing the major and minor products of the reaction of *o*-MitoPhB(OH)$_2$ and ONOO$^-$. *b,* LC-MS/MS traces corresponding to *o*-MitoPhOH, cyclo-*o*-MitoPh, and *o*-MitoPhNO$_2$, recorded during analysis of extracts of RAW 264.7 cells incubated with *o*-MitoPhB(OH)$_2$. Concentration of standards were as follows: 100 nM (*o*-MitoPhOH), 30 nM (cyclo-*o*-MitoPh), and 1 nM (*o*-MitoPhNO$_2$). *c,* quantitative analysis of the intracellular levels *o*-MitoPhOH, cyclo-*o*-MitoPh, and *o*-MitoPhNO$_2$, detected in cells stimulated to produce ONOO$^-$ in the absence or presence of Nox2 inhibitors, as indicated. RAW 264.7 cells were stimulated with IFNγ, LPS, and PMA (shown as *I/L + P*) and incubated for 1 h in the presence of *o*-MitoPhB(OH)$_2$ (50 μM). Inhibitors were added immediately before addition of PMA and the probe. Concentrations of agents are as follows: LPS, 0.5 μg/ml; IFNγ, 50 units/ml; PMA, 1 μM; DPI, 1 μM; sulconazole, 100 μM; mefloquine, 100 μM; cetylpyridinium chloride, 10 μM.

inhibits basal mitochondrial respiration in *d*HL60 cells, without affecting the Nox2 activity, as measured by the PMA-stimulated increase in the rate of oxygen consumption (8). It is also worth noting that DPI, a non-selective inhibitor of flavoenzymes, inhibits Nox2 activity at a significantly lower concentration (0.1 μM) than required for inhibiting the basal mitochondrial respiration (≈1 μM) (Fig. 5*d*).

The proposed method of high throughput screening of Nox inhibitors in intact cells will likely yield many positive hits that affect the Nox enzyme indirectly, as discussed above. The detailed mechanistic studies may provide new information on the pathways/factors controlling Nox enzyme activity and yield potentially new inhibitors for clinical trials, based on drug repurposing strategy.

Author Contributions—B. K. conceived and coordinated the study and wrote the paper. J. Z. designed, performed, analyzed, and interpreted the data, prepared the figures, and revised the paper critically. M. Z. performed the experiments and provided the technical assistance. G. C. designed and performed the Seahorse experiments and obtained cell proliferation data. M. H. and M. M. A. synthesized hydropropidine and cyclo-*o*-MitoPh product, respectively. O. O. provided assistance in these syntheses and structure analyses. R. P. synthesized *o*-MitoPhB(OH)$_2$, its oxidation/nitration products and corresponding deuterated analogs. A. S. helped in characterization of minor products of *o*-MitoPhB(OH)$_2$ oxidation. J. D. L. revised the manuscript for intellectual content. L. V. provided training, assisted in screening of the bioactive libraries at Broad Institute, and performed first pass analysis of the screening results. All authors reviewed the results and approved the final version of the manuscript.

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References

1. Bulua, A. C., Simon, A., Maddipati, R., Pelletier, M., Park, H., Kim, K. Y., Sack, M. N., Kastner, D. L., and Siegel, R. M. (2011) Mitochondrial reactive oxygen species promote production of proinflammatory cytokines and are elevated in TNFR1-associated periodic syndrome (TRAPS). *J. Exp. Med.* **208,** 519–533
2. Hecker, L., Cheng, J., and Thannickal, V. J. (2012) Targeting NOX enzymes in pulmonary fibrosis. *Cell. Mol. Life Sci.* **69,** 2365–2371
3. Leto, T. L., Morand, S., Hurt, D., and Ueyama, T. (2009) Targeting and regulation of reactive oxygen species generation by Nox family NADPH oxidases. *Antioxid. Redox Signal.* **11,** 2607–2619
4. Lambeth, J. D. (2004) NOX enzymes and the biology of reactive oxygen. *Nat. Rev. Immunol.* **4,** 181–189
5. Nisimoto, Y., Diebold, B. A., Cosentino-Gomes, D., Constentino-Gomes, D., and Lambeth, J. D. (2014) Nox4: a hydrogen peroxide-generating oxygen sensor. *Biochemistry* **53,** 5111–5120
6. Altenhöfer, S., Radermacher, K. A., Kleikers, P. W., Wingler, K., and Schmidt, H. H. (2015) Evolution of NADPH oxidase inhibitors: selectivity and mechanisms for target engagement. *Antioxid. Redox Signal.* **23,** 406–427
7. Zielonka, J., Zielonka, M., Sikora, A., Adamus, J., Joseph, J., Hardy, M., Ouari, O., Dranka, B. P., and Kalyanaraman, B. (2012) Global profiling of reactive oxygen and nitrogen species in biological systems: high throughput real-time analyses. *J. Biol. Chem.* **287,** 2984–2995
8. Zielonka, J., Cheng, G., Zielonka, M., Ganesh, T., Sun, A., Joseph, J., Michalski, R., O'Brien, W. J., Lambeth, J. D., and Kalyanaraman, B. (2014) High throughput assays for superoxide and hydrogen peroxide: design of a screening workflow to identify inhibitors of NADPH oxidases. *J. Biol. Chem.* **289,** 16176–16189
9. Daiber, A., August, M., Baldus, S., Wendt, M., Oelze, M., Sydow, K., Kleschyov, A. L., and Munzel, T. (2004) Measurement of NAD(P)H oxidase-derived superoxide with the luminol analogue L-012. *Free Radic. Biol. Med.* **36,** 101–111
10. Zielonka, J., Lambeth, J. D., and Kalyanaraman, B. (2013) On the use of L-012, a luminol-based chemiluminescent probe, for detecting superoxide and identifying inhibitors of NADPH oxidase: a reevaluation. *Free Radic. Biol. Med.* **65,** 1310–1314

11. Beckman, J. S., Beckman, T. W., Chen, J., Marshall, P. A., and Freeman, B. A. (1990) Apparent hydroxyl radical production by peroxynitrite: implications for endothelial injury from nitric oxide and superoxide. *Proc. Natl. Acad. Sci. U.S.A.* **87,** 1620–1624
12. Radi, R., Beckman, J. S., Bush, K. M., and Freeman, B. A. (1991) Peroxynitrite oxidation of sulfhydryls. The cytotoxic potential of superoxide and nitric oxide. *J. Biol. Chem.* **266,** 4244–4250
13. Beckman, J. S. (2009) Understanding peroxynitrite biochemistry and its potential for treating human diseases. *Arch. Biochem. Biophys.* **484,** 114–116
14. Al Ghouleh, I., Khoo, N. K., Knaus, U. G., Griendling, K. K., Touyz, R. M., Thannickal, V. J., Barchowsky, A., Nauseef, W. M., Kelley, E. E., Bauer, P. M., Darley-Usmar, V., Shiva, S., Cifuentes-Pagano, E., Freeman, B. A., Gladwin, M. T., and Pagano, P. J. (2011) Oxidases and peroxidases in cardiovascular and lung disease: new concepts in reactive oxygen species signaling. *Free Radic. Biol. Med.* **51,** 1271–1288
15. Pacher, P., Beckman, J. S., and Liaudet, L. (2007) Nitric oxide and peroxynitrite in health and disease. *Physiol. Rev.* **87,** 315–424
16. Ye, Y., Quijano, C., Robinson, K. M., Ricart, K. C., Strayer, A. L., Sahawneh, M. A., Shacka, J. J., Kirk, M., Barnes, S., Accavitti-Loper, M. A., Radi, R., Beckman, J. S., and Estévez, A. G. (2007) Prevention of peroxynitrite-induced apoptosis of motor neurons and PC12 cells by tyrosine-containing peptides. *J. Biol. Chem.* **282,** 6324–6337
17. Guzik, T. J., and Harrison, D. G. (2006) Vascular NADPH oxidases as drug targets for novel antioxidant strategies. *Drug Discov. Today* **11,** 524–533
18. Cifuentes-Pagano, E., Meijles, D. N., and Pagano, P. J. (2014) The quest for selective nox inhibitors and therapeutics: challenges, triumphs and pitfalls. *Antioxid. Redox Signal.* **20,** 2741–2754
19. Michalski, R., Zielonka, J., Hardy, M., Joseph, J., and Kalyanaraman, B. (2013) Hydropropidine: a novel, cell-impermeant fluorogenic probe for detecting extracellular superoxide. *Free Radic. Biol. Med.* **54,** 135–147
20. Zielonka, J., Sikora, A., Hardy, M., Joseph, J., Dranka, B. P., and Kalyanaraman, B. (2012) Boronate probes as diagnostic tools for real time monitoring of peroxynitrite and hydroperoxides. *Chem. Res. Toxicol.* **25,** 1793–1799
21. Zielonka, J., Sikora, A., Adamus, J., and Kalyanaraman, B. (2015) Detection and differentiation between peroxynitrite and hydroperoxides using mitochondria-targeted arylboronic acid. *Methods Mol. Biol.* **1264,** 171–181
22. Sikora, A., Zielonka, J., Adamus, J., Debski, D., Dybala-Defratyka, A., Michalowski, B., Joseph, J., Hartley, R. C., Murphy, M. P., and Kalyanaraman, B. (2013) Reaction between peroxynitrite and triphenylphosphonium-substituted arylboronic acid isomers: identification of diagnostic marker products and biological implications. *Chem. Res. Toxicol.* **26,** 856–867
23. Zhao, H., Joseph, J., Fales, H. M., Sokoloski, E. A., Levine, R. L., Vasquez-Vivar, J., and Kalyanaraman, B. (2005) Detection and characterization of the product of hydroethidine and intracellular superoxide by HPLC and limitations of fluorescence. *Proc. Natl. Acad. Sci. U.S.A.* **102,** 5727–5732
24. Zielonka, J., Vasquez-Vivar, J., and Kalyanaraman, B. (2008) Detection of 2-hydroxyethidium in cellular systems: a unique marker product of superoxide and hydroethidine. *Nat. Protoc.* **3,** 8–21
25. Teufelhofer, O., Weiss, R. M., Parzefall, W., Schulte-Hermann, R., Micksche, M., Berger, W., and Elbling, L. (2003) Promyelocytic HL60 cells express NADPH oxidase and are excellent targets in a rapid spectrophotometric microplate assay for extracellular superoxide. *Toxicol. Sci.* **76,** 376–383
26. Seitz, P. M., Cooper, R., Gatto, G. J., Jr., Ramon, F., Sweitzer, T. D., Johns, D. G., Davenport, E. A., Ames, R. S., and Kallal, L. A. (2010) Development of a high throughput cell-based assay for superoxide production in HL-60 cells. *J. Biomol. Screen.* **15,** 388–397
27. Zhang, J. H., Chung, T. D., and Oldenburg, K. R. (1999) A simple statistical parameter for use in evaluation and validation of high throughput screening assays. *J. Biomol. Screen.* **4,** 67–73
28. Nicholls, D. G., Darley-Usmar, V. M., Wu, M., Jensen, P. B., Rogers, G. W., and Ferrick, D. A. (2010) Bioenergetic profile experiment using C2C12 myoblast cells. *J. Vis. Exp.* **46,** 2511
29. Oba, M., Iida, M., and Nishiyama, K. (2001) Generation and reactions of transient 9-silaphenanthrene derivative. *Organometallics* **20,** 4287–4290
30. Cookson, E. A., and Crofts, P. C. (1966) Phosphorus heterocycles. Part I. A conjugated cyclic methylenephosphorane. *J. Chem. Soc. C,* 2003–2005
31. Goy, R., Apfel, U. P., Elleouet, C., Escudero, D., Elstner, M., Görls, H., Talarmin, J., Schollhammer, P., González, L., and Weigand, W. (2013) A silicon-heteroaromatic system as photosensitizer for light-driven hydrogen production by hydrogenase mimics. *Eur. J. Inorg. Chem.* **2013,** 4466–4472
32. Sikora, A., Zielonka, J., Lopez, M., Dybala-Defratyka, A., Joseph, J., Marcinek, A., and Kalyanaraman, B. (2011) Reaction between peroxynitrite and boronates: EPR spin-trapping, HPLC analyses, and quantum mechanical study of the free radical pathway. *Chem. Res. Toxicol.* **24,** 687–697
33. Zielonka, J., Sikora, A., Joseph, J., and Kalyanaraman, B. (2010) Peroxynitrite is the major species formed from different flux ratios of co-generated nitric oxide and superoxide: direct reaction with boronate-based fluorescent probe. *J. Biol. Chem.* **285,** 14210–14216
34. Van de Bittner, G. C., Dubikovskaya, E. A., Bertozzi, C. R., and Chang, C. J. (2010) *In vivo* imaging of hydrogen peroxide production in a murine tumor model with a chemoselective bioluminescent reporter. *Proc. Natl. Acad. Sci. U.S.A.* **107,** 21316–21321
35. Cohen, H. J., Chovaniec, M. E., and Ellis, S. E. (1980) Chlorpromazine inhibition of granulocyte superoxide production. *Blood* **56,** 23–29
36. Seredenina, T., Chiriano, G., Filippova, A., Nayernia, Z., Mahiout, Z., Fioraso-Cartier, L., Plastre, O., Scapozza, L., Krause, K. H., and Jaquet, V. (2015) A subset of *N*-substituted phenothiazines inhibits NADPH oxidases. *Free Radic. Biol. Med.* **86,** 239–249
37. Burkhart, R. A., Peng, Y., Norris, Z. A., Tholey, R. M., Talbott, V. A., Liang, Q., Ai, Y., Miller, K., Lal, S., Cozzitorto, J. A., Witkiewicz, A. K., Yeo, C. J., Gehrmann, M., Napper, A., Winter, J. M., *et al.* (2013) Mitoxantrone targets human ubiquitin-specific peptidase 11 (USP11) and is a potent inhibitor of pancreatic cancer cell survival. *Mol. Cancer Res.* **11,** 901–911
38. Baell, J. B., and Holloway, G. A. (2010) New substructure filters for removal of pan assay interference compounds (PAINS) from screening libraries and for their exclusion in bioassays. *J. Med. Chem.* **53,** 2719–2740
39. Baell, J., and Walters, M. A. (2014) Chemistry: chemical con artists foil drug discovery. *Nature* **513,** 481–483
40. Sikora, A., Zielonka, J., Lopez, M., Joseph, J., and Kalyanaraman, B. (2009) Direct oxidation of boronates by peroxynitrite: mechanism and implications in fluorescence imaging of peroxynitrite. *Free Radic. Biol. Med.* **47,** 1401–1407
41. Ximenes, V. F., Morgon, N. H., and de Souza, A. R. (2015) Hypobromous acid, a powerful endogenous electrophile: experimental and theoretical studies. *J. Inorg. Biochem.* **146,** 61–68
42. Kumar, K., and Margerum, D. W. (1987) Kinetics and mechanism of general-acid-assisted oxidation of bromide by hypochlorite and hypochlorous acid. *Inorg. Chem.* **26,** 2706–2711
43. Drummond, G. R., Selemidis, S., Griendling, K. K., and Sobey, C. G. (2011) Combating oxidative stress in vascular disease: NADPH oxidases as therapeutic targets. *Nat. Rev. Drug Discov.* **10,** 453–471
44. Jaquet, V., Scapozza, L., Clark, R. A., Krause, K. H., and Lambeth, J. D. (2009) Small-molecule NOX inhibitors: ROS-generating NADPH oxidases as therapeutic targets. *Antioxid. Redox Signal.* **11,** 2535–2552
45. Mukhopadhyay, P., Horváth, B., Zsengellér, Z., Zielonka, J., Tanchian, G., Holovac, E., Kechrid, M., Patel, V., Stillman, I. E., Parikh, S. M., Joseph, J., Kalyanaraman, B., and Pacher, P. (2012) Mitochondrial-targeted antioxidants represent a promising approach for prevention of cisplatin-induced nephropathy. *Free Radic. Biol. Med.* **52,** 497–506
46. Deng, Y., Thompson, B. M., Gao, X., and Hall, E. D. (2007) Temporal relationship of peroxynitrite-induced oxidative damage, calpain-mediated cytoskeletal degradation and neurodegeneration after traumatic brain injury. *Exp. Neurol.* **205,** 154–165
47. Khan, M., Dhammu, T. S., Matsuda, F., Annamalai, B., Dhindsa, T. S., Singh, I., and Singh, A. K. (2016) Targeting the nNOS/peroxynitrite/calpain system to confer neuroprotection and aid functional recovery in a mouse model of TBI. *Brain Res.* **1630,** 159–170
48. Corzo, C. A., Cotter, M. J., Cheng, P., Cheng, F., Kusmartsev, S., Sotomayor, E., Padhya, T., McCaffrey, T. V., McCaffrey, J. C., and Gabrilovich, D. I. (2009) Mechanism regulating reactive oxygen species in tumor-induced myeloid-derived suppressor cells. *J. Immunol.* **182,** 5693–5701
49. Holmström, K. M., and Finkel, T. (2014) Cellular mechanisms and physi-

ological consequences of redox-dependent signalling. *Nat. Rev. Mol. Cell Biol.* **15,** 411–421
50. Bonner, M. Y., and Arbiser, J. L. (2012) Targeting NADPH oxidases for the treatment of cancer and inflammation. *Cell. Mol. Life Sci.* **69,** 2435–2442
51. Winterbourn, C. C. (2008) Reconciling the chemistry and biology of reactive oxygen species. *Nat. Chem. Biol.* **4,** 278–286
52. Kalyanaraman, B. (2013) Teaching the basics of redox biology to medical and graduate students: oxidants, antioxidants and disease mechanisms. *Redox Biol.* **1,** 244–257
53. Murphy, M. P., Holmgren, A., Larsson, N. G., Halliwell, B., Chang, C. J., Kalyanaraman, B., Rhee, S. G., Thornalley, P. J., Partridge, L., Gems, D., Nyström, T., Belousov, V., Schumacker, P. T., and Winterbourn, C. C. (2011) Unraveling the biological roles of reactive oxygen species. *Cell Metab.* **13,** 361–366
54. Bendall, J. K., Cave, A. C., Heymes, C., Gall, N., and Shah, A. M. (2002) Pivotal role of a gp91(phox)-containing NADPH oxidase in angiotensin II-induced cardiac hypertrophy in mice. *Circulation* **105,** 293–296
55. Mukhopadhyay, P., Rajesh, M., Bátkai, S., Kashiwaya, Y., Haskó, G., Liaudet, L., Szabó, C., and Pacher, P. (2009) Role of superoxide, nitric oxide, and peroxynitrite in doxorubicin-induced cell death *in vivo* and *in vitro*. *Am. J. Physiol. Heart Circ. Physiol* **296,** H1466–H1483
56. Zhao, Y., McLaughlin, D., Robinson, E., Harvey, A. P., Hookham, M. B., Shah, A. M., McDermott, B. J., and Grieve, D. J. (2010) Nox2 NADPH oxidase promotes pathologic cardiac remodeling associated with doxorubicin chemotherapy. *Cancer Res.* **70,** 9287–9297
57. Borbély, G., Szabadkai, I., Horváth, Z., Markó, P., Varga, Z., Breza, N., Baska, F., Vántus, T., Huszár, M., Geiszt, M., Hunyady, L., Buday, L., Orfi, L., and Kéri, G. (2010) Small-molecule inhibitors of NADPH oxidase 4. *J. Med. Chem.* **53,** 6758–6762
58. Wind, S., Beuerlein, K., Eucker, T., Müller, H., Scheurer, P., Armitage, M. E., Ho, H., Schmidt, H. H., and Wingler, K. (2010) Comparative pharmacology of chemically distinct NADPH oxidase inhibitors. *Br. J. Pharmacol.* **161,** 885–898
59. Gianni, D., Taulet, N., Zhang, H., DerMardirossian, C., Kister, J., Martinez, L., Roush, W. R., Brown, S. J., Bokoch, G. M., and Rosen, H. (2010) A novel and specific NADPH oxidase-1 (Nox1) small-molecule inhibitor blocks the formation of functional invadopodia in human colon cancer cells. *ACS Chem. Biol.* **5,** 981–993
60. Heumüller, S., Wind, S., Barbosa-Sicard, E., Schmidt, H. H., Busse, R., Schröder, K., and Brandes, R. P. (2008) Apocynin is not an inhibitor of vascular NADPH oxidases but an antioxidant. *Hypertension* **51,** 211–217
61. Hirano, K., Chen, W. S., Chueng, A. L., Dunne, A. A., Seredenina, T., Filippova, A., Ramachandran, S., Bridges, A., Chaudry, L., Pettman, G., Allan, C., Duncan, S., Lee, K. C., Lim, J., Ma, M. T., *et al.* (2015) Discovery of GSK2795039, a novel small molecule NADPH oxidase 2 inhibitor. *Antioxid. Redox Signal.* **23,** 358–374
62. Li, Y., Ganesh, T., Diebold, B. A., Zhu, Y., McCoy, J. W., Smith, S. M., Sun, A., and Lambeth, J. D. (2015) Thioxo-dihydroquinazolin-one compounds as novel inhibitors of myeloperoxidase. *ACS Med. Chem. Lett.* **6,** 1047–1052
63. Kalyanaraman, B., Darley-Usmar, V., Davies, K. J., Dennery, P. A., Forman, H. J., Grisham, M. B., Mann, G. E., Moore, K., Roberts, L. J., 2nd., and Ischiropoulos, H. (2012) Measuring reactive oxygen and nitrogen species with fluorescent probes: challenges and limitations. *Free Radic. Biol. Med.* **52,** 1–6
64. Streeter, J., Thiel, W., Brieger, K., and Miller, F. J., Jr. (2013) Opportunity Nox: the future of NADPH oxidases as therapeutic targets in cardiovascular disease. *Cardiovasc. Ther.* **31,** 125–137

Mitigation of NADPH oxidase 2 activity as a strategy to inhibit peroxynitrite formation

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SUPPLEMENTAL DATA

SUPPLEMENTAL TABLE S-1: List of all the compounds tested for Nox2 activity (using three different probes) at Broad Institute Screening Facility, and the normalized scores.

Supplemental Table S-1

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1	HEMADO	BRD-A00267231-001-01-1	-16.0	-18.0	29.5	39.9	37.5	18.5
2	(+)-UH 232 maleate	BRD-A00327403-103-01-9	9.2	20.3	23.6	-4.7	12.3	24.4
3	AF-DX 116	BRD-A00520476-001-03-3	-17.6	0.7	-3.4	7.5	3.1	6.2
4	BIPERIDEN	BRD-A00546892-001-01-8	-6.4	3.5	-0.5	-9.5	1.2	7.6
5	DYPHYLLINE	BRD-A00827783-001-15-4	-14.7	3.0	-5.4	-11.1	3.1	18.6
6	ALPRENOLOL	BRD-A00993607-003-15-4	-16.4	-40.9	-21.4	-20.7	-9.4	-6.3
7	HEXESTROL	BRD-A01078468-001-08-0	-12.0	38.2	-30.9	-22.3	-7.4	-10.0
8	Salmeterol	BRD-A01320529-001-05-9	-8.7	-10.1	-18.0	-18.8	-22.3	-17.2
9	FLUMETHASONE	BRD-A01346607-001-03-4	6.7	4.3	4.6	0.8	9.8	11.5
10	WB 4101 hydrochloride	BRD-A01493904-003-05-5	2.1	-16.5	-13.6	-16.4	-0.9	-2.6
11	CHLORMADINONE ACETATE	BRD-A01593789-001-02-3	-40.9	-17.7	-34.9	-25.4	-12.4	-11.0
12	BUPIVACAINE HYDROCHLORIDE	BRD-A01636364-003-08-6	4.6	10.3	0.8	-12.8	4.4	9.6
13	NAFTOPIDIL DIHYDROCHLORIDE	BRD-A01787639-300-04-5	-10.1	-4.4	-6.2	-0.9	-11.7	-16.9
14	NITRENDIPINE	BRD-A02006392-001-09-9	-53.2	-4.3	-33.7	-27.4	-16.2	-19.2
15	BETAMETHASONE	BRD-A02180903-001-03-7	-16.4	-8.1	11.2	19.7	18.2	18.7
16	DIHYDROCELASTRYL DIACETATE	BRD-A02267565-001-02-3	20.1	-7.1	-43.6	-31.0	-33.0	-42.4
17	ETHINYL ESTRADIOL	BRD-A02367930-001-03-7	11.6	6.9	-30.6	-12.8	-4.6	0.0
18	NMDA	BRD-A02508087-001-01-1	6.5	-14.2	5.3	17.7	6.9	19.8
19	Betaxolol hydrochloride	BRD-A02759312-003-11-2	-5.8	15.2	-7.1	-3.8	12.2	7.8
20	DEOXYANDIROBIN	BRD-A02799884-001-03-7	-7.7	-3.1	-11.4	-6.1	-10.0	-7.6
21	MEPIVACAINE HYDROCHLORIDE	BRD-A03216249-003-12-8	-28.6	-1.6	-2.1	6.4	5.4	-6.8
22	ICI-89406	BRD-A03359064-001-01-5	2.4	8.4	21.4	18.1	19.5	26.1
23	ROSMARINIC ACID	BRD-A03397678-001-06-2	37.8	30.7	-8.9	3.4	-57.1	-52.8
24	METOPROLOL TARTRATE	BRD-A03623303-045-05-3	-3.3	-13.0	-9.5	-9.7	8.2	-1.3
25	CP 55,940	BRD-A03816571-001-01-0	-11.6	-15.7	-64.2	-82.3	-40.4	-45.0
26	METHSCOPOLAMINE BROMIDE	BRD-A03932035-004-03-5	-21.8	21.8	18.3	26.2	22.1	21.0
27	YO-2	BRD-A04026261-001-01-0	1.5	0.4	18.5	20.6	22.5	12.4
28	?-Funaltrexamine hydrochloride	BRD-A04231641-003-01-3	2.4	-7.9	-9.9	3.5	-4.8	-5.0
29	U-54494A hydrochloride	BRD-A04258855-003-01-7	-11.6	3.7	1.7	-3.3	0.2	2.6
30	SKF 83959 hydrobromide	BRD-A04260165-004-02-4	-32.6	-34.7	-25.6	-30.7	-54.3	-55.7
31	DEXCHLORPHENIRAMINE MALEATE	BRD-A04553218-050-08-9	-9.8	-11.8	-33.9	-41.3	-17.8	-10.9
32	2-[(4-Phenylpiperazin-1-yl)methyl]-2,3-dihydroimidazo[1,2-c]quinazolin-5(6H)-one	BRD-A04661934-001-01-1	0.5	-2.0	-25.5	-32.7	-13.3	-10.4
33	Dibutyryl-cAMP, sodium salt	BRD-A04706586-236-01-7	-7.4	-3.4	6.2	4.0	0.0	3.2
34	NORGESTIMATE	BRD-A04756508-001-01-5	-22.2	-17.5	-30.7	-9.3	-8.1	0.2
35	1,2alpha-EPOXYDEACETOXYDIHYDROGEDUNIN	BRD-A04975445-001-03-3	9.9	-5.9	-4.2	10.8	6.7	-2.7
36	BUPROPION	BRD-A05186015-003-09-9	0.4	-4.3	-0.3	-5.7	10.3	3.1
37	Ipratropium bromide	BRD-A05352148-004-02-0	12.4	-4.9	10.8	2.0	-2.9	0.7
38	TRIDESACETOXYKHIVORIN	BRD-A05422420-001-03-4	-26.0	17.0	-16.4	-11.1	-8.3	2.5
39	(?)-Bay K 8644	BRD-A05457250-001-04-3	-6.7	-5.8	-11.8	-11.4	-14.8	-9.1
40	SOLIDAGENONE	BRD-A05666893-001-03-4	-14.5	-13.0	-48.3	-40.6	-32.0	-34.3
41	HEDERAGENIN	BRD-A05987535-001-03-8	-9.6	-4.9	22.4	33.9	23.8	28.3
42	ETICLOPRIDE HYDROCHLORIDE	BRD-A05994177-003-02-5	3.3	5.1	-24.7	-8.9	-17.9	-18.9
43	EPOXYGEDUNIN	BRD-A06232236-001-03-0	-13.4	-15.3	-5.1	6.0	-5.1	-8.5

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
44	N-Benzylnaltrindole hydrochloride	BRD-A06276885-003-01-1	-34.6	-50.6	15.6	9.3	-85.3	-83.6
45	TERFENADINE	BRD-A06352418-001-15-0	-12.0	-18.8	-85.5	-84.0	-41.5	-52.5
46	HYDROQUINIDINE	BRD-A06390036-001-03-8	-7.5	-13.3	-8.0	4.8	0.6	4.1
47	DEACETYLGEDUNIN	BRD-A06561405-001-03-7	-15.5	-15.3	-29.6	-19.3	-32.7	-14.9
48	FUSIDIC ACID	BRD-A06935312-001-03-5	7.8	8.0	3.2	22.8	13.2	8.7
49	HYDROCORTISONE HEMISUCCINATE	BRD-A07000685-001-03-6	4.4	-11.2	0.4	21.4	1.8	7.9
50	.ONDANSETRON	BRD-A07195938-001-01-3	6.9	-13.7	0.6	3.2	7.4	5.1
51	4-(3-BUTOXY-4-METHOXYBENZYL)IMIDAZOLIDIN-2-ONE	BRD-A07207424-001-09-0	7.4	15.4	8.7	28.6	17.6	30.3
52	8-M-PDOT	BRD-A07232941-001-01-9	-7.1	-2.8	8.3	28.6	19.2	11.9
53	LABETALOL HYDROCHLORIDE	BRD-A07440155-003-16-3	-9.9	-8.3	9.7	15.5	3.9	9.2
54	MECLOCYCLINE SULFOSALICYLATE	BRD-A07600638-060-03-7	35.9	28.7	-24.4	-13.7	-30.7	-57.0
55	Cilnidipine	BRD-A07875874-001-01-6	-8.7	-15.8	-37.0	-44.3	-20.4	-25.8
56	Methiothepin maleate	BRD-A07932845-103-01-5	-111.0	-108.1	-101.2	-102.4	-83.8	-85.8
57	FAMPROFAZONE	BRD-A08255417-001-06-3	-24.6	1.9	-54.5	-23.9	-15.3	-10.0
58	DOXYCYCLINE HYDROCHLORIDE	BRD-A08545410-003-03-7	5.3	5.1	-86.9	-93.1	-90.1	-89.7
59	ALFLUZOSIN	BRD-A09056319-001-05-5	-24.6	-2.4	19.3	24.4	10.7	16.6
60	STRYCHNINE	BRD-A09094913-001-03-1	-9.3	-1.6	-5.6	8.5	11.4	15.3
61	NORETHINDRONE ACETATE	BRD-A09349126-001-06-5	-9.4	-12.6	-14.6	-6.3	-7.4	-14.3
62	MEBEVERINE HYDROCHLORIDE	BRD-A09467419-003-14-1	-3.9	3.8	0.8	17.2	-8.3	-0.4
63	Flecainide acetate	BRD-A09472452-015-11-9	16.3	-3.4	3.9	17.2	15.0	12.3
64	BICUCULLINE (+)	BRD-A09495397-001-03-5	-14.7	-1.7	-3.4	0.8	-2.5	12.0
65	HOMATROPINE BROMIDE	BRD-A09539288-004-03-6	0.4	-4.8	-4.0	-0.5	4.9	6.6
66	SKF 81297 hydrobromide	BRD-A09828896-004-04-5	2.9	4.4	-0.3	-14.5	-41.7	-39.8
67	ALGESTERONE ACETOPHENIDE	BRD-A09977907-001-01-9	-7.4	-5.2	-8.2	20.1	-1.7	8.9
68	PROPRANOLOL HYDROCHLORIDE (+/-)	BRD-A10070317-003-17-6	-14.0	-14.5	-74.9	-48.8	-44.1	-37.9
69	DEXAMETHASONE	BRD-A10188456-001-03-1	0.5	-2.1	21.9	22.2	-1.7	11.5
70	Norketamine hydrochloride	BRD-A10355991-003-01-8	-3.5	-16.4	-14.1	-17.0	-0.5	2.8
71	Cyclopiazonic Acid	BRD-A10420615-001-03-6	-1.3	12.4	0.0	-8.7	-4.8	3.5
72	SULPIRIDE	BRD-A10715913-001-03-8	-12.9	9.2	16.4	7.0	-7.1	5.9
73	EFAROXAN HYDROCHLORIDE	BRD-A10739734-003-05-6	-2.8	-4.6	5.9	26.4	1.6	2.0
74	Imiloxan hydrochloride	BRD-A10903566-003-02-8	-10.1	-9.6	-5.7	-12.3	6.5	5.1
75	CARVEDILOL	BRD-A10977446-001-05-5	-6.0	-15.7	-24.0	-31.8	-12.9	-17.7
76	BECLOMETHASONE DIPROPIONATE	BRD-A11319535-001-02-8	-12.1	-8.2	5.1	13.5	0.0	7.0
77	DEHYDROCHOLIC ACID	BRD-A11551002-001-03-8	5.1	11.2	-3.6	-5.6	-0.9	-3.1
78	SB 205607 dihydrobromide	BRD-A11609859-303-01-2	-3.2	-5.4	-0.7	-3.5	-4.3	-3.3
79	Wortmannin	BRD-A11678676-001-03-4	48.9	43.2	21.5	21.4	-4.7	-8.5
80	ENILCONAZOLE	BRD-A11776908-001-06-9	-7.7	-3.6	-20.5	-13.1	-4.5	1.5
81	AM 92016 hydrochloride	BRD-A11813248-003-01-6	-24.5	-17.3	-45.0	-38.1	-38.5	-39.4
82	PROTOVERATRINE A	BRD-A12055418-001-03-7	-23.7	21.6	-10.9	17.6	0.3	16.5
83	1,7-DIDEACETOXY-1,7-DIOXO-3-DEACETYLKHIVORIN	BRD-A12372458-001-03-7	-4.8	-3.4	-16.3	15.8	-9.6	-1.1
84	p-FLUOROPHENYLALANINE	BRD-A12490356-001-03-0	-13.8	-1.1	-2.6	0.9	5.1	5.4
85	(-)-U-50488 hydrochloride	BRD-A12822115-003-01-6	-0.8	3.5	5.8	13.1	-22.0	-12.0
86	FLUOROMETHOLONE	BRD-A13133631-001-03-2	8.4	-11.0	-7.0	-11.7	5.2	8.5
87	DOXAZOSIN MESYLATE	BRD-A13188892-066-13-2	-6.4	2.6	14.0	10.8	1.9	7.2
88	PERILLYL ALCOHOL	BRD-A13323580-001-03-0	-22.6	7.3	-7.8	10.0	-3.6	-7.0
89	KHIVORIN	BRD-A13569698-001-03-7	-10.8	1.7	-5.3	-19.5	-10.8	-8.3

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
90	DOBUTAMINE HYDROCHLORIDE	BRD-A13912374-003-03-6	45.3	23.9	54.3	58.2	-12.9	-12.3
91	SULINDAC	BRD-A13946108-001-08-0	1.1	16.9	-10.6	1.2	-20.7	-19.4
92	TC 1	BRD-A13964793-001-01-8	12.1	14.0	39.5	36.8	12.8	23.1
93	3alpha-ACETOXYDIHYDRODEOXYGEDUNIN	BRD-A14098586-001-03-1	-23.6	-14.7	-22.4	-29.2	1.7	4.8
94	OXYPHENONIUM BROMIDE	BRD-A14208071-004-10-7	11.3	1.9	6.5	17.5	16.9	21.4
95	SN-6	BRD-A14316475-001-01-5	-15.3	-23.0	-52.6	-45.6	-47.6	-56.6
96	IDRA 21	BRD-A14344385-001-02-4	-5.5	-35.7	-5.3	17.2	5.0	8.9
97	Scopolamine hydrobromide	BRD-A14566392-004-03-5	-6.8	14.0	5.2	17.8	10.0	7.5
98	UB 165 fumarate	BRD-A14574269-051-01-4	-8.1	-7.9	6.3	-4.9	-5.6	14.2
99	MESTRANOL	BRD-A14798026-001-01-8	8.9	5.8	30.6	44.2	9.1	-2.9
100	ALAPROCLATE	BRD-A14966924-001-03-0	-29.1	-27.3	-25.1	-22.2	-13.5	-17.9
101	Benazepril hydrochloride	BRD-A15131297-003-01-9	-16.0	57.2	12.3	25.5	6.5	7.3
102	FLUOCINONIDE	BRD-A15297126-001-03-5	-21.4	3.5	-27.5	-15.8	-3.2	-0.8
103	BMY 14802 hydrochloride	BRD-A15435692-003-01-5	3.3	-3.9	60.3	-8.2	15.9	11.5
104	6-HYDROXYANGOLENSIC ACID METHYL ESTER	BRD-A15454510-001-03-6	1.4	-1.1	0.1	1.6	-9.0	-11.2
105	SDZ 21009	BRD-A15530910-001-01-3	-4.1	-0.9	-26.6	-31.4	3.9	1.5
106	ISOFLUPREDNONE ACETATE	BRD-A15670677-001-01-0	15.1	-17.7	-6.2	-15.8	-2.8	7.9
107	TELITHROMYCIN	BRD-A15798299-001-02-5	-4.6	-3.4	23.9	25.4	1.3	3.8
108	REBAMIPIDE	BRD-A15909516-001-03-3	0.6	-11.6	20.5	18.0	3.5	7.4
109	MODAFINIL	BRD-A16332958-001-04-0	-1.2	-5.8	6.0	4.7	0.5	9.7
110	BUTOCONAZOLE	BRD-A16665823-001-01-2	-50.8	-32.1	-85.7	-82.4	-61.3	-69.1
111	BADGE	BRD-A16694057-001-03-5	2.8	-13.9	20.4	27.9	1.2	0.9
112	ISOXSUPRINE HYDROCHLORIDE	BRD-A16700644-003-03-6	16.7	16.0	-7.1	-4.9	-18.0	-16.1
113	2-Chloro-N6-cyclopentyladenosine	BRD-A16827030-001-01-7	0.2	-10.3	6.1	7.8	24.6	13.5
114	8beta-HYDROXYCARAPIN, 3,8-HEMIACETAL	BRD-A17120244-001-03-4	-6.2	15.3	-1.5	0.9	-1.8	21.0
115	CARPROFEN	BRD-A17411484-001-05-1	2.3	1.3	-13.9	-8.0	-1.9	-1.2
116	BW 723C86 hydrochloride	BRD-A17428743-003-03-3	-19.3	-23.9	-39.5	-47.7	-51.0	-39.0
117	MDL 72832 hydrochloride	BRD-A17453586-003-01-5	7.2	-8.7	-32.3	-18.8	13.5	16.3
118	BAMBUTEROL HYDROCHLORIDE	BRD-A17462676-003-06-6	-20.4	0.3	-5.4	-3.9	5.4	8.5
119	IBUPROFEN	BRD-A17655518-001-12-9	16.0	-6.5	-1.8	-10.2	6.1	10.4
120	a-Methyl-5-hydroxytryptamine maleate	BRD-A17745711-103-01-0	-25.8	-19.9	5.6	6.5	-37.3	-39.7
121	DIHYDROMUNDULETONE	BRD-A17831693-001-03-2	16.9	8.6	-11.5	6.9	-3.3	-17.5
122	TROLOX	BRD-A17846016-001-07-1	-41.4	-10.6	32.9	17.6	-30.1	-30.6
123	CPCCOEt	BRD-A18202423-001-01-6	-2.6	11.1	23.3	12.9	13.9	8.8
124	Etoposide	BRD-A18419789-001-01-4	9.9	0.6	-4.0	11.5	-12.4	-12.9
125	ESTRIOL	BRD-A18620900-001-04-5	-16.4	5.1	-22.5	-24.9	-1.1	-9.1
126	IDAZOXAN HYDROCHLORIDE	BRD-A18696154-003-14-3	-12.9	-29.3	-38.3	-45.6	-38.8	-41.6
127	DIHYDROROTENONE	BRD-A18788061-001-03-7	24.2	16.7	-8.2	3.9	-13.2	-10.9
128	7-Hydroxy-DPAT hydrobromide	BRD-A18795974-004-02-4	-0.2	22.3	20.7	30.8	12.4	3.2
129	ESTRADIOL	BRD-A18917088-001-03-1	17.4	-17.6	-16.6	-25.9	-20.1	-24.4
130	TRIMIPRAMINE MALEATE	BRD-A19195498-050-09-1	-58.3	-57.6	-103.7	-99.4	-82.3	-82.5
131	Vinpocetine	BRD-A19374631-001-01-0	-14.8	-9.4	-31.3	-27.9	-28.0	-21.0
132	METHYLPHENIDATE HYDROCHLORIDE	BRD-A19585813-003-01-7	11.1	-12.2	-9.3	6.1	4.9	13.6
133	MIANSERIN HYDROCHLORIDE	BRD-A19661776-003-16-9	-12.3	-9.6	-22.7	-11.5	-33.9	-26.7
134	Atovaquone	BRD-A19795905-001-05-6	-19.9	5.3	1.4	26.3	9.1	22.4
135	MEDRYSONE	BRD-A20126139-001-03-4	-1.0	-18.6	-33.0	-20.2	-12.2	-8.7

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
136	3-DEOXO-3beta-ACETOXYDEOXYDIHYDROGEDUNIN	BRD-A20182314-001-03-4	30.5	10.2	20.0	18.0	-1.8	0.2
137	ATENOLOL	BRD-A20239487-001-15-7	7.9	23.4	11.3	13.1	12.5	0.4
138	Danazol	BRD-A20243730-001-01-4	-63.6	-53.3	-84.3	-86.0	-37.8	-34.9
139	18alpha-GLYCYRRHETINIC ACID	BRD-A20256229-001-04-8	-21.5	-18.0	-73.8	-66.0	-29.2	-11.6
140	CHLORMEZANONE	BRD-A20348246-001-08-3	21.4	-0.1	-10.2	-22.3	-8.0	-4.6
141	DEOXYSAPPANONE B 7,3'-DIMETHYL ETHER ACETATE	BRD-A20368188-001-03-2	1.8	-4.2	12.1	43.8	-21.5	-19.0
142	IB-MECA	BRD-A20527803-001-01-2	-12.8	4.0	24.1	38.9	24.5	14.1
143	CANRENONE	BRD-A20644369-001-04-5	-12.7	-11.3	-25.0	-14.2	-21.0	-16.8
144	WAY 213613	BRD-A20968261-001-01-3	6.6	1.2	-27.7	-18.0	5.6	12.2
145	EPI(13)TORULOSOL	BRD-A21113731-001-03-3	-16.8	-0.1	-15.9	-8.4	-12.0	-23.0
146	MEROGEDUNIN	BRD-A21423998-001-03-4	3.5	-10.9	-4.7	-3.1	-6.9	-10.6
147	SNAP 5089	BRD-A21428877-003-01-9	-68.0	-85.9	-98.2	-106.5	-87.4	-90.2
148	Naltriben mesylate	BRD-A21723284-066-01-7	-7.5	-3.3	-20.4	0.0	-48.2	-52.3
149	AMLODIPINE BESYLATE	BRD-A22032524-074-04-0	-26.6	-27.2	-61.5	-67.3	-54.7	-57.5
150	SULMAZOLE	BRD-A22081593-001-06-1	-3.4	-10.2	5.2	12.0	14.1	19.1
151	PHENOTHRIN	BRD-A22106989-001-02-7	-18.5	-4.5	-7.7	25.1	25.8	36.8
152	PARAMETHADIONE	BRD-A22128695-001-01-8	-10.8	5.5	-3.9	-2.0	-5.3	7.2
153	ESTROPIPATE	BRD-A22143024-231-02-0	-5.2	-15.9	5.8	6.4	3.9	15.6
154	TERAZOSIN HYDROCHLORIDE	BRD-A22256192-003-14-4	-7.9	-8.4	103.5	129.1	0.9	2.1
155	DROFENINE HYDROCHLORIDE	BRD-A22267103-003-08-1	-9.8	-10.3	-41.0	-26.1	-37.5	-30.0
156	BENFLUOREX HYDROCHLORIDE	BRD-A22305049-003-08-6	-38.7	-33.0	-71.9	-61.0	-47.7	-52.3
157	PANTOPRAZOLE	BRD-A22380646-001-02-3	-3.1	-13.2	-0.4	15.5	3.3	-12.0
158	Procaterol hydrochloride	BRD-A22684332-003-03-1	7.1	3.4	20.6	18.2	16.3	12.4
159	SB 205384	BRD-A22707317-001-02-5	0.1	-5.2	-4.8	-3.2	2.5	6.6
160	BVT 948	BRD-A22713669-001-01-9	6.9	-6.6	19.0	25.1	-18.3	-26.8
161	Vinblastine sulfate	BRD-A22783572-065-01-3	4.6	7.4	20.2	24.1	11.8	9.0
162	TENOXICAM	BRD-A22844106-001-16-1	71.6	37.9	63.4	64.3	11.0	11.3
163	DIHYDROGEDUNIN	BRD-A22963354-001-03-6	-20.7	2.6	0.3	2.4	-27.4	-35.7
164	CLINDAMYCIN HYDROCHLORIDE	BRD-A23034328-003-06-7	-20.0	-23.1	-1.4	1.2	2.8	2.6
165	ITRACONAZOLE	BRD-A23067620-001-01-7	1.4	21.9	-11.8	2.9	-25.6	-25.3
166	PHENIRAMINE MALEATE	BRD-A23072235-050-09-4	-15.9	5.5	1.4	31.2	7.2	4.8
167	ESTRADIOL ACETATE	BRD-A23226398-001-04-3	-2.8	4.8	-13.1	-23.6	3.5	8.5
168	RIFAMPIN	BRD-A23603052-001-02-4	79.1	82.7	5.0	12.0	-51.2	-47.8
169	NAS-181	BRD-A23683907-334-01-0	32.8	23.7	34.7	18.5	11.6	17.2
170	Taxol	BRD-A23723433-001-01-2	4.5	-0.3	13.4	30.0	9.1	-0.5
171	THIAMYLAL SODIUM	BRD-A23970436-236-03-4	-20.4	-32.2	-10.9	-5.9	-8.8	-10.3
172	Saclofen	BRD-A24122750-001-02-9	-4.4	13.4	3.5	-2.7	6.8	5.3
173	OFLOXACIN	BRD-A24228527-001-19-0	3.5	-12.8	31.1	50.7	5.9	19.3
174	ANABASINE HYDROCHLORIDE	BRD-A24284985-003-03-8	27.0	16.5	8.9	32.6	3.4	10.9
175	HEAT hydrochloride	BRD-A24429032-003-01-6	-39.4	-40.4	-75.1	-79.4	-51.0	-52.9
176	PUERARIN	BRD-A24433358-001-04-2	-16.6	-6.7	-2.3	24.4	5.5	11.4
177		BRD-A24514565-236-01-6	7.7	7.8	27.8	31.3	4.6	18.4
178	ISOETHARINE MESYLATE	BRD-A24587114-066-14-2	7.0	12.7	43.6	58.2	12.8	21.8
179	HYDROCORTISONE VALERATE	BRD-A25143711-001-01-4	-15.9	-41.7	-60.1	-44.7	-40.7	-49.1
180	AMINOGLUTETHIMIDE	BRD-A25234499-001-09-2	-1.9	0.1	15.0	25.0	14.5	5.8
181	DEOXYGEDUNIN	BRD-A25243629-001-03-9	-5.9	-8.6	-27.6	-16.3	-30.9	-34.7

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	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
182	DEACETOXY-7-OXOGEDUNIN	BRD-A25408073-001-03-9	-0.9	15.4	-17.6	-7.9	0.8	-10.8
183	FENBUTYRAMIDE	BRD-A25537246-001-03-7	-8.7	-9.6	-0.9	0.1	1.4	4.9
184	EMETINE	BRD-A25687296-300-03-5	2.2	-23.0	-19.1	-7.8	-16.6	-12.1
185	ANISODAMINE HYDROBROMIDE	BRD-A25706161-001-03-9	-10.7	-11.4	-0.3	8.5	11.6	16.7
186	CGS 9343B	BRD-A26032986-050-01-3	11.9	-8.5	-2.5	-5.5	-6.9	-6.2
187	CLOBETASOL PROPIONATE	BRD-A26095496-001-03-2	29.1	1.8	3.2	-0.4	5.0	13.3
188	bulleyaconitine A	BRD-A26097136-001-01-8	-23.8	-0.8	5.5	27.2	14.7	20.9
189	PROPAFENONE HYDROCHLORIDE	BRD-A26334849-003-16-7	-21.1	-13.2	-48.5	-46.8	-15.4	-24.7
190	CHLORTHALIDONE	BRD-A26384407-001-15-2	14.4	-3.3	1.3	2.9	-2.8	14.8
191	ERGONOVINE MALEATE	BRD-A26387268-050-03-6	4.5	14.2	85.6	53.7	-15.4	-2.3
192	NICARDIPINE HYDROCHLORIDE	BRD-A26711594-003-06-4	20.4	14.2	11.5	-2.6	-10.6	-6.7
193	DESONIDE	BRD-A26858303-001-01-0	2.3	-22.8	-17.9	-0.8	-7.6	0.7
194	18-AMINOABIETA-8,11,13-TRIENE SULFATE	BRD-A27080191-065-03-6	2.9	-36.9	-96.4	-80.6	-47.6	-68.2
195	DPN	BRD-A27143604-001-01-2	7.3	0.6	-7.1	-5.7	7.0	8.4
196	ALTRENOGEST	BRD-A27554692-001-01-3	9.3	-3.9	-28.2	-25.4	-20.9	-23.2
197	PREDNISOLONE	BRD-A27887842-001-03-2	-11.8	-9.1	21.7	32.1	16.2	18.8
198	GRISEOFULVIC ACID	BRD-A27914728-001-03-3	6.5	-25.3	-36.2	6.2	13.6	8.3
199	2-Hydroxysaclofen	BRD-A27924917-001-01-7	-1.4	-3.6	1.6	19.5	6.4	-7.2
200	AMINOBENZTROPINE	BRD-A28095882-001-05-7	2.7	0.5	-1.0	0.7	-3.5	-1.0
201	AMT hydrochloride	BRD-A28318179-003-03-6	-10.6	0.5	13.1	11.5	14.7	21.8
202	L-689,560	BRD-A28422058-001-01-0	-1.5	-0.8	18.9	-9.5	23.7	21.5
203	SELEGILINE HYDROCHLORIDE	BRD-A28545468-003-10-9	4.3	6.5	9.6	-0.9	5.1	3.7
204	STRYCHNINE METHIODIDE	BRD-A28702443-005-01-0	3.9	42.7	-39.0	-0.1	4.3	6.7
205	PACLITAXEL	BRD-A28746609-001-05-7	7.9	-8.0	-13.3	-10.3	4.8	7.0
206	TETRAHYDROZOLINE HYDROCHLORIDE	BRD-A28856712-003-15-3	-10.0	8.4	1.9	12.1	13.5	15.5
207	PROXYPHYLLINE	BRD-A28887267-001-13-6	-18.2	-23.6	22.2	3.0	16.9	12.0
208	TRICHLORMETHIAZIDE	BRD-A28940325-001-15-8	-8.3	-9.2	-42.4	-6.6	3.0	-7.1
209	PUROMYCIN HYDROCHLORIDE	BRD-A28970875-300-03-1	25.5	16.4	27.5	24.6	3.8	9.1
210	ETHISTERONE	BRD-A29111201-001-03-0	6.6	-8.6	-36.4	-19.6	4.1	0.4
211	ACEBUTOLOL HYDROCHLORIDE	BRD-A29260609-003-15-3	22.4	45.9	-7.7	29.5	20.1	18.7
212	PCA 4248	BRD-A29289453-001-03-9	0.8	2.7	18.0	21.3	4.9	8.4
213	CANRENOIC ACID, POTASSIUM SALT	BRD-A29322418-237-03-2	0.3	-12.2	2.9	-0.6	14.3	19.3
214	DROPROPIZINE	BRD-A29349577-001-15-6	13.5	4.5	5.8	28.7	10.5	13.9
215	FISSINOLIDE	BRD-A29371732-001-03-8	-2.1	0.6	-10.6	-14.5	-0.5	-5.2
216	CARBINOXAMINE MALEATE	BRD-A29426959-050-07-4	-2.8	-0.4	-23.8	-27.7	-4.2	-2.1
217	RWJ 21757	BRD-A29437505-001-01-6	1.9	4.8	22.4	24.9	24.3	15.6
218	BICALUTAMIDE	BRD-A29485665-001-03-7	-27.1	8.9	-82.7	-76.2	-24.7	-33.1
219	STICTIC ACID	BRD-A29578214-001-08-4	68.1	59.9	-21.9	16.0	3.1	11.7
220	NOMIFENSINE MALEATE	BRD-A29644307-050-10-5	0.0	24.7	8.5	4.2	3.0	-0.5
221	DISOPYRAMIDE PHOSPHATE	BRD-A29734509-011-06-0	-17.9	19.6	11.9	25.4	11.3	12.9
222	LORGLUMIDE SODIUM	BRD-A29854054-236-07-6	2.9	23.2	2.4	12.6	-0.4	0.9
223	VANCOMYCIN HYDROCHLORIDE	BRD-A30133509-003-03-6	12.9	3.4	-9.1	30.0	34.7	23.8
224	MR 16728 hydrochloride	BRD-A30590053-003-01-1	3.2	9.4	-29.1	-42.3	-5.3	-8.8
225	LFM-A13	BRD-A30655177-001-06-6	-11.8	6.8	15.2	25.8	13.0	17.3
226	DIPERODON HYDROCHLORIDE	BRD-A30693873-003-06-0	-27.3	-26.9	-39.4	-37.8	-22.2	-19.1
227	TRIAMCINOLONE DIACETATE	BRD-A30717181-001-03-5	8.3	17.1	3.9	13.0	4.3	3.2

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	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
228	FLORFENICOL	BRD-A30886737-001-01-1	14.4	10.5	-16.7	-1.3	22.5	25.9
229	SDZ WAG 994	BRD-A31007383-001-01-0	-7.7	-2.3	3.3	0.9	-6.7	-6.7
230	DESACETYLCOLFORSIN	BRD-A31087826-001-01-7	14.0	30.8	7.7	8.4	6.0	6.5
231	FLUOXETINE	BRD-A31159102-003-16-3	-39.0	-19.3	-80.0	-88.4	-57.1	-58.0
232	TCB2	BRD-A31195449-004-01-9	-11.8	-5.6	-13.2	-21.4	5.4	-3.6
233	CGP 20712 dihydrochloride	BRD-A31575449-300-01-4	-14.2	-3.6	-5.1	1.4	-5.8	-1.9
234	3-AMINO-beta-PINENE	BRD-A31576716-003-03-4	-6.9	6.6	-3.1	6.3	23.5	9.7
235	PROCYCLIDINE HYDROCHLORIDE	BRD-A31800922-003-15-2	-17.7	-31.0	-24.4	9.2	7.5	-4.1
236	formestane	BRD-A31801025-001-01-0	8.9	-7.1	41.8	36.4	-8.3	-8.8
237	3-DEACETYLKHIVORIN	BRD-A31863775-001-03-8	11.6	-19.5	-0.2	1.0	2.1	-7.0
238	(S)-Timolol maleate	BRD-A31916785-103-01-0	-6.1	1.1	-9.5	-2.3	3.6	8.9
239	OLEANOIC ACID	BRD-A31962514-001-03-4	6.4	10.4	-9.3	-16.9	-17.5	-17.8
240	Methyllycaconitine citrate	BRD-A32164164-048-01-4	-0.3	10.0	7.8	-3.8	17.5	19.9
241	11alpha-HYDROXYPROGESTERONE HEMISUCCINATE	BRD-A32440707-001-01-1	-27.1	-11.6	10.3	26.7	3.3	8.5
242	TRANDOLAPRIL	BRD-A32505112-001-03-6	12.7	8.6	6.3	0.6	2.0	1.1
243	ACECLIDINE	BRD-A32673558-001-01-7	-13.8	-10.0	9.5	5.0	-9.6	3.0
244	SALINOMYCIN, SODIUM	BRD-A32757659-236-03-4	2.9	-7.1	-40.8	-20.6	-25.9	-20.3
245	MRS 1845	BRD-A32949107-001-01-7	18.9	3.0	11.0	18.6	-15.0	-19.6
246	TIOCONAZOLE	BRD-A33084557-001-01-7	-58.3	-57.5	-94.3	-88.9	-83.4	-84.1
247	DEHYDRODIHYDROROTENONE	BRD-A33119430-001-03-0	8.5	32.9	-18.2	8.8	9.1	8.4
248	Sotalol hydrochloride	BRD-A33168282-003-06-5	-7.6	-4.1	6.4	20.2	9.1	6.9
249	OXFENDAZOLE	BRD-A33447119-001-03-3	-20.4	6.0	24.2	41.1	8.3	11.5
250	LOE 908 hydrochloride	BRD-A33676200-003-01-7	23.2	34.5	23.2	40.4	7.9	1.2
251	GITOXIN	BRD-A33810106-001-03-7	23.1	17.9	13.9	26.8	35.5	32.5
252	SUPROFEN	BRD-A34006693-001-07-1	-26.4	25.6	-52.8	10.2	29.2	24.0
253	SULOCTIDIL	BRD-A34205397-001-03-7	-91.6	-90.7	-94.9	-94.1	-98.9	-101.8
254	ZOPICLONE	BRD-A34309505-001-10-1	6.2	35.7	24.9	15.5	11.7	12.8
255	4'-DEMETHYLEPIPODOPHYLLOTOXIN	BRD-A34380114-001-03-0	24.5	21.8	8.2	9.3	-17.6	-1.8
256	URSOLIC ACID	BRD-A34492468-001-04-3	2.7	-7.5	0.4	22.5	7.4	20.7
257	CGP 12177 hydrochloride	BRD-A34706053-003-01-9	-9.1	-11.1	4.6	-5.1	9.9	9.7
258	HOMOSALATE	BRD-A34751532-001-04-4	-26.1	-25.0	32.5	30.2	42.1	32.3
259	ANABASAMINE HYDROCHLORIDE	BRD-A34774643-003-06-3	-10.8	17.0	29.6	8.5	-4.1	18.1
260	DEACETOXY(7)-7-OXOKHIVORINIC ACID	BRD-A34842997-001-03-1	-14.1	-3.7	-44.6	4.7	1.9	4.4
261	1,3-DIDEACETYL-7-DEACETOXY-7-OXOKHIVORIN	BRD-A34891365-001-03-2	-25.2	-18.1	2.8	-25.1	-15.2	-15.5
262	rutin	BRD-A34907681-001-01-7	0.2	-15.6	15.5	4.8	-15.5	-17.8
263	PREGNENOLONE	BRD-A35054627-001-05-5	-9.8	-9.7	-0.9	-5.0	-4.6	0.2
264	NECA	BRD-A35338386-001-04-6	6.9	-1.1	5.3	-2.0	19.9	18.0
265	L-803,087 trifluoroacetate	BRD-A35511923-019-01-6	-25.4	-27.7	11.2	18.2	-36.3	-56.8
266	CGP 37157	BRD-A35623999-001-04-0	-16.2	-14.7	-38.3	-45.1	-22.8	-18.6
267	2-[[4-(2-Methoxyphenyl)piperazin-1-yl]methyl]-6-methyl-2,3 dihydroimidazo[1,2c]quinazolin-5(6H)-one	BRD-A35871558-001-01-4	-4.4	1.6	-12.6	15.0	3.0	-3.0
268	PREGNENOLONE SUCCINATE	BRD-A35912562-001-01-0	-0.9	-2.9	-35.7	-52.3	-27.4	-32.1
269	APOMORPHINE HYDROCHLORIDE	BRD-A35931254-003-03-5	31.5	33.3	-60.9	-25.3	-51.4	-55.3
270	MEGESTROL ACETATE	BRD-A35989968-001-03-4	-10.2	18.0	-21.2	-16.9	-12.3	-8.0
271	AMCINONIDE	BRD-A36010170-001-03-2	7.6	2.9	-2.1	-4.2	11.9	1.0
272	ESTRADIOL BENZOATE	BRD-A36066264-001-03-1	-41.6	-8.0	-68.1	-65.5	-41.0	-42.6
273	Remacemide hydrochloride	BRD-A36074203-003-03-5	-14.3	-9.0	-42.2	-54.1	-19.3	-4.5

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
274	SULFINPYRAZONE	BRD-A36217750-001-09-8	-34.3	-12.6	-12.2	0.0	4.9	3.1
275	NYLIDRIN HYDROCHLORIDE	BRD-A36267905-003-12-7	17.8	6.9	5.6	8.2	-10.2	-14.1
276	CEFUROXIME AXETIL	BRD-A36322567-001-01-6	8.6	4.0	-14.1	20.9	9.4	24.8
277	BIOTIN	BRD-A36603537-001-07-3	-10.2	5.0	13.8	-6.0	3.6	2.5
278	GLYCOCHOLIC ACID	BRD-A36636859-001-01-6	14.2	-14.5	-27.2	-24.9	15.1	13.0
279	GAMBOGIC ACID	BRD-A37011749-001-03-1	-85.4	-84.1	-101.2	-96.4	-87.2	-88.4
280	BRL 52537 hydrochloride	BRD-A37347161-003-01-8	21.0	22.8	18.1	27.0	-21.3	-17.0
281	TULOBUTEROL	BRD-A37441042-003-03-0	13.1	-9.2	24.4	22.7	17.8	13.2
282	Naloxone hydrochloride	BRD-A37541666-003-01-6	3.9	-4.0	2.2	1.4	-8.1	-2.7
283	SB 203580 hydrochloride	BRD-A37704979-003-01-2	-9.9	-20.4	-6.8	-8.7	5.7	-3.1
284	ICI 204,448 hydrochloride	BRD-A37776212-003-02-5	25.4	4.1	28.6	39.9	14.5	18.2
285	TRIAMCINOLONE	BRD-A37780065-001-03-7	12.9	-2.6	28.8	38.0	15.5	16.3
286	ANTHOTHECOL	BRD-A37828317-001-03-0	-23.7	-6.4	-46.3	-62.1	-33.3	-31.1
287	ESTRONE	BRD-A37959677-001-03-7	24.6	10.5	-8.3	-3.7	-12.4	1.0
288	KETOCONAZOLE	BRD-A38350138-001-03-1	-48.8	-24.2	-80.4	-81.2	-63.6	-70.2
289	CYCLOTHIAZIDE	BRD-A38675539-001-05-1	-7.0	2.4	-23.7	11.2	23.2	19.9
290	KU14R	BRD-A38747044-001-01-5	13.9	-5.8	5.9	19.3	30.8	24.2
291	FLUDROCORTISONE ACETATE	BRD-A38749782-001-03-3	0.1	-15.1	-1.8	-9.8	4.2	1.0
292	GW 311616 hydrochloride	BRD-A38898897-003-01-0	-2.2	-4.2	2.6	-1.3	8.6	22.7
293	METHOXAMINE HYDROCHLORIDE	BRD-A39189014-003-14-4	2.0	-9.8	10.3	-7.7	9.1	5.4
294	RABEPRAZOLE SODIUM	BRD-A39390670-236-04-0	295.6	314.3	76.7	89.4	32.0	30.0
295	NORETHINDRONE	BRD-A39415247-001-06-2	24.7	11.3	-1.7	15.9	2.1	-10.2
296	OMDM-2	BRD-A39522003-001-01-0	20.0	2.0	7.8	11.5	36.2	20.9
297	DEOXYKHIVORIN	BRD-A39660642-001-03-1	5.2	-3.3	-15.2	-13.8	-6.4	-8.9
298	ESTRADIOL VALERATE	BRD-A39747742-001-03-5	-47.6	0.1	-39.3	-51.7	0.2	10.7
299	HYDROXYPROGESTERONE	BRD-A39791822-001-04-4	4.2	3.9	-22.3	-13.4	-6.9	-12.2
300	Eplerenone	BRD-A39969961-001-01-3	-2.1	-5.5	-4.3	-10.2	2.3	6.4
301	GITOXIGENIN DIACETATE	BRD-A40022950-001-03-7	-14.2	-24.9	-41.0	-13.2	9.9	6.3
302	DICHLORISONE ACETATE	BRD-A40195998-001-01-9	-11.5	-16.9	-35.0	19.3	15.4	17.0
303	CARAPIN	BRD-A40253167-001-03-7	14.4	-0.7	-36.7	-18.0	4.2	-10.8
304	7-DESACETOXY-6,7-DEHYDROGEDUNIN	BRD-A40431293-001-01-0	-19.7	-22.4	-32.7	-20.4	-23.9	-20.8
305	KETOROLAC TROMETHAMINE	BRD-A40639672-234-09-9	13.9	11.0	24.0	17.5	18.5	16.4
306	GEMIFLOXACIN MESYLATE	BRD-A40787240-066-03-8	22.6	4.1	22.9	11.4	26.2	23.8
307	PK 11195	BRD-A41451487-001-04-7	-23.0	4.8	-63.1	-52.4	-33.1	-26.6
308	Naloxone benzoylhydrazone	BRD-A41833852-001-01-9	12.6	-13.6	9.7	11.4	8.9	0.8
309	ENTANDROPHRAGMIN	BRD-A41916216-001-03-9	17.5	28.8	-3.3	9.2	12.6	-0.2
310	BRUCINE	BRD-A41995253-001-03-7	5.3	-3.2	-2.5	-9.2	2.3	-0.5
311	L-152,804	BRD-A42553870-001-05-1	38.5	42.9	26.0	18.3	4.4	4.4
312	CETIRIZINE HYDROCHLORIDE	BRD-A42571354-300-07-0	20.7	17.1	21.8	13.8	2.3	4.5
313	IOPANIC ACID	BRD-A42628519-001-07-4	-11.2	2.5	-43.6	-49.9	-15.8	-18.3
314	API-2	BRD-A42649439-001-02-8	-11.6	-7.4	11.9	7.4	-8.9	-5.1
315	MELENGESTROL ACETATE	BRD-A42746051-001-01-1	-21.1	-9.4	-26.9	-38.5	-36.3	-31.9
316	ORNIDAZOLE	BRD-A42759514-001-09-8	13.1	6.9	12.7	3.8	9.9	2.2
317	DEHYDROABIETAMIDE	BRD-A42929532-001-03-8	21.8	-10.1	-65.5	-57.9	-12.2	-33.9
318	Cantharidin	BRD-A43076080-001-03-3	-6.2	-6.1	29.7	23.6	2.7	-3.4
319	PINACIDIL	BRD-A43882281-001-11-4	10.3	3.9	-2.6	-0.2	-0.2	9.7

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
320	L 368899 hydrochloride	BRD-A43930669-003-01-0	9.1	2.4	3.4	-9.0	8.4	12.7
321	TETRAHYDROPALMATINE	BRD-A43940795-001-03-6	-5.8	-2.3	11.9	5.7	-1.4	-2.1
322	Reboxetine mesylate	BRD-A43974499-066-01-1	-2.0	-8.6	-32.8	-45.1	-27.3	-20.3
323	TRANYLCYPROMINE SULFATE	BRD-A43974575-065-04-4	-4.1	-2.5	23.1	34.1	4.9	14.9
324	HOMATROPINE METHYLBROMIDE	BRD-A43999749-004-03-3	-19.4	-6.1	12.5	1.7	10.7	6.8
325	DOXYLAMINE SUCCINATE	BRD-A44008656-036-15-9	-16.5	-14.1	15.4	11.0	-0.7	5.6
326	INDOPROFEN	BRD-A44090213-001-15-7	-4.5	-16.4	-1.4	6.0	10.8	3.6
327	Dihydroergocristine mesylate	BRD-A44701612-066-01-9	9.6	13.4	-3.1	-30.9	-16.8	-23.8
328	Mifepristone	BRD-A44780397-001-01-1	-25.6	-32.3	-5.9	-4.3	-26.6	-17.7
329	PROGLUMIDE	BRD-A44863528-001-08-2	23.1	4.9	4.1	18.2	28.4	11.3
330	BOLDINE	BRD-A44966919-001-09-8	9.3	20.7	-15.1	42.9	-13.8	-15.4
331	METHYLPREDNISOLONE SODIUM SUCCINATE	BRD-A45044890-236-01-5	9.6	-3.1	18.5	-6.2	6.2	9.8
332	UBP 302	BRD-A45499626-001-02-8	-7.7	5.0	0.7	0.7	4.3	9.2
333	QUINACRINE HYDROCHLORIDE	BRD-A45889380-300-04-8	10.4	4.2	-43.0	-39.7	-27.6	-13.5
334	CLIDINIUM BROMIDE	BRD-A46066006-004-15-0	11.3	20.8	8.8	21.6	31.9	25.2
335	HYDROCORTISONE PHOSPHATE TRIETHYLAMINE	BRD-A46186775-369-01-2	-14.9	-21.1	1.3	14.6	-0.2	6.7
336	TETRAMIZOLE HYDROCHLORIDE	BRD-A46393198-003-10-9	9.5	10.1	13.7	9.8	5.1	5.8
337	DEOXYSAPPANONE B 7,4'-DIMETHYL ETHER	BRD-A46460777-001-03-4	29.3	8.6	10.1	-7.6	-68.3	-67.7
338	PROSCILLARIDIN	BRD-A46600320-001-01-1	-0.8	9.6	14.9	11.7	-0.8	7.3
339	Colchicine	BRD-A46684810-001-04-6	2.5	10.9	10.6	9.3	0.8	5.9
340	Ouabain	BRD-A46747628-001-01-9	-14.5	-6.2	8.9	31.1	21.1	13.6
341	CRUSTECDYSONE	BRD-A46778020-001-03-4	15.4	9.6	-50.0	21.1	12.4	13.4
342	LEVOBUNOLOL HYDROCHLORIDE	BRD-A46876182-003-01-0	12.0	21.4	-9.2	5.1	4.1	13.9
343	Citalopram hydrobromide	BRD-A47598013-004-06-1	-4.0	4.6	-16.5	-23.9	-14.4	-22.3
344	NPC 15199	BRD-A47633927-001-01-8	-17.1	-11.7	12.2	4.1	11.4	14.3
345	8-Hydroxy-DPAT hydrobromide	BRD-A48015106-004-03-0	4.4	26.6	24.8	46.8	4.7	14.1
346	TRIHEXYPHENIDYL HYDROCHLORIDE	BRD-A48180038-003-15-1	-1.3	1.5	-17.8	29.8	16.1	-2.3
347	MITOMYCIN C	BRD-A48237631-001-03-0	26.3	16.1	-1.7	4.5	10.9	19.8
348	PHCCC	BRD-A48257147-001-01-9	-17.6	15.8	-43.0	-49.3	-4.9	-2.8
349	AJMALINE	BRD-A48300215-001-03-0	3.6	7.5	30.5	34.5	7.0	2.2
350	SALSOLINE	BRD-A48323445-001-03-4	14.3	8.1	20.8	-4.5	-29.8	-31.9
351	GEDUNIN	BRD-A48397526-001-03-0	-11.5	-11.8	-62.2	-15.2	-17.7	-23.7
352	PIOGLITAZONE HYDROCHLORIDE	BRD-A48430263-003-06-5	-5.3	-7.0	-22.3	-14.4	7.8	8.0
353	IVERMECTIN	BRD-A48570745-001-01-1	-2.0	6.3	-25.7	-29.1	-29.1	-27.7
354	TESTOSTERONE PROPIONATE	BRD-A48720949-001-03-2	-9.6	6.1	5.1	16.2	-15.4	-8.8
355	METHACYCLINE HYDROCHLORIDE	BRD-A49035384-003-12-3	82.4	67.9	32.2	12.4	-12.2	-4.0
356	SKF 89976A hydrochloride	BRD-A49046702-003-03-4	-9.4	-3.2	-7.3	2.2	-8.0	0.4
357	Galanthamine hydrobromide	BRD-A49148672-004-01-6	-11.5	-3.1	21.0	4.8	2.3	3.2
358	DONEPEZIL HYDROCHLORIDE	BRD-A49160188-003-04-4	2.6	-6.5	19.7	-5.0	17.1	20.7
359	Lansoprazole	BRD-A49172652-001-13-1	-7.2	-1.5	-12.1	-3.9	6.2	11.2
360	TRIMEPRAZINE TARTRATE	BRD-A49225603-045-05-0	-64.4	-48.1	-67.0	-67.4	-82.4	-87.3
361	KHAYANTHONE	BRD-A49243397-001-03-1	13.2	7.6	-39.9	-14.0	-12.1	-15.6
362	Ro 60-0175	BRD-A49370193-051-01-7	-43.3	-39.5	-62.3	-70.3	-51.3	-47.8
363	DESOXYMETASONE	BRD-A49447682-001-01-6	-10.8	-13.0	-13.8	-15.7	4.5	9.4
364	(?)-AC 7954 hydrochloride	BRD-A49544621-003-01-0	-7.7	6.0	-25.7	-52.5	-22.0	-22.7
365	FLURANDRENOLIDE	BRD-A49765801-001-03-3	-11.2	-14.8	2.5	0.4	2.6	8.0

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
366	clindamycin	BRD-A49912425-001-01-1	42.1	-2.9	5.3	24.1	13.1	15.1
367	FLUMETHAZONE PIVALATE	BRD-A50064262-001-03-9	0.6	0.3	23.8	19.5	-2.1	5.8
368	TERBUTALINE HEMISULFATE	BRD-A50157456-065-12-3	0.4	4.0	-45.5	9.4	-9.3	-8.9
369	MECLIZINE HYDROCHLORIDE	BRD-A50311610-300-06-2	17.7	8.8	4.1	67.9	8.0	63.1
370	FIPRONIL	BRD-A50675702-001-04-8	-11.2	-24.9	-29.0	-24.9	-32.8	-23.8
371	Fenoldopam hydrochloride	BRD-A50684349-003-01-1	2.9	3.6	4.9	5.8	-14.0	-16.9
372	MDL 73005EF hydrochloride	BRD-A50764878-003-01-0	13.0	-17.2	5.6	0.8	-3.6	3.2
373	NORGESTREL	BRD-A50928468-001-03-7	-15.6	-6.5	-34.2	-28.3	-22.0	-16.6
374	8-Hydroxy-PIPAT oxalate	BRD-A51381734-034-01-1	-5.4	4.7	-19.4	0.2	-23.1	-19.2
375	Noscapine hydrochloride	BRD-A51393488-003-01-9	-14.2	-12.5	-3.4	-21.0	6.3	14.0
376	Yohimbine hydrochloride	BRD-A51410489-003-02-8	0.7	0.6	-23.1	-3.8	-7.4	-7.2
377	3 a-[(4-Chlorophenyl)phenylmethoxy]tropane hydrochloride	BRD-A51713165-003-01-8	-15.9	-20.7	-87.0	-92.8	-39.1	-48.1
378	Venlafaxine HCl	BRD-A51714012-003-01-1	11.3	16.9	13.3	30.0	6.0	0.4
379	ECONAZOLE NITRATE	BRD-A51820102-008-16-4	-41.5	-53.8	-58.6	-68.7	-62.1	-63.1
380	BRL 15572 hydrochloride	BRD-A51829654-003-02-8	-6.2	-4.4	4.2	16.6	28.7	30.4
381	ICI-185,282	BRD-A51929314-001-01-4	14.1	9.0	-26.0	-23.3	-8.6	-9.1
382		BRD-A52530684-003-01-7	-3.5	1.9	27.3	25.5	-5.4	-3.9
383	SKF 83566 hydrobromide	BRD-A52588987-004-04-1	-5.8	11.0	-16.4	-9.4	-12.3	-16.9
384	Tetrindole mesylate	BRD-A52660433-066-01-3	-90.3	-92.9	25.8	40.1	-64.2	-68.3
385	CHRYSANTHEMIC ACID	BRD-A52893269-001-03-2	1.8	-17.1	6.3	-16.9	8.5	14.9
386	Tianeptine	BRD-A53077924-236-01-4	20.3	-16.1	34.9	40.3	22.1	3.4
387	EPITESTOSTERONE	BRD-A53131506-001-01-3	-0.6	3.3	-3.8	-20.6	0.4	5.7
388	METHYLPREDNISOLONE	BRD-A53176877-001-03-5	10.2	45.7	17.3	14.8	-10.9	-11.6
389	AMIPRILOSE	BRD-A53484347-003-03-1	4.9	-6.7	6.4	5.1	2.1	12.3
390	PIPENZOLATE BROMIDE	BRD-A53561827-004-15-7	12.7	14.3	-7.1	28.1	-1.2	3.6
391	ORPHENADRINE CITRATE	BRD-A53576514-048-06-9	5.0	-16.7	-25.1	-5.3	-4.9	3.7
392	PRILOCAINE HYDROCHLORIDE	BRD-A53952395-003-15-2	-9.0	-8.4	-20.1	1.4	3.1	20.6
393	RACEPHEDRINE HYDROCHLORIDE	BRD-A54236247-003-03-5	-5.2	-6.7	10.6	22.3	10.8	5.7
394	CORTISONE ACETATE	BRD-A54487287-001-03-9	-14.1	-2.0	26.8	30.4	24.1	15.1
395	Pirlindole mesylate	BRD-A54490543-066-04-4	-53.9	-44.2	-48.8	-62.2	-50.2	-51.8
396	SOLIFENACIN SUCCINATE	BRD-A54596827-036-01-4	-37.8	4.2	-18.5	-23.2	-17.6	-21.3
397	Dihydroergotamine mesylate	BRD-A54845972-066-01-5	-1.9	-8.3	-11.3	-7.1	-8.6	-13.1
398	ETOMIDATE	BRD-A54880345-001-11-8	-11.3	-6.9	-11.1	2.9	-2.4	4.6
399	(RS)-(?)-Sulpiride	BRD-A55272860-001-08-8	-6.5	12.6	5.5	8.0	20.0	7.0
400	STROPHANTHIDIN	BRD-A55312468-001-03-9	-21.2	-3.5	-32.1	19.6	29.1	5.6
401	CGP 54626 hydrochloride	BRD-A55369275-003-01-2	-8.1	-7.6	7.8	0.1	22.2	19.4
402	TESTOSTERONE	BRD-A55393291-001-05-7	-18.3	0.8	-18.5	11.0	0.3	11.5
403	COLFORSIN	BRD-A55416093-001-03-1	3.8	4.4	4.6	-13.1	9.2	9.0
404	Methotrexate	BRD-A55424491-001-08-2	-22.3	4.5	23.6	25.0	13.2	10.8
405	BNTX maleate	BRD-A55484088-050-01-7	-23.6	-27.8	28.6	33.9	-35.6	-42.2
406	CYTISINE	BRD-A55579717-001-03-2	11.1	-1.5	-27.2	-11.5	3.8	2.1
407	H-7 dihydrochloride	BRD-A55756846-300-01-0	-22.3	-10.8	20.6	-27.2	7.6	-1.8
408	PRIMAQUINE DIPHOSPHATE	BRD-A55913614-316-06-2	-12.6	7.6	-36.9	-48.9	-29.5	-24.1
409	OMEPRAZOLE	BRD-A55962179-001-08-0	-20.7	35.2	-0.4	2.6	-12.2	-1.6
410	ZILEUTON	BRD-A56359832-001-04-6	-2.0	5.6	14.8	9.3	-12.4	-13.3
411	ALTHIAZIDE	BRD-A56675431-001-07-3	5.8	18.0	20.4	26.3	9.3	21.6

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
412	11a-ACETOXYPROGESTERONE	BRD-A56884981-001-02-6	4.6	11.8	-5.6	-2.2	13.7	26.7
413	SQ 22536	BRD-A56987319-001-05-3	0.4	-9.5	-2.0	-3.7	10.9	23.5
414	PERUVOSIDE	BRD-A57089740-001-03-1	1.9	12.9	1.2	-10.6	12.9	5.7
415	CHLORCYCLIZINE HYDROCHLORIDE	BRD-A57133233-003-06-0	10.9	2.5	-66.7	-49.1	-20.1	-19.9
416	PIROXICAM	BRD-A57382968-001-18-3	41.2	64.2	27.6	25.2	-7.1	4.7
417	(-)-Bicuculline methiodide	BRD-A57798559-005-01-2	-17.9	-3.3	-15.8	-3.5	15.2	10.2
418	NIMODIPINE	BRD-A58048407-001-09-7	-12.5	-8.1	-10.1	-20.2	-8.9	-4.5
419	OXYPHENCYCLIMINE HYDROCHLORIDE	BRD-A58193911-003-12-0	-9.6	-23.6	-28.5	16.2	1.2	0.1
420	SELAMECTIN	BRD-A58564983-001-03-8	-5.0	4.4	13.6	19.6	22.5	22.3
421	N-ACETYLPROLINE	BRD-A58587171-001-04-9	-19.4	-5.7	2.0	17.5	-0.4	1.1
422	RITODRINE HYDROCHLORIDE	BRD-A59174698-003-12-8	1.9	10.2	16.4	6.2	4.0	-6.4
423	7-Hydroxy-PIPAT maleate	BRD-A59391763-103-01-9	-10.7	-11.3	5.5	21.8	4.1	8.9
424	DEXPANTHENOL	BRD-A59413292-001-04-1	-10.7	-1.3	2.8	10.0	12.7	12.5
425	12a-HYDROXY-5-DEOXYDEHYDROMUNDUSERONE	BRD-A59471422-001-02-6	-8.0	-4.4	-13.1	-16.7	6.7	-11.5
426	7-DEACETYLKHIVORIN	BRD-A59539786-001-03-8	10.5	16.3	16.8	4.1	0.5	-6.8
427	AMYGDALIN	BRD-A59552297-001-03-3	-0.8	1.2	34.9	18.8	9.8	11.8
428	3-NOR-3-OXOPANASINSAN-6-OL	BRD-A59682351-001-03-1	23.4	-1.1	-22.6	8.3	5.6	7.9
429	Fluticasone propionate	BRD-A59943784-001-01-8	-23.8	-13.3	-9.5	-1.6	12.5	-2.1
430	Amisulpride	BRD-A60197193-001-05-4	8.3	-14.3	15.0	4.0	8.6	7.3
431	BUDESONIDE	BRD-A60571864-001-03-3	-1.7	2.4	-11.1	-19.2	-8.3	-10.7
432	CAFESTOL	BRD-A60717068-001-01-0	-22.2	-21.1	-42.0	-30.7	-24.8	-25.0
433	2'-MeCCPA	BRD-A60877539-001-01-3	-2.5	8.2	30.7	15.0	36.1	30.2
434	GLICLAZIDE	BRD-A61154809-001-08-4	-14.8	-48.2	18.6	-5.2	7.0	14.3
435	Eliprodil	BRD-A61392169-001-01-9	25.1	13.1	-18.3	-11.8	-6.5	-14.1
436	METOLAZONE	BRD-A61793559-001-08-1	-3.3	2.3	-4.5	7.3	6.0	11.4
437	WAY 161503 hydrochloride	BRD-A62021152-003-01-8	-3.9	-3.9	-6.6	11.1	1.4	-8.8
438	MDL 11,939	BRD-A62057054-001-01-5	-16.6	-8.9	6.3	-12.6	20.1	17.2
439	TOTAROL	BRD-A62129005-001-03-8	17.3	4.4	85.4	-14.0	-25.3	-20.6
440	Cycloheximide	BRD-A62184259-001-02-8	-0.1	4.5	-2.1	-17.0	11.7	13.3
441	ZM 226600	BRD-A62209527-001-03-7	-33.2	-21.6	-8.5	0.8	-9.7	-8.5
442	EDOXUDINE	BRD-A62505706-001-03-1	-1.5	17.3	6.9	-4.9	-0.5	-2.5
443	PREDNISONE	BRD-A62525898-001-04-5	8.0	3.6	18.3	-2.9	10.7	12.7
444	CORTISONE	BRD-A62731508-001-04-1	16.0	-1.3	3.6	25.7	23.6	18.0
445	RIFAXIMIN	BRD-A62879835-001-03-4	37.0	39.6	-26.4	8.2	-46.8	-47.2
446	Cabergoline	BRD-A63043573-001-01-6	-10.4	-12.0	11.5	7.7	18.7	22.9
447	Rimcazole dihydrochloride	BRD-A63346720-300-01-1	-36.3	-35.9	-91.9	-95.0	-81.1	-84.4
448	EPIESTRIOL	BRD-A63433173-001-01-3	-4.5	13.6	-42.4	1.0	9.9	15.2
449	Ro 04-5595	BRD-A63546914-003-01-2	-17.9	-18.8	-54.4	-63.4	-43.8	-48.4
450	Methylergometrine maleate	BRD-A63667919-103-01-9	34.3	33.9	68.2	82.3	4.5	3.9
451	PD 123319 ditrifluoroacetate	BRD-A63836183-362-01-1	-25.3	-18.8	11.0	-1.0	21.0	21.7
452	N-BENZYLTROPAN-4-OL	BRD-A64068566-001-01-1	-2.7	33.4	-12.7	6.7	16.7	3.7
453	MEXILETINE HYDROCHLORIDE	BRD-A64092382-003-09-2	-33.9	-1.7	0.5	15.3	16.4	7.2
454	SODIUM DEHYDROCHOLATE	BRD-A64125466-236-03-8	-12.0	-4.6	10.1	-9.2	8.5	21.3
455	SKF 77434 hydrobromide	BRD-A64227845-004-02-8	9.5	11.2	-19.7	-25.7	-25.1	-29.7
456	(-)-Terreic acid	BRD-A64228451-001-04-3	95.0	79.6	10.6	18.5	-5.3	-3.1
457	LANATOSIDE C	BRD-A64242993-001-03-1	29.5	30.8	21.8	11.1	33.6	30.9

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
458	JOSAMYCIN	BRD-A64243931-001-01-8	-2.4	9.4	18.1	-4.4	3.6	21.9
459	Cyclosporin A	BRD-A64290322-001-01-6	-18.6	-10.0	-27.3	-15.4	-16.1	-22.5
460	MEXICANOLIDE	BRD-A64523751-001-03-6	3.6	2.6	20.7	-1.9	2.5	3.5
461	CV 1808	BRD-A64933752-001-01-0	-8.9	-5.9	25.9	38.9	18.7	26.5
462	Mirtazepine	BRD-A64977602-001-04-3	0.2	-4.1	10.6	4.2	16.7	8.0
463	OXYBUTYNIN CHLORIDE	BRD-A65013509-003-13-7	-15.0	-8.3	0.0	-27.6	-17.7	-5.3
464	DIHYDROERGOCRISTINE	BRD-A65076780-001-02-1	13.2	-10.6	32.8	13.9	-31.9	-28.2
465	ATPA	BRD-A65145453-001-02-0	-14.1	-10.8	11.3	18.4	17.5	27.1
466	LOBELINE HYDROCHLORIDE	BRD-A65243462-003-03-6	-11.0	-4.3	-8.4	9.1	10.1	4.2
467	Cimaterol	BRD-A65440446-001-03-3	-15.0	-10.8	0.8	15.9	5.3	22.4
468	FLUNISOLIDE	BRD-A65449987-001-06-2	-18.3	-13.9	-3.4	9.8	1.0	1.2
469	ginsenoside-Rc	BRD-A65550283-001-01-9	3.8	-2.3	12.0	4.8	7.5	9.5
470	RX 821002 hydrochloride	BRD-A65597028-003-02-4	-6.3	-7.5	-5.3	-5.9	-5.6	2.5
471	Zacopride hydrochloride	BRD-A65615053-003-01-4	-10.2	-1.3	10.9	22.7	13.7	16.3
472	CANDESARTAN CILEXTIL	BRD-A65671304-001-03-4	-63.7	-70.0	16.3	2.1	-78.1	-78.8
473	HYDROCORTISONE ACETATE	BRD-A65767837-001-03-6	-5.6	-0.5	-11.7	-2.2	5.1	-3.8
474	(S)-WAY 100135 dihydrochloride	BRD-A66369147-300-01-5	11.1	-20.0	12.1	13.7	11.8	15.1
475	HTMT dimaleate	BRD-A66435872-313-01-8	-15.4	-20.6	-19.6	5.0	-5.8	2.4
476	ACETYLPHENYLALANINE	BRD-A66443329-001-05-3	9.3	45.5	-6.2	5.9	-1.8	-8.5
477	OXACILLIN SODIUM	BRD-A66481418-236-03-2	15.7	0.6	13.1	22.0	12.1	23.6
478	DIGOXIGENIN	BRD-A66491790-001-01-1	12.3	14.1	11.7	-12.3	20.6	12.6
479	NALTREXONE HYDROCHLORIDE	BRD-A66559694-001-03-8	17.5	10.3	-15.2	-2.6	-14.0	-13.1
480	Medetomidine hydrochloride	BRD-A66563878-003-01-8	-8.0	-7.4	-9.6	-7.9	-1.7	-6.6
481	BETAMETHASONE 17,21-DIPROPIONATE	BRD-A66861218-001-03-5	-38.9	-12.9	4.3	13.6	-9.0	6.5
482	DIFLORASONE DIACETATE	BRD-A66869276-001-01-1	-23.3	-28.5	15.0	-14.9	-3.4	-7.8
483	NORCANTHARIDIN	BRD-A66914119-001-04-0	11.6	-0.4	-2.8	-13.5	12.1	13.7
484	Nemonapride	BRD-A66927094-001-01-7	-14.0	-5.1	-19.2	-25.2	-8.3	6.3
485	7-OXOCHOLESTEROL	BRD-A67138712-001-03-8	-24.2	-14.7	0.8	21.3	0.3	9.7
486	O-BENZYL-l-SERINE	BRD-A67259561-001-02-6	-8.6	20.7	-11.1	18.7	11.7	-3.8
487	NCS-382	BRD-A67433117-001-01-8	-10.5	-4.2	-2.8	2.6	4.2	7.6
488	4-P-PDOT	BRD-A67482312-001-01-8	-11.2	1.3	-24.9	-23.4	1.4	7.1
489	3beta-HYDROXYDEOXODIHYDRODEOXYGEDUNIN	BRD-A67508925-001-03-5	5.5	-12.4	-52.8	-39.5	-18.2	-22.2
490	NAFRONYL OXALATE	BRD-A67862938-034-09-9	-4.9	3.0	-9.8	-22.4	15.7	16.1
491	BRL 44408 maleate	BRD-A67949680-103-01-4	-8.5	26.7	32.6	19.7	12.9	19.3
492	Daunorubicin hydrochloride	BRD-A68009927-003-02-9	-20.2	-1.9	-22.4	-29.0	-7.2	-6.3
493	BROMPHENIRAMINE MALEATE	BRD-A68723818-050-18-4	1.8	-33.9	-35.1	-27.8	-9.7	-10.2
494	AZELASTINE HYDROCHLORIDE	BRD-A68888262-003-07-8	-14.4	-26.3	-58.9	-50.7	-64.3	-66.6
495	DAPT	BRD-A68929948-001-01-9	-3.3	-4.1	-8.8	-20.7	1.8	8.8
496	CEDRELONE	BRD-A69143712-001-03-6	-19.0	-19.5	-44.0	-53.5	-43.5	-43.6
497	CARBIDOPA	BRD-A69512159-001-03-2	32.2	41.7	56.2	33.8	-37.4	-33.7
498	DILTIAZEM HYDROCHLORIDE	BRD-A69636825-003-03-9	25.0	15.4	-44.2	-55.4	-11.8	-6.8
499	MINOCYCLINE HYDROCHLORIDE	BRD-A69651145-003-04-9	28.3	26.4	-5.2	-8.6	-51.1	-50.0
500	FLUMEQUINE	BRD-A69777949-001-15-0	11.0	17.9	-25.7	-7.7	8.8	-6.7
501	EUCATROPINE HYDROCHLORIDE	BRD-A69786436-003-03-3	17.9	9.3	35.1	26.7	7.5	16.1
502	CYCLOSPORINE	BRD-A69815203-001-05-0	-2.1	-41.1	-20.9	-20.2	-6.8	-2.9
503	AMINOPENTAMIDE	BRD-A69917777-065-01-4	-10.6	-5.6	-17.5	16.8	5.8	10.2

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
504	Bromocriptine mesylate	BRD-A69960130-066-01-4	15.3	19.8	35.1	16.7	24.8	26.2
505	SECNIDAZOLE	BRD-A70083328-001-12-8	14.0	9.4	21.4	9.7	22.6	26.9
506	PG-9 maleate	BRD-A70268693-103-01-9	-7.6	-1.6	-41.3	-58.5	-8.2	-4.7
507	PSB 36	BRD-A70407468-001-01-2	22.8	16.1	27.1	25.4	20.9	21.4
508	SULCONAZOLE NITRATE	BRD-A70649075-008-17-5	-54.8	-61.6	-66.6	-76.1	-57.5	-62.6
509	3beta-ACETOXYDEOXODIHYDROGEDUNIN	BRD-A71001587-001-03-4	-27.5	-34.3	15.1	5.2	-20.0	-3.4
510	FENDILINE HYDROCHLORIDE	BRD-A71033472-003-15-5	9.0	9.9	-58.4	-50.6	-33.2	-35.8
511	LUFENURON	BRD-A71774530-001-02-6	15.3	9.0	-15.7	0.1	10.7	2.2
512	PRAVASTATIN SODIUM	BRD-A71816415-236-03-5	20.5	15.9	0.1	10.6	3.9	4.3
513	MUNDULONE ACETATE	BRD-A71960694-001-01-5	-3.8	0.2	28.4	35.1	5.3	8.6
514	SR 202	BRD-A72066420-001-01-1	20.3	-13.1	6.8	1.3	7.8	11.3
515	METERGOLINE	BRD-A72309220-001-03-3	-20.9	-43.0	-86.3	-84.0	-69.1	-79.5
516	Spiroxatrine	BRD-A72483914-001-02-9	-6.8	-26.6	-20.4	-24.4	-10.6	-11.0
517	GW 6471	BRD-A72596465-001-01-3	11.8	-5.5	9.7	7.7	-9.8	-5.8
518	SKF 96365	BRD-A72703248-003-03-1	0.2	-14.6	0.8	23.7	-10.7	-10.6
519	ASIATIC ACID	BRD-A72758037-001-01-8	-4.5	3.7	-29.2	-37.1	-12.6	-16.6
520	FEXOFENADINE HYDROCHLORIDE	BRD-A73368467-003-07-7	-35.8	-13.6	13.1	1.2	10.3	11.9
521	8-HYDROXYCARAPINIC ACID	BRD-A73559168-001-03-6	8.8	-5.4	-11.8	-7.0	-7.3	4.8
522	EXEMESTANE	BRD-A73741725-001-01-0	12.6	-0.9	10.8	5.0	5.3	9.2
523	Glycodeoxycholic Acid	BRD-A73859745-236-01-8	-0.9	6.5	-9.4	1.2	7.4	13.9
524	DACTINOMYCIN	BRD-A73909368-001-01-5	-1.8	6.8	5.2	7.3	-12.8	-25.7
525	TROXERUTIN	BRD-A74160776-001-03-6	0.9	3.6	-28.6	-10.4	-11.2	2.9
526	ETODOLAC	BRD-A74667430-001-15-2	-26.9	-51.7	0.3	-10.7	-4.1	1.0
527	GATIFLOXACIN	BRD-A74980173-001-06-9	5.4	-9.5	3.9	32.9	12.2	21.5
528	HYDROCORTISONE	BRD-A75172220-001-03-2	22.0	48.2	5.5	-8.7	5.9	12.7
529	DESOXYCORTICOSTERONE ACETATE	BRD-A75402480-001-03-8	-23.2	6.6	-41.8	-51.3	-17.9	-19.0
530	KAWAIN	BRD-A75455249-001-12-9	-28.2	-17.4	-9.0	-18.9	6.0	2.8
531	PD 166793	BRD-A75478957-001-01-6	-9.8	-2.7	5.6	2.6	31.8	27.4
532	ISOXICAM	BRD-A75552914-001-09-3	-9.8	-5.8	7.2	-3.8	6.5	6.7
533	CLENBUTEROL HYDROCHLORIDE	BRD-A75726477-003-14-8	9.6	6.3	25.7	33.9	38.8	31.1
534	SDM25N hydrochloride	BRD-A75769826-003-01-3	-7.3	-21.0	23.2	25.5	-37.7	-40.2
535	LOMEFLOXACIN HYDROCHLORIDE	BRD-A75850590-003-06-4	9.5	48.7	4.8	26.7	14.7	13.0
536	MUUROLLADIE-3-ONE	BRD-A75954196-001-03-3	14.0	5.8	6.6	26.8	26.0	8.9
537	Cromakalim	BRD-A76093993-001-01-8	-3.3	-1.7	3.7	-2.5	-13.0	-3.4
538	PANTETHINE	BRD-A76244192-001-01-6	17.3	4.4	-3.4	-2.8	9.1	6.6
539	alpha-DIHYDROGEDUNOL	BRD-A76417540-001-03-3	3.2	4.5	-53.0	-17.3	11.2	0.2
540	RUTOSIDE (rutin)	BRD-A76747559-001-02-3	-13.2	-22.1	-40.9	2.0	-34.1	-35.0
541	QUERCITRIN	BRD-A76899420-001-03-7	34.6	18.6	-27.3	2.9	-37.0	-40.4
542	VESAMICOL HYDROCHLORIDE	BRD-A76904477-003-05-8	14.5	9.4	0.0	37.7	14.5	12.3
543		BRD-A76941896-001-01-6	102.6	108.7	25.0	30.6	-1.6	4.3
544	D609	BRD-A77118605-237-01-2	11.6	22.2	6.5	-10.3	10.6	12.7
545	DEOXYSAPPANONE B TRIMETHYL ETHER	BRD-A77164655-001-03-1	2.3	-15.2	-44.5	-27.6	-24.0	-21.8
546	SYM 2206	BRD-A77218119-001-02-7	-7.2	-2.3	-57.3	-61.0	8.2	-0.8
547	CYCLOPENTOLATE HYDROCHLORIDE	BRD-A77291778-003-15-4	5.8	-16.5	2.4	-9.8	6.5	2.4
548	Salubrinal	BRD-A77299732-001-01-6	19.9	15.0	-9.9	-16.6	-10.6	-11.2
549	RK-682	BRD-A77349281-001-02-2	-66.5	-62.9	36.1	55.0	-60.8	-64.1

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
550	TOTAROL-19-CARBOXYLIC ACID, METHYL ESTER	BRD-A77488069-001-03-4	-11.6	-11.5	-9.1	42.1	23.5	7.6
551	FLUOCINOLONE ACETONIDE	BRD-A77824596-001-03-2	-18.9	-12.9	-3.7	-5.1	-8.6	2.9
552	HYOSCYAMINE	BRD-A78303415-001-03-5	13.3	18.2	23.8	15.0	19.4	11.1
553	Monastrol	BRD-A78377521-001-03-0	-18.9	-5.3	16.6	20.3	11.4	20.2
554	PREDNISOLONE HEMISUCCINATE	BRD-A78391468-001-01-0	-20.6	-5.9	-2.7	6.8	8.6	4.4
555	ICI-118,551 hydrochloride	BRD-A78942461-003-01-3	-13.6	-16.1	-38.9	-26.4	-20.1	-24.0
556	AGN 192403 hydrochloride	BRD-A79038507-003-01-5	-5.1	17.0	18.8	11.5	27.4	31.4
557	BETAMETHAZONE SODIUM PHOSPHATE	BRD-A79380603-304-01-6	-9.7	11.1	20.2	12.6	0.5	7.7
558	TROPICAMIDE	BRD-A79672927-001-10-8	-18.8	-9.5	4.1	21.0	13.8	2.2
559	SIROLIMUS	BRD-A79768653-001-02-1	33.1	13.8	-19.0	-33.2	-18.8	-26.6
560	Memantine hydrochloride	BRD-A79803969-003-06-2	-3.7	-1.2	13.9	6.4	30.5	31.3
561	MIDODRINE HYDROCHLORIDE	BRD-A79981887-003-09-9	8.5	-7.5	-1.2	-2.0	10.6	1.7
562	BENDROFLUMETHIAZIDE	BRD-A80017228-001-15-8	-13.3	2.4	24.2	10.9	4.4	13.2
563	NORSTICTIC ACID	BRD-A80079592-001-03-2	58.6	62.5	-67.2	-57.9	-42.3	-61.8
564	BETAMETHASONE VALERATE	BRD-A80594172-001-03-8	5.9	2.5	-49.2	-20.5	-3.0	-16.0
565	FR 139317	BRD-A80641450-001-01-4	0.8	-11.1	1.5	-3.0	19.7	26.0
566	CLOPERASTINE HYDROCHLORIDE	BRD-A80908310-003-08-8	-1.7	-12.4	-61.5	-43.4	-20.6	-32.2
567	CONVALLATOXIN	BRD-A80968824-001-03-6	-13.0	0.9	33.2	5.5	3.0	22.3
568	GLYCOPYRROLATE	BRD-A81233518-004-07-0	4.4	3.5	9.6	2.6	14.6	9.5
569	Simvastatin	BRD-A81772229-001-03-2	2.1	-1.6	-3.8	-6.6	3.1	17.0
570	U 18666A	BRD-A81795050-003-01-7	3.3	-10.0	-15.7	-32.3	-17.0	-11.0
571	CGS 21680 hydrochloride	BRD-A81866333-003-01-5	12.6	-1.6	-21.4	-26.8	-14.0	-14.7
572	6alpha-METHYLPREDNISOLONE ACETATE	BRD-A82086877-001-03-1	-3.3	-16.1	0.2	-15.3	-3.0	-1.0
573	Clofarabine	BRD-A82371568-001-01-5	8.6	-2.3	0.7	-7.4	19.0	25.0
574	MICONAZOLE NITRATE	BRD-A82396632-008-14-2	-128.3	-123.4	-126.2	-131.1	-97.9	-97.9
575	MANGIFERIN	BRD-A82440780-001-01-0	107.7	98.2	-36.1	-19.7	-26.2	-39.2
576	ARTENIMOL	BRD-A82452087-001-01-5	-4.3	-17.9	-47.0	-4.3	-1.4	4.7
577	SDZ NKT 343	BRD-A82590476-001-01-1	-8.8	-15.4	-31.2	-33.9	-9.4	-6.3
578	Naltrindole hydrochloride	BRD-A82656074-003-01-2	17.5	9.8	-25.6	-8.5	-48.4	-32.0
579	FINASTERIDE	BRD-A83081521-001-01-5	-26.5	3.8	-15.8	3.1	-3.4	2.9
580	BRAZILIN	BRD-A83326220-001-04-2	305.6	279.8	25.5	30.3	-0.3	5.4
581	2-Cl-IB-MECA	BRD-A83387524-001-01-3	-41.3	-34.6	-59.1	-86.9	-42.8	-37.2
582	ESTRADIOL METHYL ETHER	BRD-A83613346-001-03-4	-9.3	-18.8	-32.1	-50.6	-31.2	-29.6
583	A 61603 hydrobromide	BRD-A83650191-004-01-0	-6.7	7.8	11.8	4.8	-30.5	-27.6
584	Chromanol 293B	BRD-A83695761-001-01-1	1.0	-0.3	12.3	-1.0	21.9	24.2
585	DEXAMETHASONE SODIUM PHOSPHATE	BRD-A83802939-304-03-4	5.5	-3.8	5.0	20.0	10.7	-20.9
586	Tropisetron hydrochloride	BRD-A83859836-003-02-8	-8.7	-6.5	-4.0	0.5	3.9	2.6
587	Calpeptin	BRD-A84045418-001-01-5	16.2	21.1	-21.0	-13.7	2.5	-3.6
588	MELOXICAM SODIUM	BRD-A84174393-236-03-0	13.8	1.0	13.8	-2.8	15.2	8.5
589	Baclofen (R,S)	BRD-A84174873-001-06-0	-37.7	-12.3	32.4	33.3	10.6	5.9
590	MADECASSIC ACID	BRD-A84189249-001-03-2	30.9	60.8	-44.1	-30.9	28.0	16.7
591	BACCATIN III	BRD-A84189516-001-01-2	10.0	-3.5	-10.3	1.9	11.8	11.7
592	L-655,708	BRD-A84389091-001-01-1	7.6	0.8	-6.2	0.5	16.5	8.0
593	Tropanyl-3,5-dimethylbenzoate	BRD-A84389633-001-02-4	5.2	-12.1	-13.0	-20.0	-0.7	-2.4
594	NISOLDIPINE	BRD-A84465106-001-01-2	264.7	329.5	-46.6	-72.4	-16.9	-35.4
595	THIORIDAZINE HYDROCHLORIDE	BRD-A84481105-003-17-2	-96.8	-96.1	-94.0	-95.8	-71.6	-76.8

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
596	3,16-DIDEOXYMEXICANOLIDE-3beta-DIOL	BRD-A84663931-001-03-9	-10.6	-21.8	-47.9	-51.7	-29.1	-30.2
597	DEHYDROROTENONE	BRD-A84913188-001-03-8	8.7	8.4	-41.3	-5.6	2.0	0.0
598	3 a-Bis-(4-fluorophenyl) methoxytropane hydrochloride	BRD-A85216385-003-01-6	-28.4	-45.7	-83.1	-83.6	-58.9	-54.9
599	N6 -Cyclopentyladenosine	BRD-A85234536-001-04-5	8.6	-0.3	6.3	26.7	18.3	21.2
600	(-)-Quinpirole hydrochloride	BRD-A85280935-003-01-7	7.5	3.4	12.0	-18.5	10.8	12.4
601	L 670596	BRD-A85472596-001-01-4	-20.7	-22.3	-42.0	-69.6	-28.3	-31.1
602	MDL 72222	BRD-A85587465-001-02-5	-23.2	-11.7	-22.7	-15.4	-10.0	-1.6
603	USNIC ACID	BRD-A85739295-001-03-6	15.3	49.9	21.7	23.4	7.1	11.8
604	(?)-1-(1,2-Diphenylethyl)piperidine maleate	BRD-A86415025-103-01-7	-22.1	-29.6	12.2	6.6	13.0	18.4
605	Ganaxolone	BRD-A87005460-001-01-3	-9.3	4.8	-20.0	10.0	-21.2	-12.1
606	CEFPODOXIME PROXETIL	BRD-A87387433-001-01-9	19.5	16.3	12.8	37.5	9.3	5.9
607	Tenidap	BRD-A87479750-001-01-9	-18.0	-19.9	-29.3	-32.9	7.6	0.1
608	NADOLOL	BRD-A87606379-001-13-3	-0.9	0.9	-4.1	-17.6	10.2	10.5
609	PRONETALOL HYDROCHLORIDE	BRD-A87715314-003-09-4	-0.1	-31.5	-37.0	2.0	14.7	6.2
610	EQUILIN	BRD-A88080608-001-03-4	48.1	11.5	-2.9	-25.1	-24.2	-32.6
611	HALCINONIDE	BRD-A88138582-001-03-0	36.0	20.0	-3.0	4.8	4.7	-0.4
612	ALBUTEROL (+/-)	BRD-A88254928-001-05-3	16.4	10.9	2.2	-10.0	4.7	9.2
613	DIHYDROXY (3alpha,12alpha)PREGNAN-20-ONE	BRD-A88284590-001-03-2	10.1	-7.7	-37.5	-20.5	-16.1	-13.5
614	SKF 38393 hydrobromide	BRD-A88548664-004-01-9	6.3	17.7	-12.4	-12.3	-30.1	-37.4
615	BUCETIN	BRD-A88684804-001-01-9	-1.3	11.3	-2.4	0.2	23.6	19.6
616		BRD-A88691025-001-07-4	-5.7	2.4	-3.3	-0.9	5.5	10.6
617	BISOPROLOL FUMARATE	BRD-A89175223-051-05-6	7.9	-0.3	11.6	20.7	25.4	28.9
618	ICI 192,605	BRD-A89208012-001-01-4	-7.2	-8.3	-66.1	-55.0	-31.6	-16.4
619	jmw-topo1-04	BRD-A89471977-001-05-2	6.9	-2.7	22.5	26.2	6.9	16.2
620	Mefloquine	BRD-A89585551-003-08-3	-52.4	-72.9	-91.6	-105.5	-82.2	-99.4
621	CGP 55845	BRD-A89672324-001-02-2	15.6	-5.3	-4.0	-10.0	1.6	-0.4
622	ALCLOMETAZONE DIPROPIONATE	BRD-A90131694-001-02-8	-11.7	-7.1	-2.2	-4.6	-1.7	9.8
623	ALPINETIN METHYL ETHER	BRD-A90249268-001-04-0	-2.6	-2.8	-42.9	-43.7	-20.1	-19.1
624	Cilastatin sodium	BRD-A90311807-236-01-4	-3.7	-11.0	-9.6	-4.5	9.9	13.5
625	GUAIFENESIN	BRD-A90515964-001-09-0	15.5	-7.0	-11.0	4.8	3.2	-2.5
626	ESTRONE BENZOATE	BRD-A90969585-001-03-1	5.3	1.5	-11.0	-17.0	11.2	6.9
627	BEPRIDIL HYDROCHLORIDE	BRD-A91008255-003-16-4	-13.9	-33.9	-25.3	-6.1	-36.5	-7.2
628	LAPPACONITINE	BRD-A91353509-001-01-4	1.9	-3.7	-9.7	0.2	-4.0	4.6
629	ESTRADIOL CYPIONATE	BRD-A91452556-001-03-2	-33.3	-1.0	10.5	27.5	47.8	49.7
630	CHLOROQUINE DIPHOSPHATE	BRD-A91699651-316-06-7	-21.5	10.8	-3.5	-3.9	6.3	2.0
631	ESTRADIOL-3-SULFATE, SODIUM SALT	BRD-A91702150-236-03-2	-6.5	-20.3	15.9	8.2	1.1	6.8
632	CAMYLOFINE DIHYDROCHLORIDE	BRD-A91733352-300-01-1	-9.1	-11.0	8.8	-7.2	-1.0	-0.6
633	Siguazodan	BRD-A91992993-001-01-2	5.1	-5.2	-3.4	-10.4	7.2	16.6
634	BETAMETHASONE ACETATE	BRD-A92177080-001-01-3	-6.0	-1.0	-4.1	20.0	5.2	7.6
635	TRIAMCINOLONE ACETONIDE	BRD-A92439610-001-03-2	-21.8	4.0	5.8	23.9	1.1	4.0
636	DEOXYSAPPANONE B 7,3'-DIMETHYL ETHER	BRD-A92542880-001-01-0	12.5	6.1	-24.3	-2.6	-40.9	-38.5
637	RU 28318, potassium salt	BRD-A92585442-237-01-0	-18.8	-14.4	7.7	-13.9	-0.4	15.0
638	TRIMEBUTINE MALEATE	BRD-A92630576-050-14-2	6.8	-16.6	16.6	-6.3	23.1	23.9
639	NALBUPHINE HYDROCHLORIDE	BRD-A92651262-003-03-9	22.6	6.4	17.9	15.3	-18.8	-24.9
640	BICUCULLINE(-) METHIODIDE	BRD-A92652541-005-01-9	-4.2	-7.7	-23.4	-21.0	-13.2	-12.3
641	LUPANINE PERCHLORATE	BRD-A92826379-009-03-4	1.8	5.1	9.5	25.8	7.7	11.6

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
642	SM-21 maleate	BRD-A92933783-103-01-3	-8.8	-11.5	-31.3	-35.6	-23.2	-24.2
643	Ciglitazone	BRD-A93000692-001-03-2	-8.6	-20.8	22.5	5.2	-9.6	-20.8
644	DIGITOXIN	BRD-A93236127-001-03-7	-3.7	11.1	12.6	11.6	-0.2	6.4
645	(+/-)-Clopidogrel hydrochloride	BRD-A93269281-003-01-0	15.4	0.8	2.6	4.5	28.0	22.1
646	DEXAMETHASONE ACETATE	BRD-A93424738-001-03-0	-13.8	-15.9	3.6	2.6	1.1	1.9
647	AF-DX 384	BRD-A93436351-001-01-4	-4.9	-2.4	7.0	-0.4	10.4	6.8
648	PETCM	BRD-A93477898-001-03-4	6.0	33.6	8.5	7.1	7.9	7.5
649	MUNDULONE	BRD-A93572202-001-03-3	-35.2	-38.0	-58.8	-20.4	-22.6	-25.7
650	GR 89696 fumarate	BRD-A93659613-051-03-6	-14.6	-28.0	-38.5	-58.6	-19.0	-12.6
651	ATROPINE SULFATE	BRD-A93739713-065-03-5	-1.3	21.1	-33.9	0.5	-5.0	-0.3
652	17-PA	BRD-A94046266-001-01-4	-17.7	-5.5	2.3	49.8	8.2	19.2
653	TOTAROL ACETATE	BRD-A94366206-001-03-5	7.5	9.4	49.6	12.5	17.7	35.8
654	NTNCB hydrochloride	BRD-A94413429-003-01-6	6.7	-8.0	-3.6	10.3	-25.7	-26.7
655	PREDNISOLONE SODIUM PHOSPHATE	BRD-A94523291-304-01-9	10.9	18.7	9.5	38.8	7.9	11.1
656	BIFONAZOLE	BRD-A94543220-001-12-2	1.0	-14.2	-61.0	-53.3	-13.5	-18.0
657	21-ACETOXYPREGNENOLONE	BRD-A94561690-001-02-6	22.1	58.9	-14.6	19.9	43.6	36.6
658	N-Methyl-N-[(1S)-1-phenyl-2-(1-pyrrolidinyl) ethyl]phenylacetamide hydrochloride	BRD-A94675310-003-01-2	-3.0	-8.7	23.7	47.7	7.7	5.8
659	METAXALONE	BRD-A94709349-001-03-4	-12.5	-16.2	-13.9	-13.3	0.8	4.4
660	DIGOXIN	BRD-A94756469-001-03-9	-21.9	10.3	24.2	15.1	15.2	22.2
661	CYPROTERONE ACETATE	BRD-A95207036-001-03-6	-0.2	-3.9	-26.8	-43.2	-21.4	-30.6
662	ANDROSTA-1,4-DIEN-3,17-DIONE	BRD-A95513702-001-03-0	-20.3	-19.7	-9.2	-14.1	1.3	13.0
663	Nisoxetine hydrochloride	BRD-A95696066-003-06-2	-7.6	-8.1	-8.3	-0.6	3.9	12.0
664	INDAPAMIDE	BRD-A95869247-001-14-5	13.3	3.9	6.3	8.2	-8.8	-9.0
665	FPL 55712	BRD-A96456596-001-01-4	-45.0	-43.9	-83.3	-93.3	-45.4	-49.9
666	EBPC	BRD-A96485169-001-05-1	-9.9	-10.3	7.3	9.1	12.8	19.6
667	5alpha-ANDROSTAN-3,17-DIONE	BRD-A96828973-001-05-8	-3.5	-8.5	-23.0	5.9	2.6	-5.9
668	L-732,138	BRD-A96882008-001-01-3	-11.9	-9.8	-14.7	-15.6	-25.0	-27.9
669	HYDROQUININE HYDROBROMIDE HYDRATE	BRD-A96933311-337-01-4	4.0	1.2	7.4	-6.4	0.1	2.5
670	DECAHYDROGAMBOGIC ACID	BRD-A97026779-001-01-3	6.8	-0.5	-5.6	78.5	16.2	29.2
671	FENOTEROL HYDROBROMIDE	BRD-A97104540-004-08-5	1.0	-4.0	16.0	16.2	11.4	12.9
672	ISOKOBUSONE	BRD-A97152619-001-03-7	29.7	26.7	-3.5	13.6	26.0	20.3
673	ROSIGLITAZONE	BRD-A97437073-001-04-9	3.8	-8.5	-0.1	0.2	2.3	8.0
674	PIPERIDOLATE HYDROCHLORIDE	BRD-A97479839-003-08-3	-22.4	18.5	-21.1	-22.0	-16.7	-4.9
675	RANOLAZINE	BRD-A97674275-001-04-3	-2.9	14.4	16.6	-6.5	15.4	25.7
676	PINDOLOL	BRD-A97701745-001-09-5	-4.3	-10.4	20.6	7.7	18.3	22.6
677	KETOPROFEN	BRD-A97739905-001-15-8	-31.6	-32.3	2.3	-12.0	15.8	10.8
678	Talniflumate	BRD-A98378129-001-01-4	-26.0	-17.1	-13.9	-26.3	-26.2	-21.9
679	CARBENOXOLONE SODIUM	BRD-A98702003-304-03-0	1.0	-24.9	-25.2	-16.9	-10.6	5.1
680	Methysergide maleate	BRD-A98725278-103-01-9	33.9	35.3	101.9	113.9	19.1	20.3
681	HYDROXYCHLOROQUINE SULFATE	BRD-A99117172-065-02-4	12.0	3.0	-10.3	22.4	2.2	15.0
682	EVOXINE	BRD-A99268498-001-06-8	8.5	-4.8	110.4	76.1	4.1	-0.1
683	NAFCILLIN SODIUM	BRD-A99402294-236-03-8	-22.2	-30.2	13.8	7.8	-5.3	12.5
684	MT-21	BRD-A99449986-001-01-4	-12.1	5.8	21.6	24.3	-10.8	-13.5
685	ETHOSUXIMIDE	BRD-A99633051-001-05-4	9.1	6.1	13.4	-9.6	-2.7	3.2
686	TRILOSTANE	BRD-A99644790-001-01-6	-6.7	-10.7	-46.8	-29.7	-1.8	1.5
687	Nicergoline	BRD-A99721021-001-01-3	-2.1	-8.6	-23.8	-25.7	-4.4	-13.0

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
688	P1075	BRD-K00206590-001-01-2	6.7	17.7	21.1	0.9	15.4	14.8
689	PPT	BRD-K00312224-001-03-8	-38.3	-35.8	-75.2	-79.1	8.2	7.1
690	RITA	BRD-K00317371-001-01-2	-29.4	-24.3	25.4	44.3	-31.1	-37.7
691	Ro 08-2750	BRD-K00486786-001-01-4	316.8	315.9	12.8	9.3	-18.9	-3.7
692		BRD-K00535541-311-04-1	-5.6	-1.1	9.5	14.9	2.8	19.1
693	TICLOPIDINE HYDROCHLORIDE	BRD-K00603606-003-13-3	-9.3	-15.9	32.4	11.3	9.0	14.9
694	Altanserin hydrochloride	BRD-K00610438-003-01-7	4.3	2.9	-23.1	-20.9	1.1	-3.8
695	CL 218872	BRD-K00662280-001-04-5	-2.5	-4.0	3.4	7.6	5.6	5.0
696	FAMOTIDINE	BRD-K00673382-001-07-2	1.1	9.6	17.8	12.4	12.3	5.9
697	CL 82198 hydrochloride	BRD-K00675675-003-01-2	-16.4	-8.7	-4.6	12.7	21.4	24.4
698	2',4'-DIHYDROXYCHALCONE	BRD-K00721105-001-01-8	8.0	6.5	-9.3	-30.7	-19.9	-27.4
699	SULFAMETHOXYPYRIDAZINE	BRD-K00938507-001-13-7	-8.6	29.6	0.6	53.1	31.4	22.8
700	CLOXACILLIN SODIUM	BRD-K01244426-236-08-9	-7.4	-24.0	1.0	7.4	16.8	12.4
701	PIMOZIDE	BRD-K01292756-001-13-6	-20.0	-19.7	-60.0	-50.0	-43.2	-30.0
702	2,4-Dichlorophenoxyacetic acid	BRD-K01473791-001-06-3	7.7	16.3	-17.5	-5.6	-16.7	-2.7
703	APIGENIN	BRD-K01493881-001-17-9	11.1	21.3	-39.0	-35.7	-8.5	-15.0
704		BRD-K01567962-001-08-1	1.1	-1.8	25.5	21.2	13.8	20.1
705	LE 300	BRD-K01648091-001-04-2	-17.2	-22.4	19.6	13.4	-16.7	4.7
706	INDOLE-3-CARBINOL	BRD-K01815685-001-07-2	-5.2	-16.1	45.8	38.4	-0.9	2.3
707	CARAPIN-8(9)-ENE	BRD-K01818918-001-03-4	-1.1	20.0	-77.1	-37.0	27.2	-2.4
708	DPCPX	BRD-K01824921-001-10-2	-14.2	-17.2	11.8	31.1	13.1	22.7
709	RS 23597-190 hydrochloride	BRD-K01868942-003-01-9	-35.7	-3.8	20.7	24.2	0.7	6.8
710	WY 14643	BRD-K01902415-001-03-4	-5.0	-3.9	6.0	-5.5	17.8	21.8
711	SUCCINYLSULFATHIAZOLE	BRD-K01950558-001-09-7	8.5	12.5	-23.5	20.8	18.2	5.0
712	PACHYRRHIZIN	BRD-K02070226-001-03-8	22.2	7.3	9.0	-2.9	-21.4	-28.4
713	panobinostat	BRD-K02130563-001-07-2	0.0	-12.8	11.6	59.1	-15.2	-22.5
714	AMOXAPINE	BRD-K02265150-001-15-8	-50.4	-49.4	-80.3	-71.7	-31.0	-50.6
715	GR 32191 hydrochloride	BRD-K02283807-003-01-4	-15.9	-13.8	-51.5	-70.4	-27.0	-23.1
716	CAFFEINE	BRD-K02404261-001-07-6	-0.7	6.8	25.7	10.6	23.0	23.7
717	Parbendazole	BRD-K02407574-001-04-8	6.9	5.3	-2.0	1.8	26.7	33.0
718	ETHYL PARABEN	BRD-K02464583-001-01-4	23.1	21.0	-3.2	1.8	5.1	-11.1
719	O-2050	BRD-K02590140-001-01-2	-22.2	-12.8	-3.6	-13.4	-12.9	-17.5
720	CELECOXIB	BRD-K02637541-001-06-5	10.3	23.2	-32.2	-29.8	29.5	24.4
721	RESVERATROL 4'-METHYL ETHER	BRD-K02671211-001-03-0	0.5	-3.8	16.4	-18.0	-1.4	-6.7
722	HYDRASTINE (1R, 9S)	BRD-K02715688-001-01-3	-0.7	-8.9	5.2	5.3	-2.0	22.2
723	Methiazole	BRD-K02764365-001-05-2	10.9	-4.6	42.7	33.9	17.3	28.4
724	2-METHOXYXANTHONE	BRD-K02855712-001-06-6	16.1	-1.7	151.9	127.9	7.3	-4.9
725	MINAPRINE HYDROCHLORIDE	BRD-K02867583-300-06-3	-13.8	-18.8	-3.2	-14.2	5.0	12.6
726	CLOFOCTOL	BRD-K02900412-001-07-1	-19.4	-7.1	-26.7	-16.2	9.7	1.1
727	Forskolin, 7-Deacetyl-7-[O-(N-methylpiperazino)-g-butyryl]-, Dihydrochloride	BRD-K03015355-003-01-5	-7.1	-14.5	9.6	7.6	-0.4	-2.1
728	ARACHIDONIC ACID	BRD-K03070961-001-04-4	17.6	9.7	2.5	-32.4	10.8	0.0
729	A-7 hydrochloride	BRD-K03301001-003-01-7	-53.5	-58.6	-97.0	-94.9	-75.1	-78.4
730	Linomide	BRD-K03384561-001-01-9	-6.3	-8.1	19.1	-2.4	-3.7	13.4
731	DMNB	BRD-K03564313-001-02-5	28.3	21.2	-4.2	6.3	9.1	14.1
732	U0124	BRD-K03635852-001-01-2	0.1	18.4	64.8	28.1	-36.0	-38.3
733	AY 9944	BRD-K03642198-300-01-7	-27.2	-23.5	-48.0	-41.1	-35.3	-26.9

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
734	Raclopride	BRD-K04111260-001-05-0	-15.8	-6.3	0.9	-2.3	10.0	13.5
735	OXCARBAZEPINE	BRD-K04196797-001-12-9	1.9	1.3	-21.0	25.6	7.9	18.9
736	SB 222200	BRD-K04414442-001-03-4	-16.0	-7.1	-4.7	-11.1	9.4	5.8
737	7-NINA	BRD-K04430056-236-01-3	14.3	14.4	14.0	2.6	3.6	2.1
738	CLEMIZOLE HYDROCHLORIDE	BRD-K04704168-003-11-9	-10.5	11.2	-13.8	-49.3	-22.2	-19.1
739	SULFISOXAZOLE ACETYL	BRD-K05009775-001-01-2	-4.5	-15.2	-28.5	2.7	13.7	13.8
740	ZK 164015	BRD-K05151076-001-01-8	0.6	3.9	-4.0	11.2	16.4	13.1
741	NGB 2904	BRD-K05181084-003-02-9	8.9	-5.0	1.6	-1.5	15.5	1.1
742	L-741,626	BRD-K05181463-001-04-0	-17.0	-6.0	-34.8	-31.2	-6.0	-1.8
743	SC-10	BRD-K05361803-001-02-1	25.0	7.6	19.9	40.5	2.2	-9.5
744	NICOTINE DITARTRATE	BRD-K05395900-322-04-7	-6.6	-3.8	2.3	-0.3	21.6	5.9
745	HA-1004	BRD-K05434375-001-03-2	3.0	7.3	-20.4	-11.0	-7.3	-3.7
746	JX 401	BRD-K05464208-001-01-6	-8.7	-0.2	-41.8	-37.5	-32.1	-30.9
747	L-745,870 trihydrochloride	BRD-K05528470-305-01-4	-16.5	-6.5	-33.9	-40.1	-30.6	-28.7
748	FTAXILIDE	BRD-K05724540-001-04-4	4.5	0.2	-21.3	-2.9	17.5	19.2
749	MT001_073	BRD-K05878375-236-02-4	-5.1	-13.0	1.8	-1.9	16.9	19.4
750	FLUCONAZOLE	BRD-K05977355-001-09-1	-5.9	1.2	6.3	1.4	6.4	14.9
751	DH 97	BRD-K06014311-001-01-2	32.7	21.5	10.7	18.5	33.2	21.6
752	Telenzepine dihydrochloride	BRD-K06147391-300-04-3	-17.8	-13.7	14.8	18.8	15.6	20.2
753	CCMQ	BRD-K06159959-001-01-2	15.3	16.9	8.5	25.3	17.8	23.2
754	Carbetapentane citrate	BRD-K06181161-048-07-8	-6.6	-13.7	-13.4	-20.0	-2.3	-0.3
755	YS-035 hydrochloride	BRD-K06208435-003-03-3	4.1	2.7	7.7	18.7	18.9	22.2
756	DuP 697	BRD-K06221026-001-03-5	-13.3	2.2	19.8	38.2	39.7	39.1
757	LY 364947	BRD-K06234293-001-01-8	-4.3	-11.3	-13.2	-9.2	7.9	11.5
758	ROTENONIC ACID, METHYL ETHER	BRD-K06268662-001-03-5	-4.9	0.2	4.2	-27.8	-15.1	-3.6
759	N-METHYLANTHRANILIC ACID	BRD-K06439119-001-03-1	2.7	-26.1	56.7	56.3	3.4	12.2
760	Ro 31-8220 mesylate	BRD-K06543683-066-01-3	-5.7	-15.3	-49.5	-49.8	-46.8	-52.4
761	FAST GREEN FCF	BRD-K06561965-304-01-9	18.7	22.5	-9.7	-18.0	-32.9	-27.6
762	Cisapride	BRD-K06895174-001-01-0	-6.4	-11.1	-40.2	-50.5	-24.3	-24.3
763	MINOXIDIL	BRD-K06902185-001-10-2	18.5	18.9	17.2	3.5	16.7	23.7
764	PROMAZINE HYDROCHLORIDE	BRD-K06980535-003-15-0	-26.9	-57.0	-72.5	-74.0	-71.1	-69.5
765	XANTHURENIC ACID	BRD-K07327532-001-03-6	24.0	23.7	6.7	-10.7	-1.2	-3.8
766	BRL 37344, sodium salt	BRD-K07507905-236-01-8	2.4	-2.4	3.9	-5.8	8.7	7.4
767	curcumin	BRD-K07572174-001-19-6	36.6	44.7	-26.4	-18.7	-42.8	-45.7
768	ACECAINIDE HYDROCHLORIDE	BRD-K07753030-003-11-9	-1.0	0.6	1.6	-9.1	7.7	7.1
769	LINCOMYCIN HYDROCHLORIDE	BRD-K08033334-003-03-5	-37.8	-0.7	13.3	8.6	3.9	20.5
770	PRIMULETIN	BRD-K08048246-001-03-4	27.3	20.1	8.3	7.9	19.3	16.2
771	TETRANDRINE	BRD-K08078237-001-13-1	-28.4	-32.8	-66.4	-64.8	-73.6	-73.7
772	L-701,324	BRD-K08109516-001-02-9	30.0	-4.7	-5.7	14.8	9.2	11.2
773	AG 1288	BRD-K08115555-001-02-8	11.9	-2.0	-12.5	-13.4	-6.2	-0.1
774	AG 825	BRD-K08132273-001-01-6	-40.8	-9.4	-43.5	-30.9	-20.4	-21.1
775	5-Nonyloxytryptamine oxalate	BRD-K08219523-034-01-0	-96.6	-97.5	-110.4	-111.6	-81.8	-84.0
776	DICLOFENAC SODIUM	BRD-K08252256-236-17-1	3.3	10.8	-22.7	-26.4	-6.5	-8.5
777	GRISEOFULVIN	BRD-K08273968-001-09-1	22.9	0.8	4.3	32.9	11.8	2.8
778	BUTYL PARABEN	BRD-K08287586-001-08-5	-11.6	-8.1	-28.8	-37.3	-18.7	-12.1
779	CHLORPYRIFOS	BRD-K08303368-001-06-8	-3.6	-12.7	-13.3	7.9	-2.0	8.3

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
780	ROTENONE	BRD-K08316444-001-05-0	16.7	39.5	14.5	30.0	8.8	-10.2
781	XYLOMETAZOLINE HYDROCHLORIDE	BRD-K08356259-003-15-5	6.5	1.8	-22.3	-5.4	14.7	5.6
782	NNC 26-9100	BRD-K08438429-001-01-0	-88.7	-83.5	-111.0	-111.8	-88.2	-88.3
783	SARAFLOXACIN HYDROCHLORIDE	BRD-K08525451-003-03-7	4.7	1.5	4.5	-3.4	1.3	-0.6
784	RS 100329 hydrochloride	BRD-K08640512-003-01-5	15.3	-7.9	10.9	14.0	12.2	19.3
785	HETEROPEUCENIN, METHYL ETHER	BRD-K08745849-001-03-6	35.2	71.9	28.3	62.1	29.5	22.7
786	NARINGENIN	BRD-K08832567-001-06-5	22.8	7.6	-19.3	1.7	-11.1	-5.6
787	Co 102862	BRD-K08890269-001-01-5	36.9	12.9	25.5	42.1	24.9	26.3
788	Zolantidine dimaleate	BRD-K08996725-313-01-7	-28.2	-24.8	-39.4	-24.9	-31.0	-41.1
789	Fananserin	BRD-K08998509-001-01-6	80.5	50.6	59.7	84.1	60.2	69.1
790	PIPEMIDIC ACID	BRD-K08999871-001-13-9	16.6	5.7	19.2	11.0	13.9	12.7
791	D 4476	BRD-K09132007-001-01-8	-5.8	10.2	14.9	18.8	-14.3	-9.1
792	4'-METHOXYCHALCONE	BRD-K09233738-001-04-4	-33.8	-32.5	-88.1	-54.2	-21.9	-20.1
793	SR 57227 hydrochloride	BRD-K09397065-003-03-8	-1.4	10.7	-5.3	3.2	16.8	18.3
794	LOVASTATIN	BRD-K09416995-001-21-7	-5.8	-0.3	-45.7	-28.3	-25.7	-11.9
795	NU7026	BRD-K09537769-001-02-4	-3.2	-10.2	15.7	12.4	-4.1	1.9
796	Mibefradil dihydrochloride	BRD-K09549677-300-01-8	-52.0	-50.0	-89.2	-89.3	-67.2	-73.8
797	THIOTEPA	BRD-K09631521-001-05-7	-2.6	-3.9	-7.7	20.4	10.9	12.9
798	DEFEROXAMINE MESYLATE	BRD-K09821361-066-15-9	35.0	17.1	44.5	56.4	-6.3	-9.6
799	N-Desmethylclozapine	BRD-K10042277-001-04-3	-26.9	-29.1	-72.6	-72.0	-45.9	-50.8
800	DANTHRON	BRD-K10065684-001-06-6	30.3	9.4	19.7	9.0	19.0	9.1
801	L-701,252	BRD-K10176267-001-02-5	6.4	-16.4	-8.1	4.4	-3.2	8.7
802	PSB 11	BRD-K10177585-003-01-6	-20.3	26.3	-2.1	-19.4	-15.1	6.5
803	MECLOFENOXATE HYDROCHLORIDE	BRD-K10314788-003-07-7	4.7	-4.3	-23.6	1.9	-7.9	-5.5
804	SULFASALAZINE	BRD-K10670311-001-08-0	-8.2	-11.0	-55.4	-12.5	8.2	4.4
805	SULFAPHENAZOLE	BRD-K10671814-001-09-8	-13.4	-3.4	-32.9	6.3	-8.8	1.3
806	S-Isopropylisothiourea hydrobromide	BRD-K10673031-004-01-2	-7.8	-16.4	-17.2	-23.7	1.3	5.2
807	PHENYLBUTAZONE	BRD-K10843433-001-12-8	3.4	3.4	-17.9	-6.1	23.0	19.3
808	DILOXANIDE FUROATE	BRD-K10974103-001-14-6	-10.2	-22.4	-25.6	-21.8	0.9	9.0
809	PERPHENAZINE	BRD-K10995081-001-15-4	-88.0	-89.7	-103.3	-102.4	-72.8	-75.5
810	ACETANILIDE	BRD-K11094367-001-04-4	-14.2	1.2	-24.2	1.8	31.9	17.2
811	Tiotidine	BRD-K11107424-001-01-1	3.0	19.6	24.6	32.8	12.4	28.6
812	GEMFIBROZIL	BRD-K11129031-001-15-0	-11.4	4.1	10.6	-7.2	-2.2	-0.3
813	TYRPHOSTIN B44 (-)	BRD-K11158509-001-02-0	-5.6	-0.3	24.1	21.8	19.3	19.6
814	NORFLOXACIN	BRD-K11196887-001-15-4	3.5	-14.4	57.3	42.7	-0.5	10.2
815	AMBROXOL HYDROCHLORIDE	BRD-K11223672-003-04-5	-24.5	-19.8	-22.7	9.4	2.6	2.3
816	RUTILANTINONE	BRD-K11258719-001-03-2	309.9	341.8	23.8	22.8	-26.1	-35.8
817	ZD 7155 hydrochloride	BRD-K11373525-003-01-3	8.9	16.2	14.2	26.0	19.4	19.6
818	GBR 13069 dihydrochloride	BRD-K11634954-300-01-8	19.7	21.1	-32.5	-21.1	-3.2	-10.4
819	BU 239 hydrochloride	BRD-K11696279-003-01-5	-2.2	-2.0	13.2	17.7	11.3	12.9
820	BENZBROMARONE	BRD-K11717138-001-16-2	-69.6	-65.0	-95.4	-88.7	-75.1	-77.8
821	TRIPROLIDINE HYDROCHLORIDE	BRD-K11742128-003-15-0	-18.8	-19.1	1.2	-1.1	10.6	5.9
822	FURAZOLIDONE	BRD-K11756522-001-04-0	42.4	54.3	56.4	30.7	17.2	-0.3
823	NBQX	BRD-K11796549-001-02-9	4.9	13.7	14.8	21.4	-2.3	3.9
824	GR 127935 hydrochloride	BRD-K11911061-003-02-8	-73.0	-73.7	-58.4	-96.6	-89.7	-91.5
825	ER 27319 maleate	BRD-K11927976-050-01-1	-6.2	6.8	-12.2	-16.1	-8.2	-3.9

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			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
826	alpha-MANGOSTIN	BRD-K11991978-001-03-4	-9.9	-26.2	-63.7	-83.0	-23.2	-35.5
827	PD 160170	BRD-K12079898-001-01-8	8.2	11.1	2.8	-2.9	11.7	1.8
828	NIALAMIDE	BRD-K12102668-001-14-9	36.3	33.5	42.5	14.8	21.5	13.8
829	GR 144053 trihydrochloride	BRD-K12120659-305-01-4	-5.9	-5.8	-12.7	7.4	-3.4	6.6
830	Flunarizine dihydrochloride	BRD-K12184470-300-01-8	-9.2	-4.6	1.8	13.4	-5.6	25.4
831	METHYL ORSELLINATE	BRD-K12202814-001-05-8	20.4	16.7	20.2	15.5	-8.0	5.9
832	GLIPIZIDE	BRD-K12219985-001-15-4	-14.6	-15.9	-6.0	-2.5	8.9	13.4
833	XANTHOXYLIN	BRD-K12260308-001-04-2	-7.1	7.4	-9.4	0.6	9.5	17.0
834	JUAREZIC ACID	BRD-K12345912-001-03-1	14.1	-11.3	-18.5	7.0	14.4	12.1
835	AG 490	BRD-K12357156-001-01-5	7.6	19.8	-23.6	-28.7	-41.1	-46.1
836	FENBUFEN	BRD-K12513978-001-16-7	1.4	-5.5	-17.7	-16.6	-3.8	16.8
837	Zaprinast	BRD-K12516989-001-01-9	22.6	44.8	26.7	9.2	29.1	20.5
838	NOCODAZOLE	BRD-K12539581-001-14-6	9.4	12.9	40.0	60.9	0.1	8.1
839	EXALAMIDE	BRD-K12609457-001-02-3	7.8	14.2	-35.2	-36.4	-7.7	-36.9
840	KAEMPFEROL	BRD-K12807006-001-10-2	43.3	63.0	-22.4	-7.7	-16.7	-25.9
841	MECHLORETHAMINE	BRD-K12829205-001-03-0	-32.1	-18.3	-18.5	0.4	-0.3	4.5
842	YM 976	BRD-K12932420-001-01-5	23.6	13.7	10.4	12.6	33.9	22.0
843	BERGAPTEN	BRD-K12968785-001-06-7	0.2	4.4	31.6	24.0	26.4	28.7
844	GYROMITRIN	BRD-K13037776-001-01-2	7.0	-15.6	-1.9	-6.1	0.8	9.5
845	CICLOPIROX OLAMINE	BRD-K13044802-213-09-0	95.0	100.6	25.9	38.8	7.6	3.6
846	HYDROCHLOROTHIAZIDE	BRD-K13078532-001-17-7	-24.3	0.2	12.0	-7.0	12.2	17.2
847	Artemisinin	BRD-K13112821-001-08-3	-1.8	-11.9	-9.7	-6.7	9.9	-1.6
848	ppn-schn-2	BRD-K13169950-001-07-8	28.4	37.9	25.3	25.5	1.3	28.5
849	PENTAMIDINE ISETHIONATE	BRD-K13183738-317-06-0	7.0	-16.9	11.9	0.3	6.8	9.1
850	L-741,742 hydrochloride	BRD-K13211965-003-01-0	-7.9	-6.1	-54.7	-53.4	-25.9	-36.6
851	CARSALAM	BRD-K13238618-001-01-8	-6.5	-5.6	-18.2	22.1	4.6	18.3
852	LY-163,502	BRD-K13261168-001-01-4	-3.5	-10.7	10.4	5.5	14.1	0.4
853	beta-PELTATIN	BRD-K13265046-001-02-1	35.8	36.0	57.8	33.7	7.7	-2.0
854	METHAZOLAMIDE	BRD-K13356952-001-15-2	-33.2	-8.6	-34.1	5.2	5.9	7.3
855	DESOXYPEGANINE HYDROCHLORIDE	BRD-K13819402-003-06-0	-6.1	2.4	-4.0	22.2	6.5	13.8
856	VARDENAFIL HYDROCHLORIDE	BRD-K13926615-003-02-5	-8.8	-15.3	-5.5	1.8	5.3	17.4
857	DEXPROPRANOLOL HYDROCHLORIDE	BRD-K13994703-003-10-9	6.2	18.2	-13.0	27.1	15.2	5.0
858	SULFAMONOMETHOXINE	BRD-K14116214-001-07-0	8.5	2.3	-27.4	25.2	33.7	17.4
859	ISOPROPAMIDE IODIDE	BRD-K14127446-005-15-1	-34.5	12.9	-9.3	-8.6	15.0	15.7
860	AG 556	BRD-K14441456-001-01-2	11.4	7.1	-50.5	-52.1	-52.0	-50.9
861	VERATRIC ACID	BRD-K14520048-001-04-2	-3.4	-13.9	22.1	25.8	9.9	18.6
862	IKK 16	BRD-K14618467-003-01-8	-59.1	-67.3	-78.2	-77.6	-57.4	-62.0
863	CINCHONINE	BRD-K14693417-001-03-2	-7.0	-2.1	-6.5	-0.5	11.7	3.6
864	CINOXACIN	BRD-K14704277-001-15-0	7.5	36.0	-8.7	14.7	11.2	-0.5
865	SULFATHIAZOLE	BRD-K14705039-001-08-1	-1.6	7.1	-43.9	-2.3	12.6	-15.4
866	SPIRAMYCIN	BRD-K14716343-001-03-0	18.7	9.0	6.8	13.5	13.7	21.2
867	SC 560	BRD-K14767410-001-01-5	19.4	9.8	-17.8	-3.9	8.7	7.5
868	Berberine	BRD-K14796088-003-17-7	65.8	54.0	-12.0	-6.6	4.3	1.0
869	SB 221284	BRD-K14807180-001-01-7	-3.4	-6.2	14.2	13.1	9.0	9.8
870	FCCP	BRD-K14821540-001-03-9	-22.2	6.6	-33.5	-29.6	-36.6	-41.8
871	METHYL-6,7-DIMETHOXY-4-ETHYL-beta-CARBOLINE-3-CARBOXYLATE	BRD-K14844937-001-01-6	-15.8	-14.2	-11.4	-8.2	-55.7	-48.9

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
872	ERYTHROSINE SODIUM	BRD-K14920963-304-01-9	345.1	318.1	-3.3	-9.8	-5.0	-33.0
873	JNJ 10191584 maleate	BRD-K15086322-103-01-0	-10.4	-8.3	2.7	21.4	7.1	21.5
874	Apoptosis Activator 2	BRD-K15164005-001-02-3	-30.3	-6.1	-27.2	-38.7	-33.1	-23.8
875	5-HYDROXY-2',4',7,8-TETRAMETHOXYFLAVONE	BRD-K15179660-001-01-9	4.1	24.5	-35.0	-1.6	-32.6	-28.4
876	IBC 293	BRD-K15196155-001-01-5	35.2	34.8	5.3	-13.0	9.9	2.3
877	MUPIROCIN	BRD-K15262564-001-06-9	18.5	12.7	13.7	27.5	19.2	15.2
878	PENFLURIDOL	BRD-K15409150-001-01-7	-37.7	-30.9	-63.5	-62.7	-49.4	-51.0
879	1-[1-(2-BENZO[b]THIENYL)CYCLOHEXYL)]PIPERIDINE	BRD-K15519488-001-01-6	-12.7	-4.7	-6.8	-24.3	-8.4	-26.2
880	Cinanserin hydrochloride	BRD-K15522385-003-01-0	7.3	17.1	-17.0	-10.5	11.9	8.0
881	PHLORETIN	BRD-K15563106-001-10-7	-22.7	-11.1	-19.3	-29.0	5.9	5.0
882	PAPAVERINE HYDROCHLORIDE	BRD-K15567136-003-18-1	25.4	14.1	-12.5	-14.2	17.7	6.0
883	R-96544 hydrochloride	BRD-K15588452-003-01-9	-37.4	-45.9	-92.1	-94.4	-60.1	-64.4
884	SEW 2871	BRD-K15601958-001-01-3	17.9	39.3	4.9	12.1	5.7	11.0
885	CCCP	BRD-K15616905-001-01-5	-3.3	-10.2	28.0	32.6	6.9	-2.3
886	FLUPERLAPINE	BRD-K15715913-001-01-5	-37.9	-21.4	-33.1	-37.9	-21.2	-32.9
887	L-733,060 hydrochloride	BRD-K15791587-003-01-7	-25.5	-20.6	-69.1	-71.2	-18.2	-26.4
888	LOBENDAZOLE	BRD-K15834839-001-01-5	2.7	1.8	3.5	12.3	8.3	4.1
889	SDZ 205-557 hydrochloride	BRD-K15868788-003-02-8	-4.6	3.1	23.8	13.0	13.7	7.4
890	CLOTRIMAZOLE	BRD-K15916496-001-14-7	-46.2	-51.5	-92.6	-96.8	-48.9	-33.8
891	ANTHRAQUINONE	BRD-K15957397-001-03-4	-6.6	-2.7	-0.5	-8.2	8.6	9.8
892	OXYMETAZOLINE HYDROCHLORIDE	BRD-K16195444-003-16-1	-13.6	6.0	23.1	34.3	-15.7	-10.1
893	Ibudilast	BRD-K16444452-001-03-4	-0.6	-0.6	23.0	16.0	28.3	25.8
894	METACETAMOL	BRD-K16474819-001-05-4	-3.8	1.2	13.7	19.9	-2.3	10.1
895	MGCD-0103	BRD-K16485616-001-04-8	10.3	9.8	-22.1	17.4	-4.7	3.2
896	GALANGIN	BRD-K16503581-001-04-9	34.1	44.6	-26.9	-21.4	-37.3	-37.3
897	PNU 22394 hydrochloride	BRD-K16551401-003-02-6	-11.8	-12.9	-0.5	4.6	-9.6	-5.3
898		BRD-K16598630-001-05-7	30.6	20.2	17.2	11.3	17.9	7.4
899	TRIMETHADIONE	BRD-K16606819-001-07-7	6.5	0.3	-7.4	8.7	20.2	14.5
900	GTP 14564	BRD-K16664969-001-02-5	-13.1	3.6	-41.3	-27.9	-4.8	4.1
901	(R)-(+)-Bay K 8644	BRD-K16695519-001-01-6	27.6	51.5	4.6	9.5	20.2	22.7
902	CHLOROXINE	BRD-K17075857-001-06-9	41.0	31.7	4.3	12.2	-24.9	-23.1
903	CHLOROXYLENOL	BRD-K17223896-001-06-8	14.5	25.5	24.7	24.3	-4.1	3.1
904	5,7-DIHYDROXY-4-METHYLCOUMARIN	BRD-K17275330-001-03-9	1.4	67.2	116.3	102.3	-3.3	-14.1
905	Tyrphostin B44, (+) enantiomer	BRD-K17415526-001-02-7	-3.4	-12.8	-44.8	-47.8	-41.4	-43.0
906	Butein	BRD-K17497770-001-01-0	-21.6	-11.5	-15.4	-12.9	-35.4	-37.0
907	Alsterpaullone	BRD-K17516382-001-02-5	-0.6	-9.5	-23.0	-2.9	6.4	13.6
908	AMIODARONE HYDROCHLORIDE	BRD-K17561142-003-16-8	-73.1	-81.9	-95.3	-93.3	-69.2	-66.3
909	PRIDINOL METHANESULFONATE	BRD-K17565903-066-15-7	5.1	-15.7	5.6	-1.1	8.1	9.8
910	DECOQUINATE	BRD-K17641316-001-01-4	5.4	23.1	10.6	31.5	21.2	13.7
911	N-[2-(Acetoxy)ethyl]-3-pyridinecarboxamide	BRD-K17693482-001-03-9	10.8	-9.1	4.8	32.6	17.5	18.2
912	DEMETHYLNOBILETIN	BRD-K17726681-001-01-0	-15.2	-24.1	-79.1	-64.3	-53.2	-53.4
913	KB-R7943 mesylate	BRD-K17743697-066-02-8	-20.6	-11.4	-74.5	-76.5	-41.7	-42.8
914	JWH 015	BRD-K17796732-001-02-0	26.7	33.7	9.1	6.9	23.3	18.9
915	Tranilast	BRD-K17849083-001-03-0	-14.5	-5.2	0.7	-7.9	26.6	31.6
916	(?)-Cloprostenol sodium salt	BRD-K17850764-236-03-6	-5.9	11.7	17.7	13.6	30.4	38.6
917	BRL 54443	BRD-K17868609-001-02-7	31.4	28.9	2.8	12.6	-18.6	-21.2

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
918	2-Pyridylethylamine dihydrochloride	BRD-K17874705-300-02-4	0.8	-7.4	15.9	22.4	16.1	13.7
919	OXELAIDIN CITRATE	BRD-K17977438-048-01-6	7.4	2.9	0.4	-7.5	9.0	6.4
920	ETHOXZOLAMIDE	BRD-K18131774-001-10-1	6.5	11.2	-27.7	4.5	-1.7	-11.6
921	MEPHENTERMINE SULFATE	BRD-K18194590-065-05-6	5.8	4.4	-3.6	-4.5	-3.4	6.3
922	O-1918	BRD-K18316707-001-01-9	11.4	-4.0	15.8	1.4	17.1	27.2
923	BERGENIN	BRD-K18550767-002-01-8	-10.3	5.9	-26.9	13.8	0.2	1.7
924	Cimetidine	BRD-K18618618-001-01-6	20.6	1.0	-2.5	19.8	8.6	20.1
925	FOLIC ACID	BRD-K18673820-001-07-2	-2.0	16.7	27.6	80.0	22.7	18.1
926	Bifemelane hydrochloride	BRD-K18779551-003-03-7	-21.1	-14.1	-53.7	-55.9	-25.8	-28.3
927	BAY 59-3074	BRD-K18799075-001-01-0	-17.1	-6.9	-4.0	-18.8	-18.1	-6.1
928	L-694,247	BRD-K18816859-001-01-4	0.1	0.7	3.4	20.6	17.3	18.0
929	NEOSTIGMINE BROMIDE	BRD-K18922609-004-14-0	-4.4	-12.3	28.5	17.2	-4.8	15.4
930	CLOFIBRIC ACID	BRD-K19111024-001-10-0	3.6	-3.6	-45.2	-17.2	-6.1	4.4
931	PHENOLPHTHALEIN	BRD-K19227686-001-12-9	-19.4	-2.8	-76.6	-78.1	-34.1	-40.0
932	SALVINORIN A	BRD-K19284129-001-01-8	6.3	4.8	11.7	36.0	17.9	20.3
933	GOSSYPOL	BRD-K19295594-001-10-1	1.0	30.6	-96.9	-92.4	-75.4	-77.9
934	CNQX	BRD-K19438463-001-02-2	-16.6	7.1	15.0	8.6	11.3	7.4
935	BUFLOMEDIL HYDROCHLORIDE	BRD-K19462402-003-13-9	24.0	4.0	9.5	12.1	12.1	11.1
936	Ozagrel hydrochloride	BRD-K19525698-003-01-1	24.2	28.2	-1.2	29.6	24.2	22.5
937	ZM 241385	BRD-K19605405-001-01-9	-47.9	-40.1	-59.4	-56.9	-50.4	-49.1
938	PECTOLINARIN	BRD-K20043699-001-03-1	40.6	35.7	-13.8	8.6	-27.8	-31.5
939	Impentamine dihydrobromide	BRD-K20049318-303-01-3	-5.6	10.0	24.6	22.3	27.1	16.1
940	Tomoxetine hydrochloride	BRD-K20141153-003-03-8	-10.0	-20.5	-15.3	-14.3	-8.1	0.8
941	CEAROIN	BRD-K20420220-001-03-9	51.2	60.6	5.6	52.9	-33.3	-48.0
942	BENZOYLPAS	BRD-K20431737-001-04-0	-13.5	4.6	-28.0	5.7	-13.1	-3.8
943	cjd-pdi-3	BRD-K20482099-341-01-1	25.9	20.7	-12.5	-6.0	-32.7	-30.3
944	2-METHOXYRESORCINOL	BRD-K20559594-001-03-2	24.6	45.4	14.6	28.9	-6.3	-4.0
945	MEFEXAMIDE	BRD-K20655524-003-07-0	-10.8	3.4	-21.5	-3.6	11.1	21.8
946	RS 56812 hydrochloride	BRD-K20714604-003-01-1	4.6	-7.9	6.0	10.0	25.8	32.4
947	RS 39604 hydrochloride	BRD-K20742498-003-01-1	-87.2	-89.0	-124.8	-122.7	-72.5	-75.8
948	CROMOLYN SODIUM	BRD-K20920669-304-06-7	-25.7	7.1	-4.0	-1.6	-2.3	-3.3
949	beta-NAPHTHOL	BRD-K21164796-001-01-0	9.6	-8.6	-48.8	-33.8	-72.3	-76.1
950	Riluzole hydrochloride	BRD-K21283037-003-06-2	-14.1	-9.4	-52.2	21.1	-51.9	13.1
951	BENZTHIAZIDE	BRD-K21450440-001-08-8	-12.8	0.8	-10.7	0.7	17.5	14.7
952	SULFACETAMIDE	BRD-K21520694-001-12-3	2.3	12.9	11.9	32.8	29.3	20.8
953	XYLAZINE	BRD-K21565985-001-15-9	-0.8	9.3	24.5	31.5	15.2	30.5
954	MITOXANTRONE HYDROCHLORIDE	BRD-K21680192-300-09-4	-110.6	-105.6	-104.1	-103.9	-84.0	-82.2
955	ROFECOXIB	BRD-K21733600-001-06-7	2.2	0.0	-11.0	-2.7	8.7	4.8
956	2,4-DINITROPHENOL	BRD-K21910317-001-06-5	-6.6	1.1	-6.2	-3.8	-11.5	6.3
957	FLUORESCEIN	BRD-K21913543-001-01-6	298.5	333.8	-50.7	-17.0	9.7	1.3
958	DIFLUNISAL	BRD-K22031190-001-13-7	-7.9	1.2	-26.9	-24.4	0.5	-6.9
959	1-(2-hydroxy-4-morpholin-4-yl-phenyl)ethanone	BRD-K22160761-001-01-8	0.2	-17.9	18.7	19.3	35.3	29.8
960	DIOXYBENZONE	BRD-K22193694-001-08-6	5.3	16.0	-34.3	-19.7	4.0	1.7
961	LY 303511	BRD-K22385716-001-01-7	-6.0	-2.7	17.5	17.2	23.3	16.7
962	RETINOL	BRD-K22429181-001-06-8	16.5	11.8	-1.4	-0.7	5.3	3.4
963	IRIDIN	BRD-K22550622-001-03-5	27.2	16.8	0.7	31.2	4.1	-5.2

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
964	HIERACIN	BRD-K22585547-001-03-3	83.6	128.3	-18.0	-8.0	-38.1	-56.9
965	2-BFI hydrochloride	BRD-K22745370-003-01-5	-4.0	-11.3	18.7	9.0	11.0	3.9
966	CHRYSIN	BRD-K22861715-001-12-5	23.1	4.9	-14.3	-15.0	-21.9	-18.0
967	DIPHENYLPYRALINE HYDROCHLORIDE	BRD-K22936972-003-15-2	-14.7	24.4	0.6	4.7	1.6	-9.5
968	CHLORAMPHENICOL	BRD-K22969690-001-03-4	-2.7	3.0	-35.9	-19.5	9.4	2.0
969	RHOIFOLIN	BRD-K23327891-001-03-1	9.6	3.6	20.6	-1.2	20.8	15.2
970	AMN 082 dihydrochloride	BRD-K23335153-300-01-7	-2.2	24.3	51.8	61.9	44.5	48.7
971	T 0901317	BRD-K23383398-001-01-6	-7.8	2.1	-21.2	-16.1	-0.1	-2.5
972	SL 327	BRD-K23432132-001-01-2	-15.2	-7.7	31.1	-1.4	1.8	21.0
973	Dimaprit 2HCl	BRD-K23541596-300-05-6	0.1	-5.8	5.5	-1.0	4.8	8.7
974	NILUTAMIDE	BRD-K23566484-001-09-4	-17.2	-5.5	-35.9	6.9	-5.9	-10.8
975	DFB	BRD-K23623876-001-01-6	5.1	5.8	15.0	9.1	15.5	25.7
976	3,4'-DIMETHOXYFLAVONE	BRD-K23644387-001-01-4	13.0	11.2	13.3	33.6	12.6	16.0
977	3,4-Dichloroisocoumarin	BRD-K23704908-001-02-4	-12.9	11.5	-0.9	4.4	23.8	14.0
978	COUMARIN	BRD-K23913458-001-13-2	7.9	6.1	14.4	9.7	17.6	21.6
979	Arecaidine propargyl ester tosylate	BRD-K23922020-075-01-1	-32.2	-15.6	-1.9	-8.1	0.4	10.4
980	DEXTROMETHORPHAN HYDROBROMIDE	BRD-K24053527-004-03-8	-7.9	-5.8	-1.6	-4.5	-1.0	-7.0
981	PARAXANTHINE	BRD-K24084088-001-06-3	7.2	-1.6	-13.9	-12.5	-10.8	-2.8
982	SB 269970 hydrochloride	BRD-K24201553-003-02-4	1.4	-11.5	16.9	-2.2	3.0	4.3
983	GYKI 52466 hydrochloride	BRD-K24240364-003-02-1	15.2	0.5	-12.4	-10.8	-0.3	15.7
984	HELICIN	BRD-K24265569-001-01-7	7.3	2.9	-21.9	0.7	8.2	-1.3
985	Levcromakalim	BRD-K24526313-001-08-6	5.8	-19.4	3.7	0.9	5.6	5.5
986	PROCAINE HYDROCHLORIDE	BRD-K24616672-003-10-2	-7.1	-1.8	1.2	30.3	15.3	-7.0
987	ACTINONIN	BRD-K24621118-001-03-3	12.3	0.3	-40.4	-12.6	-8.9	-12.1
988	LY 288513	BRD-K24675965-001-02-5	32.4	31.1	21.3	22.6	-29.3	-19.3
989	3-Bromo-7-nitroindazole	BRD-K24689407-001-05-5	-15.7	-0.8	-1.8	13.3	8.5	1.1
990	ETHACRIDINE LACTATE	BRD-K24715592-043-01-4	45.2	27.8	38.4	30.1	-9.4	-6.3
991	EPIAFZELECHIN TRIMETHYL ETHER	BRD-K25064302-001-03-1	16.9	5.2	-33.8	-20.1	-11.8	-7.2
992	1-BCP	BRD-K25140590-001-02-2	-8.6	-8.7	81.3	104.5	13.4	17.8
993	TANGERITIN	BRD-K25186396-001-04-7	16.8	-4.4	29.9	34.1	-8.3	-10.8
994	PIRENPERONE	BRD-K25224017-001-15-1	1.9	-0.3	-11.8	6.7	3.0	10.8
995	OXAPROZIN	BRD-K25394294-001-08-1	4.1	0.5	-10.5	-18.3	4.0	9.8
996	MAPROTILINE HYDROCHLORIDE	BRD-K25433859-003-14-8	-1.3	-14.8	-63.7	-63.3	-30.3	-24.7
997	2-Iodomelatonin	BRD-K25649279-001-01-2	-14.2	-8.7	8.5	-7.7	4.4	1.6
998	PHYSOSTIGMINE SALICYLATE	BRD-K25650355-059-12-2	7.1	9.5	11.1	2.2	9.0	14.5
999	METHYL ROBUSTONE	BRD-K25811799-001-03-5	-23.5	-46.3	-47.5	-36.9	6.1	4.9
1000	SC-9	BRD-K25875056-001-01-2	2.0	-19.7	24.0	8.9	-9.8	-5.5
1001	Immepip dihydrobromide	BRD-K25906698-303-01-9	17.1	3.3	8.9	9.5	19.4	18.3
1002	GRAMINE	BRD-K26005076-001-06-0	-57.3	5.1	-32.9	9.7	13.7	12.9
1003	RS 45041-190 hydrochloride	BRD-K26160755-003-01-8	-0.8	13.9	-11.4	18.5	-1.4	-2.5
1004	SC-514	BRD-K26373640-001-02-8	23.9	39.2	22.7	12.8	22.2	18.4
1005	EUPARIN	BRD-K26383086-001-03-6	29.8	-2.6	-37.3	-11.5	-16.3	-19.1
1006	J 104129 fumarate	BRD-K26429091-051-01-9	11.2	3.3	5.4	0.5	18.0	20.1
1007	DMAB-anabaseine dihydrochloride	BRD-K26573499-300-01-3	1.0	-6.8	18.6	6.7	11.5	11.8
1008		BRD-K26657438-001-01-2	-4.8	9.9	22.4	22.1	23.4	34.9
1009	PIPAMPERONE	BRD-K26801045-001-01-1	-2.5	2.8	25.6	22.6	15.4	19.5

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1010	AKLOMIDE	BRD-K26807903-001-03-5	12.7	3.3	-9.8	-8.3	-5.3	-1.7
1011	PROTOPORPHYRIN IX	BRD-K26813314-001-04-4	1.1	7.4	-26.7	3.6	13.0	27.6
1012	Costunolide	BRD-K26833429-001-01-0	-11.2	-20.9	-50.9	-8.6	-15.4	-13.6
1013	3-HYDROXYPHENETHYLAMINE	BRD-K26842203-001-01-3	1.6	-5.4	10.6	-6.3	-2.2	0.3
1014	DIOSMETIN	BRD-K26862302-001-03-7	10.8	6.8	-14.7	-28.8	-35.4	-38.3
1015	3-ACETYLCOUMARIN	BRD-K26954192-001-06-8	3.0	3.8	-15.3	-15.4	3.8	-2.1
1016	SB 203186 hydrochloride	BRD-K27141178-003-02-4	-5.5	-2.1	-4.0	19.1	12.7	8.2
1017	SR 11302	BRD-K27216882-001-01-7	-4.8	-5.6	-51.2	-21.5	-16.2	-21.8
1018	BUTAMBEN	BRD-K27217864-001-15-7	2.9	5.2	1.1	24.9	-0.6	6.8
1019	H 89 dihydrochloride	BRD-K27737647-300-01-4	-35.2	-47.5	-87.3	-88.4	-75.7	-83.7
1020	(-)-[3R,4S]-Chromanol 293B	BRD-K27911943-001-01-0	-0.4	-2.5	22.2	32.8	31.0	23.2
1021	XANTHYLETIN	BRD-K28108221-001-07-2	35.2	8.2	74.8	80.2	0.2	4.5
1022	WEB 2086	BRD-K28115081-001-01-9	3.0	-6.4	-8.0	2.4	2.6	1.0
1023	Loreclezole hydrochloride	BRD-K28137194-003-01-3	-4.0	11.9	-22.4	-19.8	2.7	2.8
1024	CYPROHEPTADINE HYDROCHLORIDE	BRD-K28143534-003-14-3	-24.0	-14.6	-80.0	-78.9	-50.2	-57.6
1025	CHLOROGUANIDE HYDROCHLORIDE	BRD-K28183345-003-07-2	8.1	-12.3	-4.0	-0.5	6.1	14.7
1026	Demethylasterriquinone B1	BRD-K28452984-001-01-4	-59.9	-67.5	-105.7	-103.1	-88.1	-85.7
1027	Nitrocaramiphen hydrochloride	BRD-K28453807-003-05-4	-15.2	-6.2	-0.9	-0.6	8.7	12.6
1028	SULFAMETHOXAZOLE	BRD-K28494619-001-15-9	-2.9	1.8	21.7	33.5	9.0	13.5
1029	BENZYDAMINE HYDROCHLORIDE	BRD-K28542495-003-07-7	-21.0	-13.4	-74.9	-66.7	-14.5	-28.9
1030	Cilostamide	BRD-K28578425-001-02-1	33.2	22.1	3.6	27.3	12.6	15.8
1031	METHYL-beta-CARBOLINE-3-CARBOXYLATE	BRD-K28680267-001-01-8	-4.0	-18.4	-16.1	-10.1	-12.3	-16.6
1032	ANTIAROL	BRD-K28698314-001-02-1	-3.7	3.1	-64.3	-10.5	-50.8	-43.7
1033	PNU 282987	BRD-K28863208-001-01-2	-3.9	2.1	10.9	17.7	18.6	19.1
1034	KETOTIFEN FUMARATE	BRD-K28936863-051-18-1	-30.9	-19.4	-39.3	-40.7	-5.2	-10.9
1035	DIPTERYXIN	BRD-K29004214-001-01-4	-2.6	-3.9	43.3	23.0	-39.0	-39.2
1036		BRD-K29113274-001-11-9	-29.4	-22.7	-71.8	-70.2	-46.3	-45.2
1037	7-[2-TRIFLUOROMETHYL-4-(2-HYDROXYPHENYL)-1,3-DIOXAN-cis-5-YL]-HEPT-5Z-ENOIC ACID	BRD-K29133151-001-02-4	-2.4	-4.0	-4.8	-1.1	10.9	18.2
1038	THIRAM	BRD-K29254801-001-06-3	-56.9	-59.9	18.5	17.7	-66.2	-69.6
1039		BRD-K29359156-001-23-6	-30.5	-19.5	-87.6	-93.1	-61.3	-59.9
1040	CHLORAMBUCIL	BRD-K29458283-001-17-4	27.5	26.6	10.8	18.0	-12.0	-12.6
1041	1-Naphthyl PP1	BRD-K29542628-001-01-3	-6.9	8.4	-28.7	-19.0	-1.1	-2.1
1042	SNC 80	BRD-K29546239-001-01-5	-1.5	-10.7	-4.9	-13.9	3.5	-5.4
1043	SCH 202676 hydrobromide	BRD-K29562203-004-02-6	24.3	-0.8	12.0	10.0	-3.2	-2.4
1044	FLUNARIZINE HYDROCHLORIDE	BRD-K29582677-300-06-4	6.4	13.3	9.0	24.8	4.5	-5.4
1045	BD 1063 dihydrochloride	BRD-K29668683-300-01-4	2.0	-6.3	-5.2	6.7	-0.2	0.8
1046	MEBHYDROLIN NAPHTHALENESULFONATE	BRD-K29713308-077-03-3	-1.5	-4.1	30.9	36.7	-18.2	-0.5
1047	CLOMIPHENE CITRATE	BRD-K29950728-048-08-3	-57.8	-57.3	3.5	0.8	-84.7	-88.6
1048	ALISKIREN HEMIFUMARATE	BRD-K30020243-051-01-7	-9.1	-11.8	13.7	1.9	18.2	22.3
1049	MEXAMINE	BRD-K30197592-003-02-9	0.1	-4.9	16.9	13.5	10.1	12.1
1050	1400W dihydrochloride	BRD-K30237152-300-01-7	-18.9	-20.9	14.3	4.6	21.4	24.6
1051	CLEMASTINE	BRD-K30240666-051-08-4	-22.9	-23.4	-2.4	3.3	-35.1	-39.2
1052	TIMOLOL MALEATE	BRD-K30421593-050-03-1	2.5	5.5	5.0	0.3	13.8	13.8
1053	ELLAGIC ACID	BRD-K30466858-001-05-4	58.8	100.1	-26.4	-3.8	3.5	-4.2
1054	HESPERETIN	BRD-K30553453-001-08-2	34.5	-0.5	46.3	62.5	8.6	6.0
1055	LEVOTHYROXINE	BRD-K30685142-001-08-9	57.1	43.7	10.3	23.7	0.0	-12.4

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1056	SB 216641 hydrochloride	BRD-K30867024-003-01-7	-46.0	-41.3	-96.0	-96.1	-74.6	-74.5
1057	AT-DYRK-01	BRD-K30984264-003-06-8	-2.0	-2.9	86.3	88.4	45.0	32.7
1058	FR 122047 hydrochloride	BRD-K30990140-003-01-6	-29.8	-26.1	-35.0	-35.4	-48.9	-56.3
1059	PURPUROGALLIN	BRD-K31023358-001-10-7	32.3	29.2	52.2	32.1	-7.1	-8.8
1060	BMY 7378 dihydrochloride	BRD-K31054881-300-01-3	5.1	0.3	-6.6	3.7	10.7	11.1
1061	Devazepide	BRD-K31238592-001-01-6	-6.1	-10.2	-39.3	-39.3	-4.6	-0.8
1062	Diacylglycerol Kinase Inhibitor II	BRD-K31273080-001-01-2	2.1	-13.5	-9.8	-20.6	12.7	7.7
1063	SDZ SER 082 fumarate	BRD-K31339597-051-01-2	9.3	7.4	12.0	21.1	9.1	11.1
1064	1-PHENYLBIGUANIDE HYDROCHLORIDE	BRD-K31491153-003-04-2	44.0	-15.8	28.5	18.7	20.1	28.9
1065	Mycophenolic acid	BRD-K31542390-001-01-5	47.1	34.0	21.2	15.6	12.2	14.8
1066	DAU 5884 hydrochloride	BRD-K31633810-003-01-0	4.1	16.5	6.6	20.0	21.1	35.8
1067	ISOBERGAPTENE	BRD-K31678817-001-06-1	-2.7	-5.7	3.9	2.9	6.6	12.2
1068	SULFAMETHIZOLE	BRD-K31682896-001-15-8	-3.4	-6.1	18.4	14.5	9.1	10.1
1069	DMeOB	BRD-K31699485-001-01-9	-3.9	-3.8	0.3	9.0	7.1	4.0
1070	T 0070907	BRD-K31843556-001-01-7	-1.2	1.9	-17.4	3.0	1.9	13.8
1071	CGP 71683 hydrochloride	BRD-K31912990-003-01-0	-51.9	-77.4	-81.2	-78.3	-70.0	-73.7
1072	Oleylethanolamide	BRD-K31987754-001-01-2	0.7	6.9	-12.7	-19.5	15.5	29.5
1073	SULFACHLORPYRIDAZINE	BRD-K32021043-001-09-3	21.1	17.6	51.2	46.7	29.8	31.4
1074	temozolomide	BRD-K32107296-001-04-5	10.9	8.7	6.4	30.4	18.4	25.4
1075	TOLAZAMIDE	BRD-K32164935-001-17-5	11.1	36.2	23.7	56.3	-1.6	-2.8
1076	PRIMIDONE	BRD-K32247306-001-17-9	5.8	-4.1	6.6	1.6	-4.6	-8.9
1077	CINNARAZINE	BRD-K32256916-001-03-2	-13.5	-5.0	22.1	19.5	-1.3	-1.8
1078	SULFADIAZINE	BRD-K32273377-001-09-6	-1.5	-0.5	10.4	13.5	4.3	0.0
1079	CGP 53353	BRD-K32292990-001-01-0	23.1	51.8	55.5	38.6	12.1	15.0
1080	R(-)-2,11-DIHYDROXY-10-METHOXYAPORPHINE	BRD-K32412559-001-01-7	55.8	57.5	23.8	9.6	-18.8	-18.7
1081	3,6-DIMETHOXYFLAVONE	BRD-K32480606-001-01-7	16.1	-6.7	8.9	30.4	3.2	-3.9
1082	GBR 12909 dihydrochloride	BRD-K32501161-300-04-7	-13.9	10.2	-30.7	-3.9	-25.9	-19.4
1083	DCEBIO	BRD-K32526544-001-01-2	-5.8	-8.8	-25.4	-22.6	-2.7	-4.2
1084	DIPROPYL-5CT	BRD-K32645441-001-01-4	-5.6	-9.5	25.9	17.7	-3.8	13.5
1085	2-Aminobenzenesulfonamide	BRD-K32681104-001-03-3	13.8	4.6	9.8	28.7	15.0	12.9
1086	tetraethylthiuram disulfide	BRD-K32744045-001-17-1	-34.9	-31.7	-39.1	-35.7	-32.0	-48.6
1087	AZATHIOPRINE	BRD-K32821942-001-10-6	-9.7	3.1	10.5	-0.6	22.6	18.5
1088	Guanfacine hydrochloride	BRD-K32830106-003-11-3	1.2	4.6	8.7	32.7	19.9	18.1
1089	EUGENOL	BRD-K32977963-001-03-5	3.3	-1.1	0.7	23.6	-25.9	-30.4
1090	SPHONDIN	BRD-K33260002-001-06-1	-19.6	-15.9	-2.7	17.0	32.0	32.7
1091	INCA-6	BRD-K33308633-001-01-6	1.2	-7.0	-108.6	-109.5	-85.6	-85.5
1092	CRYPTOTANSHINONE	BRD-K33336844-001-05-3	31.9	30.2	33.5	54.2	20.2	15.2
1093	A 68930	BRD-K33400588-003-01-2	2.8	-4.6	78.1	84.6	34.1	36.9
1094	meta-CRESYL ACETATE	BRD-K33442414-001-01-8	3.5	6.9	25.1	21.7	19.4	24.2
1095	DTG	BRD-K33459542-001-02-5	3.1	18.6	11.8	20.1	18.5	18.2
1096		BRD-K33583600-001-03-9	15.0	-6.4	4.9	1.7	-16.6	-17.1
1097	Lavendustin B	BRD-K33781562-001-02-7	-54.4	-36.8	-14.4	-13.4	7.2	1.8
1098	GW 3965 hydrochloride	BRD-K33818169-003-01-2	-60.2	-64.6	-92.1	-91.4	-86.4	-88.4
1099	LY 225910	BRD-K33864865-001-01-7	-3.0	-10.6	-5.5	-1.1	1.5	-2.5
1100	ZK 93423	BRD-K33882852-003-01-0	7.4	6.3	-11.0	-18.9	-10.6	-17.7
1101	NAPROXOL	BRD-K34014345-001-03-4	-1.7	-8.9	-19.2	7.5	-1.1	-11.9

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1102	GBR 12783 dihydrochloride	BRD-K34034388-300-01-0	-8.9	12.2	-24.0	-9.5	-1.9	-4.8
1103	Arvanil	BRD-K34092021-001-02-3	12.4	8.1	10.3	11.2	-23.7	-21.8
1104	DENATONIUM BENZOATE	BRD-K34122555-057-06-5	3.5	-3.1	9.6	23.1	20.6	19.2
1105	Tracazolate hydrochloride	BRD-K34154330-003-04-9	20.2	-6.7	-32.0	-4.5	14.2	1.9
1106	Fexaramine	BRD-K34170797-001-01-1	7.0	-10.5	0.9	8.3	1.4	12.1
1107	METHICILLIN SODIUM	BRD-K34388247-236-04-1	-22.9	18.6	23.4	14.3	10.5	6.0
1108	TRIMETHOBENZAMIDE HYDROCHLORIDE	BRD-K34415467-003-08-0	0.2	4.8	19.4	39.3	32.8	38.0
1109	AG 494	BRD-K34533029-001-01-0	25.5	5.2	-26.6	-36.4	-45.5	-41.6
1110	TILORONE	BRD-K34568562-001-03-5	-15.9	-21.7	1.1	-16.8	-19.9	-19.7
1111	GP 2a	BRD-K34608650-001-01-6	7.7	6.5	4.9	35.3	31.7	30.6
1112	6-Chloromelatonin	BRD-K34663752-001-02-6	-10.0	-8.4	10.5	7.4	-3.8	-1.6
1113	METHYLERGONOVINE MALEATE	BRD-K34685430-050-06-7	19.3	14.8	12.4	-5.7	3.2	-7.3
1114	THEOBROMINE	BRD-K34888156-001-08-8	2.1	1.1	18.7	3.0	5.1	9.8
1115	SU1498	BRD-K34995470-001-03-1	8.8	5.1	27.7	19.3	26.7	9.1
1116	3,7-DIHYDROXYFLAVONE	BRD-K35133923-001-03-1	48.5	-3.5	27.9	35.0	-4.7	4.2
1117		BRD-K35240538-001-11-4	21.9	-1.5	6.7	33.7	5.9	8.1
1118	SR 59230A hydrochloride	BRD-K35430135-003-01-5	-7.6	-3.8	-33.3	-33.1	-28.4	-27.0
1119	MCI-186	BRD-K35458079-001-12-5	17.5	14.2	20.3	22.1	-2.2	2.6
1120	BPIQ-II	BRD-K35473459-001-01-7	0.4	4.8	12.4	23.7	7.0	21.2
1121	ALRESTATIN	BRD-K35498378-001-05-3	-4.7	-2.1	-5.2	14.1	20.1	15.7
1122		BRD-K35520305-001-07-8	-2.6	0.7	0.4	1.0	11.1	14.9
1123	2,6-DIHYDROXY-4-METHOXYTOLUENE	BRD-K35568433-001-03-1	14.2	-11.2	21.4	10.4	-4.1	-5.2
1124	SR 27897	BRD-K35629949-001-01-2	1.5	2.2	-13.8	-9.8	0.9	7.8
1125	niclosamide	BRD-K35960502-001-11-9	2.7	6.7	8.5	20.0	-9.5	-11.3
1126	NNC 63-0532	BRD-K36009368-001-01-8	-3.9	-7.0	12.0	18.1	11.1	21.2
1127	ABT 702 dihydrochloride	BRD-K36021395-300-01-6	-35.5	-34.2	-62.5	-59.8	-28.8	-32.3
1128	PYRITHYLDIONE	BRD-K36116267-001-08-8	-10.5	-17.1	33.8	19.9	9.5	22.7
1129	PLUMBAGIN	BRD-K36137799-001-03-2	26.0	28.4	8.8	22.8	-47.4	-50.1
1130	WAY 170523	BRD-K36198571-001-01-2	3.6	-17.9	7.0	8.8	18.5	11.0
1131	AZ 10417808	BRD-K36258877-001-01-5	5.7	1.2	4.5	25.5	15.5	17.7
1132	SB 206553 hydrochloride	BRD-K36395411-003-01-4	-17.4	-16.7	13.3	17.2	16.1	25.6
1133	AZTREONAM	BRD-K36547807-001-02-4	0.0	-5.6	14.5	-1.2	-3.4	5.8
1134	Doxepin hydrochloride	BRD-K36616567-003-01-5	-8.1	-6.9	-35.8	-6.6	-3.4	1.4
1135	IPRIFLAVONE	BRD-K36646537-001-02-1	-2.1	-1.3	10.4	29.8	14.5	14.0
1136	BUFEXAMAC	BRD-K36660044-001-15-0	10.6	0.0	-12.3	-8.5	11.4	-0.4
1137	GUAIAZULENE	BRD-K36719159-001-04-9	2.6	-0.7	10.5	12.1	10.0	11.7
1138	ETHAVERINE HYDROCHLORIDE	BRD-K36756879-003-06-1	-15.6	-15.3	23.1	28.4	6.7	7.5
1139	5-alpha-PREGNANE-3-alpha-2,1-DIOL-20-ONE	BRD-K36764776-001-01-4	-6.6	-8.8	4.3	-2.8	-9.6	-8.2
1140	TRIM	BRD-K36851334-001-05-5	10.4	-3.2	-20.1	-12.1	-3.9	-13.6
1141	HYDROFLUMETHIAZIDE	BRD-K36862742-001-15-7	12.7	3.7	40.4	20.6	-5.9	10.5
1142	BD 1047 dihydrobromide	BRD-K36864847-303-01-7	-4.4	-11.8	-28.6	-24.9	-2.0	2.8
1143		BRD-K36927236-001-17-7	11.9	2.4	10.2	-0.3	11.8	21.6
1144	m-Chlorophenylbiguanide hydrochloride	BRD-K36965586-003-03-9	6.2	19.1	26.4	2.4	18.3	19.4
1145	S-ISOCORYDINE (+)	BRD-K37049577-001-08-5	1.7	2.6	6.8	15.5	-25.3	-27.0
1146	ASTEMIZOLE	BRD-K37249724-001-16-6	-32.1	-34.7	11.6	25.0	-51.0	-48.2
1147	CLOZAPINE	BRD-K37289225-001-23-2	12.5	12.1	-22.8	-11.0	-10.1	-8.6

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1148	Kenpaullone	BRD-K37312348-001-06-9	6.9	-0.4	-9.6	0.0	8.0	9.4
1149	NSC 632839 hydrochloride	BRD-K37392901-003-01-7	-37.2	-19.9	-41.5	-41.9	-19.8	-20.3
1150	IDEBENONE	BRD-K37516142-001-01-4	6.9	14.7	20.2	25.9	-26.0	-29.2
1151	Zardaverine	BRD-K37561857-001-06-4	41.1	16.4	28.8	34.1	25.5	24.9
1152	MRS 1220	BRD-K37618799-001-01-4	-8.1	-9.0	-3.7	1.3	-1.1	10.1
1153	PIROMIDIC ACID	BRD-K37682401-001-06-9	18.0	-4.1	6.8	20.8	10.6	16.7
1154	FIPEXIDE HYDROCHLORIDE	BRD-K37688416-003-08-1	-1.5	-1.3	31.4	39.7	-1.1	-3.0
1155	ABT 724 trihydrochloride	BRD-K37714784-305-01-3	8.0	-9.4	26.1	22.0	22.4	11.5
1156	Denbufylline	BRD-K37792168-001-01-0	2.4	-14.0	18.0	25.9	24.6	38.3
1157		BRD-K37798499-001-05-8	6.9	6.2	14.3	1.8	-2.2	-8.1
1158	ACEPROMAZINE MALEATE	BRD-K37814297-050-05-4	-20.0	-28.4	29.7	6.5	-3.7	-7.7
1159	3,3'-DIINDOLYLMETHANE	BRD-K37846922-001-06-0	32.2	26.8	19.8	12.6	-8.9	-15.5
1160	N-(4-BROMOBENZYL)-5-METHOXYTRYPTAMINE	BRD-K37883585-001-01-2	-8.3	-1.4	-6.9	-5.3	8.9	1.2
1161	CAMPTOTHECIN	BRD-K37890730-001-10-2	2.1	6.8	123.2	135.1	26.6	28.2
1162	Paroxetine maleate	BRD-K37991163-050-05-1	-15.4	-21.5	-47.1	-47.8	-38.3	-40.0
1163	ETHAMIVAN	BRD-K38055836-001-13-8	18.7	14.3	15.0	31.8	1.4	-2.1
1164	BUMETANIDE	BRD-K38197229-001-17-4	9.4	5.4	12.6	40.8	26.6	27.0
1165	Paxilline	BRD-K38251852-001-06-6	-18.4	-27.4	20.2	8.9	-18.3	-24.1
1166	DOMPERIDONE	BRD-K38305202-001-08-3	-15.6	-11.7	-11.9	-10.3	20.0	16.1
1167	PHENACETIN	BRD-K38323065-001-09-0	-2.9	18.6	-1.0	-6.1	0.5	-1.7
1168	8-CYCLOPENTYLTHEOPHYLLINE	BRD-K38347298-001-06-4	5.0	1.7	6.1	4.8	25.6	20.7
1169	3-(4-Allylpiperazin-1-yl)-2-quinoxalinecarbonitrile maleate	BRD-K38370968-103-01-0	-4.0	-7.0	-2.4	9.2	-9.0	0.2
1170	IMIPRAMINE HYDROCHLORIDE	BRD-K38436528-003-15-4	-10.1	2.9	-26.0	-8.8	-28.9	-32.3
1171	Bohemine	BRD-K38622899-001-01-4	-4.8	16.9	-10.6	-23.5	8.8	8.3
1172	ROXITHROMYCIN	BRD-K38684403-001-03-9	5.1	0.4	27.4	11.5	14.1	20.3
1173		BRD-K38775274-001-06-4	-6.9	-8.8	9.3	7.9	15.4	12.8
1174	CINCHONIDINE	BRD-K39079086-001-05-0	22.9	11.7	37.6	34.5	21.6	20.1
1175	BITHIONATE SODIUM	BRD-K39120595-304-03-9	-27.9	-25.5	-94.7	-94.5	-69.9	-66.4
1176	4-Chlorophenylguanidine hydrochloride	BRD-K39160765-003-01-1	10.3	20.1	-21.5	4.6	-22.0	3.4
1177	R(-)-2,10,11-TRIHYDROXYAPORPHINE	BRD-K39187410-001-01-7	48.5	48.5	-13.3	-24.1	-57.9	-60.0
1178	NITHIAMIDE	BRD-K39467894-001-01-8	1.7	2.8	37.4	25.9	23.8	25.7
1179	Amthamine dihydrobromide	BRD-K39670393-303-01-3	11.8	0.5	36.8	17.1	13.3	15.1
1180	L 161982	BRD-K39733634-001-01-8	-28.6	-33.6	-68.8	-53.5	-20.1	-28.9
1181	LOXAPINE SUCCINATE	BRD-K39915878-036-15-2	-5.4	3.1	-18.1	-25.0	-7.6	-14.5
1182	BISACODYL	BRD-K39987650-001-15-9	18.8	-10.0	38.2	36.0	28.4	16.8
1183	TYRPHOSTIN 9	BRD-K40255344-001-04-4	-10.7	-23.4	-29.0	-41.8	-25.0	-32.5
1184	GR 79236	BRD-K40578143-001-01-8	-8.8	-7.3	0.0	12.5	-6.6	8.5
1185	LARIXINIC ACID	BRD-K40619305-001-12-1	0.7	10.9	12.5	10.3	1.7	-0.2
1186	ZM 39923 hydrochloride	BRD-K40624912-003-02-3	-60.8	-61.4	15.4	14.5	-71.3	-74.8
1187	L-165,041	BRD-K40656405-001-01-5	-36.9	-39.1	-80.2	-81.4	-30.1	-22.0
1188	QX 222	BRD-K40782193-003-01-1	10.8	4.3	-0.4	4.7	7.1	8.3
1189	RITANSERIN	BRD-K40887525-001-14-4	15.0	-3.7	-28.3	-11.9	16.5	6.5
1190	CINANSERIN	BRD-K40901640-001-01-0	-2.2	-2.0	4.8	-4.6	1.1	0.4
1191	PHENACEMIDE	BRD-K40905133-001-03-1	-5.6	-11.0	-3.3	11.2	5.4	6.8
1192	CYANOPINDOLOL	BRD-K40965114-001-01-2	1.5	-3.7	-6.0	-7.0	-4.5	-4.9
1193	N,N-HEXAMETHYLENEAMILORIDE	BRD-K40990712-001-02-4	-4.1	-18.6	3.1	1.5	-8.8	12.8

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1194	PARACHLOROPHENOL	BRD-K40992116-001-05-5	1.5	-1.8	5.2	7.8	-16.4	-10.9
1195	N20C hydrochloride	BRD-K41143549-003-01-6	-13.7	-14.8	-15.2	-7.3	4.0	11.4
1196	Fenobam	BRD-K41160163-001-01-9	15.4	9.1	25.9	35.3	3.5	6.4
1197	ZM 306416 hydrochloride	BRD-K41337261-003-01-0	-4.9	-7.9	-36.0	-25.9	-33.5	-22.9
1198	SULFAPYRIDINE	BRD-K41406082-001-09-7	3.5	-5.9	9.1	-4.5	1.4	-1.9
1199	A23187, free acid	BRD-K41431477-001-05-6	35.4	28.8	-62.7	-76.4	-61.1	-68.6
1200	BISPHENOL A	BRD-K41494493-001-04-7	8.2	-12.5	22.7	17.3	-1.3	-6.5
1201	Acetaminophen	BRD-K41524689-001-08-6	-0.2	2.3	14.9	13.7	-33.0	-25.7
1202	6,2'-DIMETHOXYFLAVONE	BRD-K41557448-001-01-3	10.9	-0.4	32.8	23.9	-8.7	-3.3
1203	Purvalanol B	BRD-K41564320-001-01-2	4.7	-17.6	26.6	17.2	27.5	29.0
1204	SB 334867	BRD-K41567364-001-01-2	11.4	-16.3	-45.7	-46.5	-19.1	-12.2
1205	GANGALEOIDIN	BRD-K41603276-001-03-8	-3.6	4.5	15.5	28.5	-21.4	-24.0
1206	E-4031 dihydrochloride	BRD-K41713976-300-01-8	12.2	-3.8	2.6	30.8	11.8	13.4
1207	TRICLOSAN	BRD-K41731458-001-04-5	-5.9	-9.7	-2.2	2.3	-35.2	-36.3
1208	IRIGENIN, DIBENZYL ETHER	BRD-K41762421-001-03-6	7.3	-10.2	20.3	31.6	7.1	13.4
1209	1,3-Dipropyl-8-phenylxanthine	BRD-K41853443-001-01-1	4.7	0.8	1.3	-2.7	-10.7	-13.3
1210	W-5 hydrochloride	BRD-K41868777-003-02-9	-1.9	-7.9	0.8	-10.8	4.9	3.1
1211	2-Phenylmelatonin	BRD-K41869275-001-01-0	-21.8	-25.9	4.1	6.7	18.0	28.1
1212	TIOXOLONE	BRD-K41876534-001-06-1	20.0	55.5	9.6	15.2	-25.3	-30.1
1213	Daidzein	BRD-K42095107-001-08-0	0.9	-9.2	7.1	24.0	-7.9	-11.4
1214	PROTRYPTYLINE HYDROCHLORIDE	BRD-K42098891-003-13-0	-22.4	-37.3	25.8	33.5	-28.4	-40.2
1215	NNC 711	BRD-K42221274-003-02-8	24.8	14.2	24.4	15.7	14.7	14.7
1216	CYCLOBENZAPRINE HYDROCHLORIDE	BRD-K42348709-003-08-1	-38.8	-21.2	30.2	17.1	-36.2	-33.9
1217	EO 1428	BRD-K42452249-001-01-7	-9.7	10.5	-8.8	-8.4	-3.1	4.2
1218	CGP 57380	BRD-K42500029-001-01-9	22.3	38.7	30.6	47.4	1.6	10.0
1219	2-(1-Thienyl)ethyl 3,4-dihydroxybenzylidenecyanoacetate	BRD-K42663584-001-01-2	20.8	15.0	-31.2	-20.9	-30.7	-35.7
1220	Y-27152	BRD-K42679050-001-01-3	2.8	4.5	-24.8	-21.5	-3.1	-1.7
1221	Glimepiride	BRD-K42693031-001-01-8	-3.1	-11.2	-6.8	9.2	24.6	18.3
1222	XE 991 dihydrochloride	BRD-K42748308-300-01-2	10.3	5.9	-20.1	-20.9	9.5	9.6
1223	CFM-2	BRD-K42859542-001-02-5	-5.6	-6.6	-2.1	-7.5	-0.4	-1.7
1224	PD 156273	BRD-K43030839-001-01-6	6.4	1.9	5.0	-0.8	17.6	19.5
1225	AMG 9810	BRD-K43068349-001-01-9	-2.9	-9.5	-6.5	-8.2	1.1	12.4
1226	2',5'-DIHYDROXY-4-METHOXYCHALCONE	BRD-K43285163-001-02-0	29.4	28.4	28.9	27.9	-49.1	-54.9
1227	RO 04-6790	BRD-K43290182-001-01-9	-3.2	-2.8	-4.6	6.0	7.0	14.5
1228	JTE 013	BRD-K43330982-001-01-5	15.2	12.1	-8.4	0.6	-34.4	-28.1
1229	FLOPROPIONE	BRD-K43383936-001-03-7	-12.4	-5.0	32.0	22.9	43.2	46.9
1230		BRD-K43389675-003-03-5	15.4	11.1	-16.9	-5.7	8.1	4.2
1231	Tamoxifen citrate	BRD-K43744935-048-01-6	-60.8	-67.1	-73.8	-73.4	-62.8	-70.3
1232	PSEUDO-ANISATIN	BRD-K43770188-001-02-2	2.0	-5.3	25.5	21.3	23.5	19.4
1233	RLM-1-127	BRD-K43796186-001-01-1	-1.8	-4.3	-1.9	-10.0	-12.7	-9.6
1234	GENISTEIN	BRD-K43797669-001-10-6	-6.2	-10.5	8.0	0.8	7.7	1.4
1235	PENICILLIN V POTASSIUM	BRD-K43966364-237-03-0	3.7	-1.9	28.0	14.9	21.7	27.2
1236	ISOSAFROLE	BRD-K44005821-001-07-4	1.0	-16.4	13.0	-12.8	-0.2	7.5
1237	FLUFENAMIC ACID	BRD-K44067360-001-16-2	-7.8	-4.9	-59.0	-67.4	-23.8	-27.6
1238	Y-27632	BRD-K44084986-300-02-7	-5.9	-11.3	-19.0	-3.0	-1.4	6.5
1239	L-PHENYLALANINOL	BRD-K44204252-001-04-8	-0.6	1.6	19.5	8.6	22.5	26.3

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1240	TRYPTAMINE	BRD-K44218819-001-05-1	24.7	7.5	19.6	34.6	11.8	8.2
1241	TOLNAFTATE	BRD-K44273375-001-14-4	-6.9	-15.3	29.8	37.7	27.2	32.3
1242	(R)-(-)-Niguldipine hydrochloride	BRD-K44309363-003-01-3	-12.3	-10.8	-27.5	-20.5	-46.2	-44.2
1243	N-METHYLBENZYLAMINE HYDROCHLORIDE	BRD-K44558320-003-01-7	3.6	0.2	8.3	14.5	11.0	11.1
1244	BECLAMIDE	BRD-K44824027-001-01-3	2.4	0.6	8.4	11.5	-4.3	4.0
1245	S-(-)-Atenolol	BRD-K44993696-001-05-7	-4.7	18.5	17.0	14.0	17.0	10.3
1246	FAMCICLOVIR	BRD-K45033733-001-05-6	-8.6	-7.7	12.0	6.1	2.2	-2.1
1247	SNC-162	BRD-K45042519-001-01-6	-0.1	-4.5	4.5	6.6	14.3	9.4
1248	W-13 hydrochloride	BRD-K45068323-003-02-1	-29.6	-26.5	-39.7	-61.9	-16.4	-39.2
1249	TETRACAINE HYDROCHLORIDE	BRD-K45071273-003-15-7	-4.8	-3.2	38.5	37.7	-11.6	-12.5
1250	Y-26763	BRD-K45117373-001-01-1	12.1	5.9	-19.8	38.8	11.8	42.9
1251	VALSARTAN	BRD-K45158365-001-05-6	-7.7	-3.4	23.3	20.4	15.5	9.8
1252	CLOFIBRATE	BRD-K45252063-001-06-0	13.2	13.9	5.8	10.4	4.5	7.2
1253	ZD 7114 hydrochloride	BRD-K45296539-003-01-0	-2.6	-6.9	-8.5	-14.3	2.0	9.2
1254	DIETHYLSTILBESTROL	BRD-K45330754-001-09-2	6.5	5.1	32.5	12.1	2.2	3.2
1255	SCH 23390 hydrochloride	BRD-K45435259-003-03-8	-4.6	2.2	24.3	29.0	12.3	16.0
1256	5-Methylfurmethiodide	BRD-K45437867-005-01-7	7.8	-6.9	3.0	12.0	24.5	25.5
1257	BP 554 maleate	BRD-K45479396-103-01-2	4.2	20.3	10.9	23.8	11.4	5.9
1258	Broad-PET-Sai-52	BRD-K45528773-001-03-1	-8.6	-9.3	3.2	-18.5	-1.8	-9.0
1259	DIETHYLCARBAMAZINE CITRATE	BRD-K45542189-048-15-5	-1.5	-15.8	6.4	-0.2	3.9	8.0
1260	3'-Fluorobenzylspiperone maleate	BRD-K45662124-103-01-2	-5.6	-6.7	-0.2	-2.0	-6.6	-5.3
1261	AZAPERONE	BRD-K45861246-001-08-4	13.2	3.4	42.6	8.5	13.6	24.0
1262	AMRINONE	BRD-K45924332-001-07-7	33.5	39.1	-4.5	14.7	-12.0	-12.2
1263	LUPININE	BRD-K45978015-001-03-6	-11.6	-1.1	11.5	17.1	2.7	-2.2
1264	TMS	BRD-K45988865-001-01-0	6.2	-7.7	-1.9	11.3	-17.8	31.9
1265	BEZAFIBRATE	BRD-K46018455-001-17-7	-8.8	-5.1	19.1	6.9	15.9	24.2
1266	RS 67333 hydrochloride	BRD-K46142322-003-01-6	2.8	-2.1	28.6	17.4	18.9	9.4
1267	TOLAZOLINE HYDROCHLORIDE	BRD-K46211610-003-15-0	-11.4	0.2	2.9	7.7	3.1	8.4
1268	PROADIFEN HYDROCHLORIDE	BRD-K46317332-003-10-3	-17.2	-11.7	-31.9	-29.8	-8.7	-12.1
1269	o-3M3FBS	BRD-K46384212-001-01-1	16.0	-0.1	10.9	-6.4	14.7	7.4
1270	Hymecromone	BRD-K46424862-001-04-2	0.2	5.7	19.9	16.1	12.3	14.3
1271	LIOTHYRONINE	BRD-K46428823-001-01-7	5.0	-1.3	8.9	6.0	-32.1	-22.6
1272	VALACYCLOVIR HYDROCHLORIDE	BRD-K46435977-003-03-8	1.3	-4.1	16.5	-2.7	11.0	16.7
1273	GR 55562 dihydrochloride	BRD-K46441700-300-01-4	-27.6	-13.4	9.1	7.9	-62.1	-30.0
1274	SCH 442416	BRD-K46469693-001-01-8	10.6	5.2	5.6	34.1	15.5	22.6
1275	SACCHARIN	BRD-K46493214-001-03-4	-10.3	-10.9	-3.0	8.0	13.7	2.1
1276	PRAMOXINE HYDROCHLORIDE	BRD-K46523383-003-14-6	-22.3	-6.2	14.3	43.4	-26.5	-29.5
1277	METHYLBENZETHONIUM CHLORIDE	BRD-K46531780-003-09-8	-55.4	-57.8	21.9	14.7	-65.3	-70.0
1278	DIPLOSALSALATE	BRD-K46585355-001-09-3	2.1	-7.1	15.9	17.2	24.8	19.3
1279	S 14506 hydrochloride	BRD-K46766488-003-01-2	-7.7	4.1	-20.0	-22.6	-10.3	-11.9
1280	6,4'-DIHYDROXYFLAVONE	BRD-K46836114-001-04-3	-8.3	-3.0	19.2	33.1	6.8	4.6
1281	Metyrapone	BRD-K46862739-001-03-6	6.8	9.9	20.4	3.5	8.4	1.3
1282	ANTIPYRINE	BRD-K46937689-001-08-5	-4.1	-8.9	19.1	7.1	1.9	5.8
1283	CLOXYQUIN	BRD-K46982791-001-04-5	34.8	13.0	15.2	33.0	-25.1	-26.9
1284	DIPHENHYDRAMINE HYDROCHLORIDE	BRD-K47278471-003-15-6	18.7	-2.3	2.3	14.5	11.8	9.9
1285	METHAPYRILENE HYDROCHLORIDE	BRD-K47323024-003-15-2	-11.3	-9.9	2.8	4.5	9.6	16.9

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1286	4-(4-Fluorobenzoyl)-1-(4-phenylbutyl)-piperidine oxalate	BRD-K47337578-034-01-7	-10.1	-11.2	-0.6	-2.3	0.1	3.7
1287	NIFENAZONE	BRD-K47407372-001-09-8	-9.3	11.4	18.9	21.4	8.0	7.1
1288	NORHARMAN	BRD-K47467075-001-13-4	-0.1	-1.8	7.5	-1.9	15.1	15.1
1289	PP 1	BRD-K47598052-001-06-7	-9.6	-6.8	-13.4	5.3	2.4	-0.8
1290	DIPYROCETYL	BRD-K47608922-001-02-1	-4.9	13.2	14.3	14.4	3.1	17.6
1291	BROMHEXINE HYDROCHLORIDE	BRD-K47631482-003-03-9	-7.6	-3.0	-42.4	-47.5	-40.9	-26.0
1292	EMD 386088 hydrochloride	BRD-K47659338-003-01-0	-6.5	-10.9	-16.4	-15.0	-17.9	-27.5
1293	NBQX disodium salt	BRD-K47717570-304-01-5	50.8	25.9	-9.3	-11.6	-11.1	-7.7
1294	6,3'-DIMETHOXYFLAVONE	BRD-K47724892-001-03-0	3.8	-3.1	52.5	10.8	25.7	21.5
1295	PD 168077 maleate	BRD-K47761761-103-01-8	11.5	-6.0	27.8	33.6	25.9	25.6
1296	DUARTIN (-)	BRD-K47814830-001-03-4	-21.4	26.7	14.6	9.7	-35.3	-33.3
1297	PODOFILOX	BRD-K47869605-001-18-9	24.6	44.3	36.5	38.5	3.6	6.6
1298	Piribedil dihydrochloride	BRD-K47936004-003-04-9	23.4	23.4	12.2	18.3	2.1	10.9
1299	TYRPHOSTIN 51	BRD-K47943470-001-03-6	29.5	63.0	-2.8	-0.4	-40.1	-40.1
1300	OBAA	BRD-K48029790-001-01-0	-19.3	-5.6	-48.6	-43.7	-40.6	-31.7
1301	YM 298198, Desmethyl-	BRD-K48059230-003-01-1	10.5	-27.1	-9.0	-2.3	-18.0	-16.8
1302	PROPYLTHIOURACIL	BRD-K48168960-001-08-5	-28.1	-55.9	25.1	26.3	20.9	15.7
1303	QUININE SULFATE	BRD-K48278478-065-03-3	39.5	9.7	11.8	24.8	0.7	6.1
1304	Zonisamide	BRD-K48300629-001-03-8	-8.2	-1.1	-3.3	13.1	21.6	27.2
1305	ICI 215,001 hydrochloride	BRD-K48311056-003-01-7	7.7	13.2	-5.4	29.6	19.6	29.4
1306	FEBUXOSTAT	BRD-K48367671-001-01-8	-16.4	4.4	15.8	-2.8	25.5	20.2
1307	Y 29794 oxalate	BRD-K48449073-034-01-9	-60.7	-65.8	17.3	8.5	-69.4	-72.8
1308	NU 1025	BRD-K48692744-001-01-2	5.3	-4.3	3.4	10.1	7.1	-0.7
1309	TL HSV 09	BRD-K48722258-300-06-0	14.2	-0.1	10.2	-15.4	-5.0	-10.3
1310	PD 158780	BRD-K48735772-001-01-4	15.1	18.4	-11.4	-4.0	-36.0	-32.4
1311	PSB 1115	BRD-K49027941-237-01-1	8.0	-1.2	91.8	114.8	1.9	6.3
1312	CGS 15943	BRD-K49049886-001-03-8	18.3	17.2	0.5	4.5	-6.6	-2.7
1313	ETHYL-beta-CARBOLINE-3-CARBOXYLATE	BRD-K49061529-001-01-0	-25.2	-47.1	-16.4	1.3	-1.0	0.0
1314	SECURININE	BRD-K49071277-001-03-9	-9.9	0.6	2.5	6.3	-12.0	-9.4
1315	PRAZOSIN HYDROCHLORIDE	BRD-K49111258-003-16-4	-75.1	-73.5	10.2	26.4	-65.8	-69.7
1316	TMPH hydrochloride	BRD-K49119234-003-01-8	-4.1	-6.6	-20.5	-20.4	-9.9	-8.9
1317	CYCLOVERATRYLENE	BRD-K49154891-001-02-1	4.9	-5.2	8.9	4.9	-8.1	-7.8
1318	RETUSIN	BRD-K49158532-001-02-7	6.8	-4.5	55.3	15.0	23.4	28.4
1319	4-METHYLDAPHNETIN	BRD-K49207204-001-04-5	40.7	3.8	26.2	18.6	-45.2	-45.5
1320	6-Iodo-nordihydrocapsaicin	BRD-K49236613-001-01-5	-6.1	13.3	-14.1	1.1	-18.6	-20.9
1321	BIBU 1361 dihydrochloride	BRD-K49294207-300-01-2	-46.2	-45.7	-98.6	-98.9	-77.7	-81.4
1322	Immethridine dihydrobromide	BRD-K49519092-303-01-4	-5.4	-15.2	9.5	2.0	13.6	11.9
1323	7,8-DIHYDROXYFLAVONE	BRD-K49535716-001-03-2	-6.7	27.2	37.6	43.3	-48.1	-53.6
1324	AG 18	BRD-K49657628-001-05-6	42.1	32.5	13.7	25.5	-31.5	-32.7
1325	CLARITHROMYCIN	BRD-K49668410-001-07-1	14.9	7.7	29.6	16.2	9.4	14.1
1326	TTNPB	BRD-K49685476-001-05-0	-3.0	-8.7	4.5	-2.7	-3.7	-21.9
1327	2-METHYL-3-HYDROXYETHYLENEPYRAN-4-ONE	BRD-K49745710-001-02-5	-18.2	-3.8	2.3	5.3	6.9	8.6
1328	4-HYDROXYANTIPYRINE	BRD-K49759007-001-06-9	-73.1	-76.1	-10.0	-9.3	-41.2	-37.0
1329	Gavestinel	BRD-K49890030-236-01-6	-43.4	-36.0	-77.0	-84.6	-16.3	-12.3
1330	GR 113808	BRD-K49945136-001-03-5	34.0	5.9	13.1	4.1	6.6	-7.2
1331	RS 67506 hydrochloride	BRD-K50018155-003-01-3	23.5	-11.0	23.7	29.6	13.8	11.0

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			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1332	2-METHYL GRAMINE	BRD-K50054100-001-03-4	-9.1	1.0	24.5	22.9	-3.6	0.1
1333	TOLFENAMIC ACID	BRD-K50133271-001-10-4	-20.5	-27.0	41.0	38.8	-15.0	-21.4
1334	GBR 12935 dihydrochloride	BRD-K50135270-300-01-5	-6.6	-7.6	21.3	20.8	-11.0	-10.5
1335	MM 77 dihydrochloride	BRD-K50293352-300-01-3	3.3	-7.6	23.2	9.2	0.1	5.0
1336	UCL 2077	BRD-K50325075-001-01-3	-2.2	-14.5	4.4	7.0	54.8	37.0
1337	7,4'-DIHYDROXYFLAVONE	BRD-K50384076-001-01-9	18.1	-28.7	20.0	30.1	-3.3	-6.5
1338	Fenofibrate	BRD-K50388907-001-20-5	-6.9	33.5	18.7	29.3	32.8	40.8
1339	Chlormethiazole hydrochloride	BRD-K50422030-003-01-8	-27.0	5.9	0.1	21.0	-7.2	6.9
1340	POMIFERIN	BRD-K50660510-001-04-0	-63.2	-69.6	-8.9	16.3	-85.0	-85.5
1341	EPICATECHIN MONOGALLATE	BRD-K50660797-001-03-6	17.1	23.6	-42.3	-17.3	-40.4	-19.3
1342	PENTACHLOROPHENOL	BRD-K50711164-001-07-3	-15.8	-14.9	18.3	23.2	-32.3	-33.0
1343	BERBAMINE HYDROCHLORIDE	BRD-K50754849-300-03-1	-12.9	0.6	17.8	42.4	12.2	9.6
1344	Purvalanol A	BRD-K50836978-001-01-7	12.3	19.6	-58.9	-56.9	-10.4	-6.7
1345	PAC 1	BRD-K50841342-001-01-6	-29.4	-34.9	-55.3	-48.2	-29.1	-27.7
1346	SULFISOXAZOLE	BRD-K50859149-001-10-4	24.1	-10.7	23.3	31.6	11.3	13.1
1347	GR 103691	BRD-K50891186-001-03-6	7.0	-16.6	21.0	32.0	13.1	3.5
1348	TRAMADOL HYDROCHLORIDE	BRD-K51033547-003-01-8	17.7	-9.1	15.1	34.8	7.1	14.1
1349	ETHIONAMIDE	BRD-K51207550-001-09-9	-17.1	-16.8	31.7	27.2	20.4	18.9
1350	A-3 hydrochloride	BRD-K51215422-003-01-1	-21.3	-17.2	17.8	17.5	-34.5	-22.6
1351	AG 99	BRD-K51223576-001-01-3	103.9	134.4	16.9	11.6	-44.8	-47.1
1352	FENBENDAZOLE	BRD-K51318897-001-07-0	25.3	3.9	14.0	40.0	9.9	9.2
1353	TOREMIPHENE CITRATE	BRD-K51350053-048-06-6	-54.5	-54.8	15.9	3.5	-77.6	-80.1
1354	DIFFRACTAIC ACID	BRD-K51370144-001-06-4	-48.8	-40.1	31.9	19.9	-38.5	-42.4
1355	ST638	BRD-K51476772-001-01-9	12.5	11.2	-10.6	-17.5	-15.0	-22.7
1356	Ro 25-6981 maleate	BRD-K51541829-001-01-3	22.1	-1.0	-18.9	6.8	-1.6	5.9
1357	(S)-(-)-Sulpiride	BRD-K51671335-001-04-9	-9.2	2.2	19.7	12.6	10.8	12.9
1358	ESCULIN MONOHYDRATE	BRD-K51742987-002-02-1	8.3	10.6	91.0	98.9	16.4	17.6
1359	Iodophenpropit dihydrobromide	BRD-K51918615-303-01-1	-11.1	-16.3	-42.0	-28.0	4.9	-2.0
1360	deoxyrhapontin	BRD-K52015643-001-01-1	20.2	34.2	-0.6	10.3	4.8	1.8
1361	METRONIDAZOLE	BRD-K52020312-001-15-1	1.7	7.6	16.8	16.7	30.7	14.5
1362	BENZYL BENZOATE	BRD-K52072429-001-06-1	-0.1	6.6	13.5	24.7	17.5	20.5
1363	OXIBENDAZOLE	BRD-K52075715-001-03-4	9.7	-1.0	59.8	57.3	44.8	38.8
1364	PIPERONYLIC ACID	BRD-K52148119-001-02-3	2.7	4.5	16.2	21.8	9.1	13.4
1365	Domoic acid	BRD-K52217427-001-02-3	12.5	1.7	10.0	42.2	18.6	11.9
1366	ICI 63197	BRD-K52219182-001-01-6	67.3	38.0	32.8	24.6	23.6	25.6
1367	CHLORHEXIDINE	BRD-K52256627-300-03-3	-88.4	-67.8	47.9	25.9	-64.0	-76.3
1368	CHINIOFON	BRD-K52284881-236-01-6	57.7	50.3	3.7	27.5	0.8	2.2
1369	CI-994	BRD-K52313696-001-08-1	7.2	-7.4	11.3	-4.2	-3.4	-2.0
1370	APIIN	BRD-K52379519-001-02-0	-12.6	3.5	-2.1	-5.3	15.3	8.6
1371	GR 159897	BRD-K52394958-001-01-9	25.6	-11.0	17.5	13.2	12.4	14.4
1372	Alprostadil	BRD-K52459643-001-10-2	-1.4	-15.4	14.2	6.4	23.8	23.4
1373	SC 19220	BRD-K52512893-001-03-0	-10.7	-3.2	-11.6	-4.3	10.6	18.5
1374	STO-609 acetate	BRD-K52620403-015-02-6	16.8	17.7	6.7	19.2	0.7	4.0
1375	LIDOCAINE HYDROCHLORIDE	BRD-K52662033-003-14-7	20.6	8.7	4.8	0.1	8.9	14.6
1376	JAK3 Inhibitor II	BRD-K52850071-001-01-2	-12.4	-4.8	-4.4	-14.4	-63.0	-65.6
1377	ACETOHEXAMIDE	BRD-K52960356-001-06-4	-20.6	19.8	41.7	30.2	18.1	15.7

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1378	CLOMIPRAMINE HYDROCHLORIDE	BRD-K52989797-003-16-5	-52.2	-52.6	54.8	47.0	-45.5	-52.3
1379	Niridazole	BRD-K53123955-001-03-0	0.5	-23.0	-2.2	4.2	14.9	12.7
1380	BUTYLATED HYDROXYTOLUENE	BRD-K53153417-001-06-2	1.2	-0.4	-1.7	7.5	0.6	-2.6
1381	TRIMETOZINE	BRD-K53220666-001-01-8	-7.4	-1.0	14.0	-2.2	-2.8	5.3
1382	HESPERIDIN	BRD-K53229386-001-03-4	16.2	5.9	27.3	26.7	8.1	12.2
1383	CITCO	BRD-K53263234-001-02-9	30.5	8.0	8.7	36.2	29.7	22.9
1384	(?)-U-50488 hydrochloride	BRD-K53532120-003-03-8	2.9	0.3	-2.4	10.9	-25.9	-20.7
1385	CNQX disodium salt	BRD-K53545112-304-01-6	-6.2	-2.2	-4.8	-4.3	15.9	13.4
1386	IRIGENIN, 7-BENZYL ETHER	BRD-K53634892-001-03-2	5.2	2.9	39.0	30.5	-11.9	-5.7
1387	AMITRIPTYLINE HYDROCHLORIDE	BRD-K53737926-003-14-6	-2.1	4.1	-35.9	-56.3	-24.7	-32.8
1388	Risperidone	BRD-K53857191-001-10-2	22.3	-4.6	0.9	3.6	1.2	0.3
1389	MMPX	BRD-K53878242-001-02-4	5.7	2.8	17.9	13.0	7.1	7.6
1390	4-HYDROXYPHENETHYLAMINE	BRD-K53893978-001-03-1	19.7	-11.8	15.3	19.9	7.5	15.1
1391	2,3,4'-TRIHYDROXY-4-METHOXYBENZOPHENONE	BRD-K53923343-001-03-4	46.3	47.7	32.8	42.0	-30.2	-28.2
1392	ALX 5407 hydrochloride	BRD-K53979406-003-01-0	-10.5	-17.5	-7.2	-17.2	-10.7	-14.6
1393	Remoxipride hydrochloride	BRD-K54094468-003-05-3	24.1	-23.8	3.4	7.5	5.1	5.8
1394	CMPD-1	BRD-K54095730-001-01-5	2.4	9.7	-54.3	-36.0	-39.2	-28.3
1395	Cirazoline hydrochloride	BRD-K54142781-003-02-7	-7.5	-12.0	-4.5	2.8	14.0	14.0
1396	Dorsomorphin dihydrochloride	BRD-K54233340-300-01-0	-20.4	-18.5	-47.2	-44.9	-20.1	-23.9
1397	SB 202190	BRD-K54330070-001-07-1	-7.2	-1.5	-24.9	-23.2	-19.4	-19.9
1398	Doxepine HCl	BRD-K54462405-003-16-5	14.5	-17.3	-6.5	-24.3	1.1	3.2
1399	CAPTOPRIL	BRD-K54529596-001-15-6	-4.1	2.4	16.1	15.6	12.0	11.2
1400	3-DEOXY-3beta-HYDROXYANGOLENSIC ACID METHYL ESTER	BRD-K54554531-001-02-0	-18.8	-11.5	13.0	6.7	0.8	0.3
1401	R 59-022	BRD-K54665485-001-04-6	16.3	9.0	12.8	-5.0	-12.8	-4.8
1402	BAY 36-7620	BRD-K54704028-001-01-3	-0.3	29.7	2.2	12.4	4.9	-1.9
1403	nTZDpa	BRD-K54708045-001-01-3	-94.9	-94.5	-96.7	-95.9	-70.6	-73.6
1404	TRIOXSALEN	BRD-K54790157-001-10-6	35.8	-0.6	1.6	21.3	-2.6	0.5
1405	PEFLOXACINE MESYLATE	BRD-K55034111-066-07-2	28.1	-5.9	42.0	34.8	16.2	9.7
1406	FLUPHENAZINE HYDROCHLORIDE	BRD-K55127134-300-07-0	-78.3	-82.5	-103.5	-104.7	-89.0	-88.2
1407	3-HYDROXYFLAVONE	BRD-K55150756-001-05-7	27.0	47.0	3.0	17.8	-18.2	-11.7
1408	2-MERCAPTOBENZOTHIAZOLE	BRD-K55160477-001-03-9	-47.3	-41.7	15.9	34.7	-4.8	-11.3
1409	EFLOXATE	BRD-K55166090-001-03-3	-8.0	-12.7	3.2	32.9	-18.3	-8.8
1410	PENICILLIN G POTASSIUM	BRD-K55191674-237-12-6	13.9	-1.9	28.9	19.6	10.5	12.7
1411	2',4'-DIHYDROXYCHALCONE 4'-GLUCOSIDE	BRD-K55250255-001-03-6	6.9	-4.4	27.9	27.0	25.8	23.3
1412	SULFADOXINE	BRD-K55250441-001-06-4	2.3	5.3	17.7	15.8	19.0	27.6
1413	5-FLUOROINDOLE-2-CARBOXYLIC ACID	BRD-K55273157-001-13-6	-10.2	-8.2	26.4	30.5	24.9	23.4
1414	CPD5	BRD-K55292075-001-01-0	26.3	19.8	-66.4	-61.8	-59.9	-60.8
1415	BU 224 hydrochloride	BRD-K55344148-003-01-8	2.5	16.7	24.1	32.7	10.9	18.7
1416	Anpirtoline hydrochloride	BRD-K55424922-003-01-0	17.5	-4.9	7.1	7.2	-0.1	0.0
1417	WAY 629 hydrochloride	BRD-K55430733-003-01-6	-0.5	-19.9	-25.9	-5.8	-32.7	-27.4
1418	TAS 301	BRD-K55454768-001-01-8	-5.0	-4.4	-22.4	-15.8	-1.5	-2.0
1419	Spiperone hydrochloride	BRD-K55468218-003-01-0	6.1	-38.2	-34.0	-17.6	-19.1	-19.4
1420	FORMONONETIN	BRD-K55567017-001-06-5	-5.1	-5.9	18.6	1.8	7.3	3.9
1421	Co 101244 hydrochloride	BRD-K55677650-003-01-1	-15.1	0.8	0.6	-21.5	-40.0	-41.9
1422	TOPOTECAN HYDROCHLORIDE	BRD-K55696337-003-08-7	77.5	73.3	31.5	24.6	8.9	2.9
1423	SCH 28080	BRD-K55748775-001-01-4	0.6	-8.3	-0.8	11.0	12.0	6.6

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1424	HYMECROMONE METHYL ETHER	BRD-K55766625-001-04-2	31.1	-8.4	38.4	33.6	18.1	19.1
1425	VEGF Receptor 2 Kinase Inhibitor II	BRD-K55823969-001-01-1	0.5	1.7	-14.5	-22.2	6.7	1.6
1426	PHENYTOIN SODIUM	BRD-K55930204-236-11-0	4.5	0.9	14.6	23.6	31.3	34.2
1427	RHC 80267	BRD-K56047318-001-03-0	-6.1	5.6	16.9	46.9	22.4	15.8
1428	METHOXYVONE	BRD-K56057104-001-03-7	-14.6	-19.0	16.2	19.1	18.0	9.7
1429	HBDDE	BRD-K56064827-001-04-7	158.4	144.3	118.3	145.4	23.7	21.5
1430	OXICONAZOLE NITRATE	BRD-K56104152-008-03-3	16.9	-9.5	40.1	37.0	-17.9	-10.6
1431	BU 226 hydrochloride	BRD-K56115039-003-01-3	-0.1	-8.0	0.5	4.8	7.5	13.9
1432	3,4',5,6,7-PENTAMETHOXYFLAVONE	BRD-K56148010-001-01-1	-6.4	-5.5	19.8	4.1	-11.4	-15.9
1433	benznidazole	BRD-K56156805-001-05-4	-12.6	-6.9	0.3	8.8	14.1	11.5
1434	trans-Triprolidine hydrochloride	BRD-K56231354-003-01-5	12.5	-3.5	18.1	11.9	14.7	18.6
1435		BRD-K56309460-001-03-0	-0.6	-0.8	38.6	6.9	3.9	4.8
1436	ZK 756326	BRD-K56403959-300-01-9	9.2	22.1	-11.0	-18.1	4.6	-7.0
1437	Calcipotriol	BRD-K56429665-001-03-9	-1.5	-7.7	-70.4	-81.1	-27.0	-30.0
1438	7-HYDROXYFLAVONE	BRD-K56450366-001-03-7	17.6	27.0	19.4	42.3	14.7	24.0
1439	CHICAGO SKY BLUE	BRD-K56483981-342-04-9	33.4	35.0	13.8	9.2	11.9	15.9
1440	BMS 182874 hydrochloride	BRD-K56509348-003-01-3	32.7	15.4	-2.3	6.8	13.7	9.4
1441	CLOFAZIMINE	BRD-K56614220-001-10-9	-9.8	-16.2	-18.8	8.4	8.8	8.0
1442	CARBADOX	BRD-K56735750-001-03-5	30.8	28.6	27.5	29.5	7.0	13.4
1443	NARINGIN	BRD-K56759808-001-03-7	18.6	12.6	18.7	23.9	3.5	4.1
1444	Ethoxyquin	BRD-K56792340-001-05-8	-27.4	-22.3	2.4	4.7	-65.9	-64.0
1445	GUANABENZ ACETATE	BRD-K56800335-015-03-1	3.3	0.9	24.7	10.3	25.6	14.3
1446	OXETHAZAINE	BRD-K56940463-001-08-8	-41.2	-48.7	28.9	8.9	-58.0	-62.0
1447	MARMESIN ACETATE	BRD-K57001030-001-02-5	-9.9	-16.9	4.7	23.7	5.1	16.9
1448	TRIPELENNAMINE CITRATE	BRD-K57033106-048-03-6	30.2	4.7	17.9	9.4	9.1	5.5
1449	CROTAMITON	BRD-K57179821-001-08-9	-0.3	-3.8	9.6	0.3	5.9	-0.5
1450	INDOMETHACIN	BRD-K57222227-001-18-6	-12.2	-16.6	1.3	4.6	-2.1	0.2
1451	5-CHLOROINDOLE-2-CARBOXYLIC ACID	BRD-K57244822-001-03-1	-9.2	-7.1	24.3	15.4	12.1	18.9
1452	MOROXYDINE HYDROCHLORIDE	BRD-K57291914-003-05-2	9.6	-17.2	21.3	21.3	15.6	27.7
1453	PRE-084 hydrochloride	BRD-K57304726-003-03-6	34.9	38.6	-15.5	-8.6	-2.8	-1.5
1454	IRIGENOL	BRD-K57398215-001-03-0	51.4	53.4	11.5	19.1	12.6	10.3
1455	TIAPRIDE HYDROCHLORIDE	BRD-K57432881-003-14-3	4.8	0.9	24.3	29.9	12.0	29.1
1456	ENALAPRIL MALEATE	BRD-K57545991-050-16-5	22.4	-14.2	7.3	20.8	8.4	2.0
1457	PENTOXIFYLLINE	BRD-K57569181-001-16-8	-37.0	1.0	-0.9	23.8	8.9	5.8
1458	1-[1-(2-BENZO[B]THIENYL)CYCLOHEXYL]PYRROLIDINE	BRD-K57586808-001-01-7	-8.1	-19.9	17.1	17.9	15.9	20.4
1459	PENTYLENETETRAZOL	BRD-K57718010-001-08-5	-12.4	-11.6	13.3	9.0	14.6	11.2
1460	Roscovitine, (S)-Isomer	BRD-K57810622-001-01-5	-5.3	-9.7	-12.1	-6.1	8.7	8.3
1461	TYRPHOSTIN AG 1295	BRD-K57926513-001-03-7	-0.8	-5.5	-5.5	-11.8	9.5	7.9
1462	ESCULETIN	BRD-K58149231-001-10-1	17.5	4.3	10.4	7.0	-50.5	-45.5
1463	METICRANE	BRD-K58265391-001-06-9	22.3	-13.1	18.6	34.8	0.5	9.8
1464	Ro 90-7501	BRD-K58299615-001-02-7	-10.3	-16.0	-6.1	-10.5	-34.2	-23.1
1465	ACETAMINOSALOL	BRD-K58464880-001-02-5	1.4	10.5	3.6	-0.4	-18.6	-20.6
1466	PALMATINE CHLORIDE	BRD-K58466253-003-07-4	13.2	18.5	22.1	10.6	7.3	1.4
1467	ROCCELLIC ACID	BRD-K58612873-001-03-6	3.1	16.2	25.9	20.4	20.5	27.9
1468	CIANIDANOL	BRD-K58736316-001-08-7	7.6	-1.2	9.7	14.0	-23.5	-29.5
1469	SANTONIN	BRD-K58787433-001-08-8	7.0	15.3	29.4	1.0	-0.9	2.0

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1470	OXYBENZONE	BRD-K59037100-001-09-7	-36.2	-13.9	10.4	3.2	-6.6	-14.3
1471	CHLORPROTHIXENE HYDROCHLORIDE	BRD-K59058766-003-15-1	-60.1	-56.7	-94.7	-93.9	-80.6	-79.7
1472	SB 216763	BRD-K59184148-001-04-2	146.0	85.6	5.4	2.3	27.4	19.2
1473	NAPROXEN(+)	BRD-K59197931-001-03-7	3.2	-3.0	19.6	16.3	21.9	16.7
1474	CHRYSOPHANOL	BRD-K59284035-001-03-8	34.1	19.2	13.6	31.8	12.2	14.8
1475	Go 6976	BRD-K59304176-001-03-3	-15.7	-5.3	-36.7	-32.2	-14.5	-12.8
1476	SB 366791	BRD-K59331372-001-01-2	37.8	-4.1	0.6	6.1	10.1	15.3
1477	Linopirdine dihydrochloride	BRD-K59332007-300-01-9	-1.9	-4.7	-2.2	-14.9	8.5	-0.7
1478	(S)-(+)-Niguldipine hydrochloride	BRD-K59333713-003-01-2	-11.2	-5.3	-29.5	-5.3	-29.2	-29.4
1479	AH 6809	BRD-K59339270-001-01-8	-7.9	-8.1	-3.7	0.2	27.1	19.5
1480	Tozasertib VX-680 (MK-0457)	BRD-K59369769-001-02-1	-21.8	-13.9	-16.9	-24.8	-14.4	-3.3
1481	AM 281	BRD-K59419204-001-01-9	0.9	-4.4	-38.2	-41.1	-16.0	-15.4
1482	AG-879	BRD-K59469039-001-03-1	2.7	21.5	-9.1	-11.7	1.5	0.2
1483	PIPERINE	BRD-K59522102-001-08-8	2.1	-2.6	-0.7	6.9	19.8	12.5
1484	Bestatin	BRD-K59574735-001-05-0	36.9	0.8	9.3	33.4	-0.7	-7.0
1485	QUINIDINE GLUCONATE	BRD-K59632282-052-02-3	1.6	-1.2	19.7	10.9	17.5	24.6
1486	7,2'-DIHYDROXYFLAVONE	BRD-K59633395-001-01-4	78.1	26.3	20.1	24.3	16.6	3.6
1487	YM 298198 hydrochloride	BRD-K59650319-003-01-7	-14.4	-18.0	8.8	23.8	-35.4	-29.2
1488	MDL 29951	BRD-K59753853-001-01-5	-4.6	24.1	7.7	-0.4	-3.9	-1.8
1489	(R)-(+)-8-Hydroxy-DPAT hydrobromide	BRD-K59765110-004-03-8	13.0	1.8	19.1	8.9	-11.3	-17.4
1490	SULFABENZAMIDE	BRD-K59983611-001-15-1	-15.6	-28.3	6.7	4.7	13.1	8.8
1491	4a-Phorbol	BRD-K60024823-001-01-5	-5.9	8.8	0.6	-14.5	-1.0	-26.6
1492	GENTIAN VIOLET	BRD-K60025295-003-03-3	-96.7	-98.2	33.9	14.3	-85.8	-87.9
1493	IRBESARTAN	BRD-K60038276-001-03-3	-4.7	0.1	35.1	27.5	60.8	55.0
1494	N-Methyllidocaine iodide	BRD-K60060639-005-01-4	28.5	8.9	-18.7	-14.1	10.7	4.7
1495	TYRPHOSTIN 46	BRD-K60184833-001-03-1	88.3	87.3	-6.3	-2.5	-43.2	-43.5
1496	MG-132	BRD-K60230970-001-04-3	15.3	5.0	28.4	14.8	-14.0	-5.0
1497	4-NAPHTHALIMIDOBUTYRIC ACID	BRD-K60241851-001-06-9	-5.7	1.6	22.7	25.4	23.1	22.7
1498	Dephostatin	BRD-K60274257-001-01-1	89.4	78.5	41.8	39.1	-6.2	-3.0
1499	5,7-Dichlorokynurenic acid	BRD-K60287130-001-04-0	-5.0	-5.2	10.0	24.6	15.8	17.3
1500	ITE	BRD-K60298136-001-01-7	7.2	-8.9	2.3	7.1	3.4	8.1
1501	alpha-CYANO-4-HYDROXYCINNAMIC ACID	BRD-K60302405-001-04-5	4.1	-3.8	32.9	26.5	22.2	18.0
1502	1-HYDROXY-3,6,7-TRIMETHOXY-2,8-DIPRENYLXANTHONE	BRD-K60465509-001-01-1	3.6	-3.4	8.5	21.3	5.4	11.8
1503	Pravastatin	BRD-K60511616-236-02-2	-6.4	21.4	29.2	8.0	6.0	9.5
1504	DIMPYLATE	BRD-K60567437-001-04-5	-5.0	-3.6	14.8	26.5	5.2	7.6
1505	DESIPRAMINE HYDROCHLORIDE	BRD-K60762818-003-15-3	-10.1	-22.6	22.4	31.2	-31.3	-36.4
1506	PERGOLIDE MESYLATE	BRD-K60770992-066-15-1	14.0	-2.4	20.0	16.3	0.9	10.0
1507	ADIPHENINE HYDROCHLORIDE	BRD-K60907894-003-14-4	-0.9	-7.6	5.1	6.8	-14.7	-16.3
1508	R(+)-6-BROMO-APB	BRD-K60932973-001-01-7	-49.1	-49.0	-48.9	-51.7	-62.6	-62.9
1509	SB 218795	BRD-K61097567-001-03-6	-6.4	2.2	4.9	-0.3	0.0	-10.8
1510	NBI 27914 hydrochloride	BRD-K61177364-003-01-1	15.6	46.9	11.9	11.4	49.2	39.4
1511	LOPERAMIDE HYDROCHLORIDE	BRD-K61250553-003-16-5	-3.7	17.1	8.6	35.5	-10.3	-10.0
1512	Daphnetin	BRD-K61269089-001-02-2	20.4	16.8	18.9	26.3	-30.4	-29.6
1513	sb 225002	BRD-K61323504-001-03-2	27.4	1.5	2.5	3.8	-29.6	-38.5
1514	DEGUELIN(-)	BRD-K61401890-001-04-6	26.8	24.4	-15.2	3.8	-10.5	-14.4
1515	THIMEROSAL	BRD-K61443650-236-06-5	-77.8	-74.4	-92.0	-90.6	-71.3	-71.1

no.	Compound		Normalized scores					
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			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1516	AG 43	BRD-K61590534-001-01-4	18.3	47.2	16.4	14.1	26.8	28.2
1517	2,3-DCPE hydrochloride	BRD-K61734568-003-01-3	-23.3	-39.1	-24.8	-12.4	-18.7	-23.4
1518	CHLORINDIONE	BRD-K61802864-001-04-7	-2.7	-26.8	3.4	21.6	-14.6	-9.8
1519	FG 7142	BRD-K61951118-001-02-0	23.2	-12.7	28.8	22.9	10.8	12.6
1520		BRD-K62008436-001-05-6	-3.8	-15.7	18.1	16.2	11.0	17.7
1521	N-Methylquipazine dimaleate	BRD-K62056274-313-01-8	-0.5	-30.9	20.5	26.9	-11.5	-3.4
1522	WIN 55,212-3 mesylate	BRD-K62085719-066-01-4	-8.9	23.4	2.4	21.2	-1.5	12.6
1523	ANAGRELIDE HYDROCHLORIDE	BRD-K62200014-003-05-5	10.5	-16.2	19.1	14.0	4.7	15.2
1524	VUF 5681 dihydrobromide	BRD-K62206109-303-01-1	-2.6	-23.7	-10.0	-1.2	13.5	14.9
1525	T 98475	BRD-K62221994-001-01-8	8.1	-7.5	-69.2	-69.1	-14.6	-12.5
1526	Lylamine hydrochloride	BRD-K62289640-003-01-9	-93.1	-87.8	-106.9	-107.9	-82.0	-83.6
1527	KOPARIN	BRD-K62331715-001-02-1	80.0	76.2	15.0	19.0	-3.9	-1.1
1528	DY131	BRD-K62353524-001-01-8	47.5	7.7	29.3	29.8	6.8	16.0
1529	DAPSONE	BRD-K62363391-001-15-7	11.4	-4.5	10.2	9.1	7.0	1.1
1530	(+)-PD 128907 hydrochloride	BRD-K62456038-003-02-2	-6.1	-1.2	4.0	15.2	-26.2	-29.2
1531	4-IBP	BRD-K62537556-001-01-7	1.7	-2.3	14.5	19.3	9.0	6.1
1532	SR 2640 hydrochloride	BRD-K62562723-003-01-9	5.2	-5.5	-16.4	-13.5	5.8	19.8
1533	PODOPHYLLIN ACETATE	BRD-K62577500-001-03-6	24.9	0.3	12.9	24.7	-12.6	-10.1
1534	3-[2-[4-(2-Methoxyphenyl)piperazin-1-yl]ethyl]pyrimido[5,4-b] indole-2,4-dione	BRD-K62581435-001-02-0	-8.8	-8.2	8.0	7.6	13.4	12.2
1535	GR 125487 sulfamate	BRD-K62594868-082-03-7	-8.1	0.0	12.3	1.3	-7.3	1.8
1536	PD 98059	BRD-K62810658-001-06-4	10.9	1.1	23.4	31.5	4.2	0.2
1537	Aminopurine, 6-benzyl	BRD-K62929068-001-05-8	45.2	21.8	-10.3	0.7	20.6	-5.8
1538	NSC 625987	BRD-K62949423-001-02-3	34.5	-7.5	38.7	34.6	3.6	-0.7
1539	ORBIFLOXACIN	BRD-K63001556-001-03-9	-24.2	9.9	3.9	14.6	10.8	4.3
1540	JTE 907	BRD-K63150726-001-01-3	7.1	9.9	18.7	27.2	29.7	26.0
1541	MNITMT	BRD-K63151507-001-01-6	32.8	42.7	-1.1	16.3	9.1	9.5
1542	METHOXSALEN	BRD-K63430059-001-09-9	-6.7	-8.7	18.1	16.0	7.4	4.8
1543	SU 5416	BRD-K63504947-001-05-5	24.5	3.0	-29.6	12.2	-15.6	4.3
1544	T 0156 hydrochloride	BRD-K63516691-003-01-2	3.5	10.8	24.6	19.8	18.3	15.8
1545	AM 630	BRD-K63533170-001-01-1	7.3	-24.9	-37.6	-33.4	-15.6	-19.1
1546	ERYTHROMYCIN STEARATE	BRD-K63550407-028-03-9	15.0	-15.3	8.1	3.2	-10.7	-13.2
1547	Bufalin	BRD-K63606607-001-02-6	25.9	31.7	38.1	26.9	28.1	40.5
1548	ETHACRYNIC ACID	BRD-K63630713-001-15-9	-6.9	-1.6	7.8	8.8	-40.0	-7.9
1549	TRIFLUPROMAZINE HYDROCHLORIDE	BRD-K63675182-003-14-5	-47.4	-54.4	-79.7	-78.3	-62.2	-58.0
1550	10-HYDROXYCAMPTOTHECIN	BRD-K63784565-001-03-9	48.8	45.4	41.7	41.5	18.3	11.8
1551	Arecaidine but-2-ynyl ester tosylate	BRD-K63792901-075-01-3	34.7	-30.1	-0.4	19.2	2.8	1.9
1552	RALOXIFENE HYDROCHLORIDE	BRD-K63828191-003-11-5	-18.8	-5.3	-0.1	8.7	-31.8	-29.6
1553	Thioperamide maleate	BRD-K63874012-103-01-5	-13.5	-12.6	32.2	22.7	3.3	-1.9
1554	DIHYDROSAMIDIN	BRD-K63945320-001-03-2	-4.5	-13.5	-25.5	-36.9	-13.0	-9.5
1555	2-Methyl-5-hydroxytryptamine hydrochloride	BRD-K64137799-003-01-7	31.0	21.0	15.1	32.7	-13.7	-15.8
1556	ZD 2079 hydrochloride	BRD-K64157027-003-01-9	-1.4	0.9	-7.0	6.9	6.8	6.8
1557	BTS	BRD-K64178227-001-04-1	-7.9	-17.7	8.3	13.5	7.5	8.4
1558	DIFUCOL HEXAMETHYL ETHER	BRD-K64246525-001-02-9	4.2	-6.2	13.2	19.5	24.9	20.2
1559	CFM 1571 hydrochloride	BRD-K64341947-003-01-6	-14.5	-15.4	-65.2	-64.2	-34.8	-36.9
1560	DNQX	BRD-K64400208-001-02-6	13.9	23.7	-12.6	-21.6	3.6	-6.6
1561	Ivachtin	BRD-K64402243-001-01-1	14.9	24.4	34.8	38.6	24.3	17.4

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	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1562	TOLTRAZURIL	BRD-K64514229-001-01-1	-24.5	-23.3	-79.3	-86.7	-41.5	-32.9
1563	SALICIN	BRD-K64614248-001-06-5	-8.4	-3.3	14.8	10.5	1.3	5.4
1564	JNJ 16259685	BRD-K64670467-001-01-2	-7.9	13.4	2.8	-4.9	12.6	22.1
1565	Etazolate hydrochloride	BRD-K64755930-003-02-4	15.1	10.3	9.6	18.8	22.8	23.7
1566	PHLORACETOPHENONE	BRD-K64824948-001-03-0	13.6	14.2	-13.1	-6.5	26.6	34.1
1567	NABUMETONE	BRD-K65146499-001-14-7	7.0	-0.1	-14.2	-6.2	2.8	-2.0
1568	BPDQ	BRD-K65185756-001-01-0	-6.2	-3.7	17.3	5.5	11.1	14.9
1569	N- (9-FLUORENYLMETHOXYCARBONYL)-L-LEUCINE	BRD-K65275554-001-03-9	8.6	3.5	-48.0	-48.9	-6.6	-13.8
1570	GP 1a	BRD-K65285700-001-01-5	-22.2	-35.1	-51.8	-56.0	-32.9	-13.7
1571	MONOCROTALINE	BRD-K65508953-001-08-9	31.2	14.7	58.8	59.4	24.9	24.7
1572	ICARIIN	BRD-K65639003-001-05-8	10.4	19.4	13.1	13.5	7.8	-0.9
1573	KINETIN	BRD-K65667145-001-07-4	6.1	14.3	24.6	21.4	25.4	21.0
1574	CGP 7930	BRD-K65786282-001-02-6	-23.5	-11.2	-29.0	-18.1	-23.3	-23.2
1575	Diphenyleneiodonium chloride	BRD-K65814004-003-01-1	-93.2	-98.0	-73.7	-73.4	-56.4	-60.3
1576	(S)-(+)-Rolipram	BRD-K65856711-001-01-0	-12.7	20.2	-9.7	5.2	5.7	7.3
1577	FGIN-1-43	BRD-K66093087-001-02-3	2.8	1.6	3.8	7.5	-2.2	1.6
1578	FLUVASTATIN	BRD-K66296774-001-02-0	-15.2	-11.8	-53.2	-57.9	-18.7	-27.3
1579	ZOXAZOLAMINE	BRD-K66353228-001-08-8	21.1	30.2	13.5	34.4	16.2	13.9
1580	ACETOSYRINGONE	BRD-K66643401-001-04-0	20.0	27.7	-4.6	20.3	-17.4	-24.5
1581	(+)-UH 232	BRD-K66715657-001-01-3	24.8	-8.5	34.6	-4.6	12.9	18.0
1582	ICI-162,846	BRD-K66782112-001-01-2	-13.7	-9.2	5.6	6.1	13.1	20.1
1583	Pifithrin- a hydrobromide	BRD-K66874953-004-01-3	-9.6	-15.2	12.9	4.9	10.5	16.2
1584	Luzindole	BRD-K67013324-001-01-5	7.6	-2.7	7.1	25.7	33.8	40.6
1585	CILOSTAZOL	BRD-K67017579-001-16-6	39.7	-3.6	-3.9	9.4	2.0	3.0
1586	ALTRETAMINE	BRD-K67043667-001-15-7	2.7	2.5	-1.6	-4.3	26.1	7.0
1587	Milrinone	BRD-K67080878-001-05-5	-8.6	-12.8	0.9	14.4	11.6	12.5
1588	4-Phenylbutyrate, sodium salt	BRD-K67102207-236-01-0	18.4	-19.2	-6.8	-2.3	18.4	19.2
1589	FENTHION	BRD-K67217586-001-04-9	-4.0	-7.4	-13.7	19.9	12.1	13.3
1590	GIBBERELLIC ACID	BRD-K67237946-001-04-2	-0.7	-6.7	11.7	12.5	44.8	32.1
1591	SB 431542	BRD-K67298865-001-03-3	14.9	-5.6	3.2	16.3	6.6	12.0
1592	TC 2559 difumarate	BRD-K67352070-364-01-5	-13.6	17.2	4.1	1.6	16.8	9.2
1593	SIB 1893	BRD-K67439147-001-01-7	-4.7	0.4	-0.1	12.7	8.3	10.2
1594	Flurofamide	BRD-K67445247-001-01-3	14.9	36.4	-11.6	-18.3	12.6	13.9
1595	AG-126	BRD-K67506692-001-04-6	23.0	25.1	-27.0	-9.2	7.7	17.7
1596	PQ 401	BRD-K67537649-001-01-1	-4.1	-7.8	-65.0	-56.6	-28.7	-31.2
1597	MYOSMINE	BRD-K67556876-001-04-9	-12.3	-14.9	-20.9	-21.2	16.0	12.1
1598	ACEMETACIN	BRD-K67563174-001-09-3	-0.3	15.7	17.0	0.2	32.2	30.3
1599	CI 966 hydrochloride	BRD-K67680372-003-01-8	-8.7	10.1	-51.2	-60.7	-35.1	-29.4
1600	PHYSCION	BRD-K67772619-001-03-6	20.0	4.0	13.1	15.2	13.2	-1.5
1601	Haloperidol hydrochloride	BRD-K67783091-003-03-6	29.0	14.7	-4.2	-9.7	19.5	11.1
1602	ZM 323881 hydrochloride	BRD-K67831364-003-01-7	16.7	34.8	6.0	7.2	15.5	19.7
1603	Palmitoylethanolamide	BRD-K68095457-001-04-4	-9.6	-21.2	-5.2	-4.5	5.2	5.9
1604	CGS 20625	BRD-K68103045-001-01-1	-2.2	1.0	-4.1	-4.9	-20.4	-15.0
1605	TERBINAFINE HYDROCHLORIDE	BRD-K68132782-003-05-4	-5.9	4.5	24.8	56.6	38.8	14.2
1606	GR 46611	BRD-K68190965-001-01-4	-9.8	5.9	-23.8	-31.8	-15.6	-13.3
1607	UK 14,304 tartrate	BRD-K68264559-045-01-6	48.1	61.9	24.3	45.0	27.5	25.9

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1608	Statil	BRD-K68332390-001-03-3	-27.7	-5.2	15.3	3.4	11.3	24.2
1609	W-9 hydrochloride	BRD-K68341547-003-01-6	-44.9	-35.3	-75.0	-61.2	-51.3	-60.8
1610	ZK 93426 hydrochloride	BRD-K68392338-003-01-2	-17.6	-15.0	-51.1	-55.9	-24.8	-26.0
1611	ML 9 hydrochloride	BRD-K68402494-003-01-9	-35.2	-34.3	-67.3	-63.5	-58.9	-52.8
1612		BRD-K68432770-001-08-0	-0.9	-2.0	-0.1	-1.0	10.8	3.6
1613	DICYCLOMINE HYDROCHLORIDE	BRD-K68507560-003-15-4	-24.4	-21.8	-61.0	-75.1	-26.9	-29.7
1614	Phorbol 12-Myristate 13-Acetate	BRD-K68552125-001-04-6	-3.5	-7.8	85.6	82.1	30.4	32.4
1615	TODRALAZINE HYDROCHLORIDE	BRD-K68553471-003-07-3	10.1	5.1	8.8	18.0	-28.5	-32.8
1616	DERACOXIB	BRD-K68558722-001-03-2	-0.3	27.2	-69.7	-77.4	-4.8	17.0
1617	ACDPP hydrochloride	BRD-K68633617-003-01-1	12.7	24.9	18.9	22.4	21.0	21.6
1618	QUETIAPINE	BRD-K68867920-001-05-2	-19.5	-29.8	-76.2	-80.1	-44.2	-50.3
1619	VISNAGIN	BRD-K68995359-001-06-9	-11.6	-4.5	-3.1	1.3	20.2	7.2
1620	2,4-DICHLOROPHENOXYBUTYRIC ACID	BRD-K69188402-001-04-2	47.9	3.0	-41.7	-26.6	18.3	8.7
1621	NAN-190 hydrobromide	BRD-K69195780-004-03-5	8.4	6.8	3.5	21.3	2.8	-6.1
1622	RYANODINE	BRD-K69556541-001-02-6	-1.6	-12.6	28.2	25.7	24.6	21.0
1623	3-HYDROXYMETHYL-beta-CARBOLINE	BRD-K69585439-001-01-2	-23.5	-36.7	52.8	39.1	4.6	1.0
1624	TACROLIMUS	BRD-K69608737-001-03-7	-9.1	-8.8	-58.5	-34.4	-13.5	-20.5
1625		BRD-K69650333-001-02-9	7.6	0.9	-29.1	-26.4	-4.7	-11.0
1626	LY 341495	BRD-K69763916-001-01-7	24.6	16.3	-4.1	20.2	13.9	21.1
1627	Trap 101	BRD-K69837166-003-01-2	6.4	-3.1	-22.6	-3.0	-8.6	16.1
1628	L-692,585	BRD-K70241288-001-01-1	-9.0	2.1	22.5	16.5	33.9	45.9
1629	RIBOFLAVIN	BRD-K70246307-001-03-3	294.8	308.9	-6.6	0.3	11.3	3.7
1630	U 99194 maleate	BRD-K70281171-103-01-1	10.1	-4.2	17.1	17.0	10.6	20.0
1631	ESCITALOPRAM OXALATE	BRD-K70301876-034-06-1	38.9	58.4	-3.2	19.8	12.3	9.5
1632	SURAMIN	BRD-K70327167-348-09-2	12.2	-8.4	7.1	4.0	1.5	8.5
1633	BENZOXIQUINE	BRD-K70327191-001-01-4	8.7	2.2	16.6	18.5	-3.5	-4.5
1634	AMANTADINE HYDROCHLORIDE	BRD-K70330367-003-03-8	17.4	33.9	12.3	5.4	3.5	6.4
1635	1-(2-METHOXYPHENYL)PIERAZINE HYDROCHLORIDE	BRD-K70343553-003-06-8	2.2	13.6	11.8	3.0	5.8	-6.1
1636	ARIPIPRAZOLE	BRD-K70358946-001-06-6	-9.9	-38.9	-70.1	-53.4	-52.0	-44.5
1637	RANITIDINE	BRD-K70505054-001-02-9	-2.0	-5.3	-5.7	-2.2	5.0	-3.3
1638	H-9 dihydrochloride	BRD-K70577657-300-04-1	5.3	-3.2	-7.6	5.5	-0.6	6.0
1639	1-EBIO	BRD-K70586315-001-01-6	0.5	17.5	28.2	29.6	26.2	27.4
1640	TRAZODONE HYDROCHLORIDE	BRD-K70778732-003-15-0	-8.4	-0.2	6.6	3.4	3.4	2.4
1641	10-DEBC hydrochloride	BRD-K70792160-003-01-2	-100.3	-93.3	-100.0	-100.8	-82.7	-82.5
1642	HOMOPTEROCARPIN	BRD-K71093375-001-03-5	17.2	12.6	-9.8	-14.5	4.5	6.7
1643	SULFADIMETHOXINE	BRD-K71125014-001-17-2	-2.8	-11.3	6.3	7.7	12.3	13.7
1644	SULFAQUINOXALINE SODIUM	BRD-K71133585-236-08-6	5.4	7.6	-6.2	2.2	10.9	-1.0
1645	ISOPEONOL	BRD-K71175374-001-02-3	9.2	2.2	4.8	15.8	11.2	1.4
1646	Clobenpropit dihydrobromide	BRD-K71430621-303-01-5	3.1	7.5	4.1	-2.6	11.8	2.7
1647	MORANTEL CITRATE	BRD-K71454870-048-03-0	-8.5	-22.4	-4.9	-4.3	12.4	6.1
1648	GW 9508	BRD-K71534238-001-03-5	-2.1	-5.7	-47.7	-46.5	-5.4	0.3
1649	PNU 120596	BRD-K71731651-001-01-9	2.1	-6.8	14.8	19.9	-1.0	4.8
1650	CARBAMAZEPINE	BRD-K71799949-001-18-2	22.1	-2.3	-8.8	4.1	4.9	5.3
1651	Cdk2/5 Inhibitor	BRD-K71860425-001-01-1	33.9	1.7	43.1	31.1	23.3	15.6
1652		BRD-K71879491-001-15-0	-10.4	12.0	1.4	5.3	-0.1	-4.6
1653	MRS 1754	BRD-K72024482-001-01-3	-2.6	-3.3	22.5	19.9	16.1	17.2

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1654	PROBUCOL	BRD-K72029282-001-15-4	14.3	3.9	-6.5	-7.4	4.0	5.3
1655	DERRUSNIN	BRD-K72066653-001-03-3	2.8	-9.6	-19.5	-16.9	2.7	-8.1
1656	BPIQ-I	BRD-K72211743-001-01-1	-3.4	-5.2	15.7	9.0	7.0	4.6
1657	QUINAPRIL HYDROCHLORIDE	BRD-K72222507-003-07-7	-6.4	-13.8	8.5	9.6	27.5	21.9
1658	ISOPIMPINELLIN	BRD-K72253829-001-07-7	6.6	1.3	-4.1	23.1	33.5	24.8
1659	DYCLONINE HYDROCHLORIDE	BRD-K72259270-003-15-7	-62.3	-62.5	-93.1	-92.7	-86.4	-85.1
1660	BAICALEIN	BRD-K72327355-001-06-3	86.7	59.0	49.8	65.8	-12.6	-16.5
1661	C-1	BRD-K72462751-001-01-9	-7.8	-11.4	-9.0	-17.6	-8.4	8.9
1662	Fluvoxamine maleate	BRD-K72676686-103-01-8	-9.2	-15.2	-53.5	-57.6	-18.2	-24.4
1663	ZM 447439	BRD-K72703948-001-02-8	7.4	-7.9	-25.4	-19.0	-16.3	-9.7
1664	BENZETHONIUM CHLORIDE	BRD-K72723676-003-10-3	-77.2	-76.5	-98.0	-97.5	-87.9	-86.7
1665	Arcyriaflavin A	BRD-K72726508-001-01-3	41.0	31.4	-13.5	-9.6	-19.3	-19.0
1666	AG 555	BRD-K72783841-001-01-0	3.3	5.7	-44.5	-54.1	-53.5	-60.0
1667	SSR 69071	BRD-K72895815-001-01-4	-32.2	-24.7	-87.2	-87.5	-50.8	-54.2
1668	ZIDOVUDINE [AZT]	BRD-K72903603-001-14-5	16.7	18.0	-2.8	-2.6	0.1	-2.2
1669	CINCHOPHEN	BRD-K72915123-001-11-6	-4.0	-4.0	-11.1	13.1	20.0	14.5
1670	PEUCENIN	BRD-K73103240-001-03-3	18.7	2.6	-36.4	-26.9	-17.3	-24.4
1671	DIAZOXIDE	BRD-K73109821-001-10-2	-18.1	-4.6	18.9	44.0	26.0	17.3
1672	PHENYL AMINOSALICYLATE	BRD-K73157543-001-03-3	8.3	12.6	7.2	16.8	-0.3	12.3
1673	ALIZARIN	BRD-K73191876-001-04-7	8.7	7.0	13.2	22.1	-12.6	-21.0
1674	URAPIDIL HYDROCHLORIDE	BRD-K73196317-003-07-2	-8.5	-13.5	-13.2	-0.5	4.2	1.7
1675	TRIPTOPHENOLIDE	BRD-K73210450-001-03-1	-13.3	-9.5	-43.1	-39.7	-54.0	-54.0
1676	CLORGILINE HYDROCHLORIDE	BRD-K73251053-003-13-1	3.5	-7.9	-17.8	-13.6	-8.4	-11.1
1677	ICI-199,441 hydrochloride	BRD-K73290745-003-01-8	-27.1	-27.8	-65.4	-72.7	-59.2	-49.4
1678	BIOCHANIN A	BRD-K73303757-001-12-5	-1.8	-0.8	-28.3	-19.5	8.4	-0.5
1679	OXOLINIC ACID	BRD-K73394555-001-08-6	-4.1	3.8	-2.2	-1.8	14.2	10.4
1680	ARP 101	BRD-K73395020-001-01-5	-6.6	-23.8	-44.0	-54.0	-24.7	-18.7
1681	Purmorphamine	BRD-K73397362-001-01-7	4.3	-8.4	1.3	18.0	26.8	23.2
1682	DIBUTYL PHTHALATE	BRD-K73477617-001-04-4	5.8	8.0	20.0	35.9	19.4	22.9
1683	NIZATIDINE	BRD-K73589491-001-05-4	-10.0	-4.2	4.5	2.4	4.1	2.3
1684	BROMOPRIDE	BRD-K73642618-001-08-3	9.4	-3.1	-1.2	-4.6	7.2	11.8
1685	N-Acetyltryptamine	BRD-K73700643-001-04-7	8.6	13.9	37.8	39.3	9.8	15.2
1686	ZM 336372	BRD-K73789395-001-05-7	-32.4	-19.3	27.7	44.3	48.2	40.8
1687	SKATOLE	BRD-K73824630-001-03-2	6.7	7.0	27.2	11.6	34.8	38.0
1688	N-hydroxy-2-phenylacetamide	BRD-K74112339-001-03-5	7.2	10.8	5.8	-9.2	8.1	9.3
1689	(-)-Cytisine	BRD-K74186897-001-04-1	5.4	-1.4	-0.3	-3.1	23.5	22.3
1690	RESORCINOL	BRD-K74190368-001-02-7	4.8	5.7	7.5	15.4	-16.9	-20.7
1691	Irsogladine maleate	BRD-K74195153-050-03-0	6.6	-8.9	18.5	16.7	13.0	2.7
1692	DCB	BRD-K74430258-001-01-2	-17.5	20.7	-4.1	-1.2	6.9	-1.5
1693	AZITHROMYCIN	BRD-K74501079-001-07-4	28.2	37.2	16.5	22.2	32.7	33.0
1694	2-METHYL-4-(PIPERIDIN-1-YLCARBOXY)-5-ISOPROPYLPHENYLTRIMETHYLAMMONIUM CHLORIDE	BRD-K74534237-003-01-3	-11.7	4.3	11.9	43.5	16.3	24.1
1695	CATECHIN TETRAMETHYLETHER	BRD-K74727418-001-03-4	-13.9	-15.0	-16.4	3.1	7.2	-7.1
1696	BW 373U86	BRD-K74990253-001-01-0	-2.7	-12.1	32.1	16.6	10.4	11.3
1697	PROCAINAMIDE HYDROCHLORIDE	BRD-K75089421-003-15-3	9.9	2.7	9.7	8.5	12.0	10.5
1698	Cdk1 Inhibitor III	BRD-K75127215-001-01-5	-0.7	18.6	20.1	32.7	4.1	17.1
1699	PROTIONAMIDE	BRD-K75360161-001-09-9	2.6	4.6	5.5	17.7	10.2	14.3

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1700	BENZOCAINE	BRD-K75466013-001-08-6	1.6	5.0	48.2	57.2	26.3	23.4
1701	GS39783	BRD-K75478907-001-01-5	11.6	19.1	1.5	13.9	-2.8	31.9
1702	(R)-(-)-Rolipram	BRD-K75516118-001-01-7	-3.9	25.7	-16.3	17.0	39.2	41.8
1703	HYDROXYTOLUIC ACID	BRD-K75608666-001-03-4	-4.7	4.8	0.6	2.6	10.3	10.6
1704	B-HT 920	BRD-K75615183-300-02-1	30.8	32.4	12.7	26.9	16.3	24.0
1705	METOCLOPRAMIDE HYDROCHLORIDE	BRD-K75641298-003-16-9	8.5	-1.4	9.2	16.3	5.8	-3.9
1706	RIZATRIPTAN BENZOATE	BRD-K75699339-057-03-2	-1.5	13.7	10.3	5.8	0.6	5.7
1707	3,7-DIMETHOXYFLAVONE	BRD-K75745696-001-03-8	-10.8	-14.1	-31.2	-31.6	-4.8	-3.9
1708	m-CPP hydrochloride	BRD-K75844781-003-03-1	-2.3	-0.7	-8.1	-1.2	5.6	0.0
1709	IODOQUINOL	BRD-K75855670-001-06-8	36.3	45.7	-25.1	-10.9	-12.6	-10.0
1710	PIZOTYLINE MALATE	BRD-K75958195-037-04-5	-3.9	-4.8	-41.8	-37.0	-7.1	-1.7
1711	LOSARTAN	BRD-K76205745-001-04-1	12.4	4.8	23.0	20.3	16.0	19.6
1712	PHENAZOPYRIDINE HYDROCHLORIDE	BRD-K76304753-003-08-8	3.6	4.1	-10.3	2.2	0.7	-8.5
1713	NITROMIDE	BRD-K76381435-001-04-5	1.7	-0.3	8.2	29.1	17.3	18.8
1714	ENROFLOXACIN	BRD-K76534306-001-11-0	-10.0	-6.5	21.8	33.1	25.4	30.4
1715	PHTPP	BRD-K76568384-001-01-4	18.0	31.0	36.3	20.6	32.8	29.4
1716	HA-1077	BRD-K76617868-300-04-4	-10.6	-0.4	-14.2	-20.3	-10.0	8.4
1717	Homoharringtonine	BRD-K76674262-001-01-7	-6.5	-3.4	14.9	9.3	6.3	7.0
1718	(+)-AJ 76 hydrochloride	BRD-K76677554-003-01-3	1.1	11.9	-4.5	12.7	16.7	9.3
1719	NIMESULIDE	BRD-K76775527-001-18-7	-6.8	-13.1	-28.8	-24.7	-11.3	-17.0
1720	SB 415286	BRD-K76805682-001-05-0	62.5	50.8	-29.6	-21.1	-37.5	-40.5
1721	DIPYRONE	BRD-K76812510-236-08-0	-17.2	-40.3	31.8	42.5	-24.8	-28.5
1722	RS 17053 hydrochloride	BRD-K76840893-003-01-7	-62.4	-64.5	-74.3	-76.9	-67.7	-70.5
1723	SULFANITRAN	BRD-K76845197-001-02-1	6.0	5.9	-13.6	-22.5	0.2	-4.8
1724	Proxyfan maleate	BRD-K77171813-050-01-4	18.6	8.3	7.1	7.6	7.2	2.8
1725	4-HYDROXY-6-METHYLPYRAN-2-ONE	BRD-K77202630-001-03-7	4.4	-1.2	8.4	17.9	27.8	15.3
1726	RAUWOLSCINE HYDROCHLORIDE	BRD-K77474816-003-09-1	13.8	12.9	6.5	21.2	22.2	16.7
1727	A 205804	BRD-K77627880-001-01-6	4.5	21.9	-11.8	-11.6	18.8	26.5
1728	AEG 3482	BRD-K77634909-001-02-7	-3.8	-13.9	-12.9	-24.4	6.4	13.2
1729	NAPHAZOLINE HYDROCHLORIDE	BRD-K77641333-003-15-6	-1.3	14.5	-3.8	12.1	17.1	14.6
1730	SB 200646 hydrochloride	BRD-K77677632-003-01-8	-24.7	-27.8	-16.0	-5.3	-1.3	-13.3
1731	ACACETIN	BRD-K77685744-001-07-7	9.0	-12.7	-8.7	7.7	11.7	14.0
1732	THIABENDAZOLE	BRD-K77695569-001-16-9	3.0	8.0	19.8	-6.6	17.4	18.6
1733	Moxonidine hydrochloride	BRD-K77771411-003-03-2	12.2	5.5	-7.9	4.9	6.3	10.5
1734	HA 1100 hydrochloride	BRD-K77793136-003-02-2	-1.9	5.1	31.5	15.3	11.9	7.0
1735	MS-275	BRD-K77908580-001-04-7	2.5	3.6	20.0	10.6	-0.8	8.2
1736	PD 81723	BRD-K77951111-001-01-1	2.1	2.7	0.1	21.7	15.9	8.6
1737	MEBENDAZOLE	BRD-K77987382-001-08-2	10.2	17.4	37.3	38.3	-6.1	8.6
1738	FUROSEMIDE	BRD-K78010432-001-10-8	-2.4	10.4	-27.3	3.8	19.6	16.3
1739	4-PPBP maleate	BRD-K78061844-103-01-6	22.3	7.5	29.2	29.5	16.3	15.4
1740	ENOXACIN	BRD-K78113049-001-07-1	3.6	3.9	10.1	7.3	10.0	12.9
1741	NNC 55-0396 dihydrochloride	BRD-K78122587-300-01-9	-106.4	-104.0	-94.2	-93.6	-79.0	-81.4
1742	MENADIONE	BRD-K78126613-001-16-0	-16.1	-15.8	-56.0	-54.1	-61.6	-62.2
1743	ANHYDROBRAZILIC ACID	BRD-K78414110-001-03-6	21.6	20.0	15.2	19.8	26.7	30.8
1744	OLMESARTAN MEDOXOMIL	BRD-K78485176-001-03-7	10.4	17.2	7.9	26.3	30.8	25.5
1745	SCS	BRD-K78496197-001-02-1	9.5	7.4	-9.6	-4.8	-9.3	-10.3

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1746	LONIDAMINE	BRD-K78513633-001-06-6	2.8	4.4	58.1	25.7	26.3	9.9
1747	ELETRIPTAN HYDROBROMIDE	BRD-K78537690-004-01-0	9.1	5.2	22.4	-11.2	5.8	8.4
1748	CITROPTEN	BRD-K78612426-001-05-9	-7.7	-1.9	81.8	89.9	-7.5	-20.5
1749	Exo1	BRD-K78633253-001-04-6	10.6	-0.5	14.5	36.2	9.2	22.5
1750	LY 320135	BRD-K78637815-001-01-4	-9.3	-3.1	-2.9	-2.0	13.3	2.4
1751	BROMPERIDOL	BRD-K78643075-001-06-6	-28.3	-23.2	-60.2	-67.6	-53.1	-63.4
1752	Leflunomide	BRD-K78692225-001-11-2	-8.9	-11.1	3.5	11.5	10.0	4.7
1753	SUXIBUZONE	BRD-K78815826-001-08-8	1.6	8.1	0.4	24.1	5.2	-5.2
1754	ASPARTAME	BRD-K78841970-001-06-2	6.9	12.0	-10.8	13.2	10.0	8.9
1755	N-[2-(Piperidinylamino)ethyl]-4-iodobenzamide	BRD-K78844995-001-01-8	-8.8	23.1	-4.4	-9.9	-4.8	0.8
1756	FPL 64176	BRD-K78959463-001-05-8	-0.6	6.7	-4.1	10.7	-2.2	-3.2
1757	NITROFURAZONE	BRD-K79092138-001-06-0	11.7	22.5	8.8	44.7	17.0	17.9
1758	ALBENDAZOLE	BRD-K79131256-001-08-8	23.5	22.6	-11.7	33.0	6.6	31.3
1759	CY 208-243	BRD-K79353516-001-03-5	22.4	11.9	-19.9	-15.9	-7.9	-10.9
1760	COTARNINE CHLORIDE	BRD-K79535367-003-02-5	7.1	2.5	-18.8	-11.0	9.8	-13.2
1761	Metformin (1,1-Dimethylbiguanide, Hydrochloride)	BRD-K79602928-003-04-1	-13.8	-15.3	28.9	11.5	0.1	9.9
1762	Ro 10-5824	BRD-K79684402-300-01-0	0.7	9.9	-0.7	-12.6	9.4	1.0
1763	THIAMPHENICOL	BRD-K79711234-001-11-8	7.0	1.1	3.9	7.6	-0.1	-0.9
1764	SILDENAFIL CITRATE	BRD-K79759585-048-01-4	-0.9	-0.7	5.8	18.7	23.6	31.7
1765	Gabazine	BRD-K79905821-001-01-6	-10.8	-8.0	16.8	15.7	11.5	15.4
1766	GW 583340 dihydrochloride	BRD-K79930101-300-01-1	-18.9	-19.8	-13.9	-16.9	-21.3	-4.8
1767	CLOPIDOL	BRD-K80036624-001-03-2	5.2	-0.9	6.2	30.0	10.9	16.2
1768	DPPE fumarate	BRD-K80315159-051-01-2	-17.7	-17.2	-15.1	-15.7	-13.6	-6.0
1769	(+/-)-abscisic acid	BRD-K80342836-001-01-2	-2.0	-22.0	-9.2	3.7	25.3	22.5
1770	SILIBININ	BRD-K80353138-001-07-1	32.5	43.5	-31.2	-14.9	-22.3	-32.6
1771	KHELLIN	BRD-K80353807-001-16-2	-22.3	-9.8	-0.3	25.4	21.5	29.8
1772	Zamifenacin fumarate	BRD-K80451230-051-01-8	-3.8	-16.6	-8.1	-20.6	1.5	0.5
1773	6,7-DICHLOROQUINOXALINE-2,3-DIONE	BRD-K80576679-001-03-1	7.7	2.7	17.5	35.1	0.7	5.3
1774	SB 258585 hydrochloride	BRD-K80639402-003-01-1	-0.2	-1.8	-31.0	-35.9	-30.3	-29.4
1775	RS 16566 hydrochloride	BRD-K80725821-300-01-1	7.9	32.7	-7.1	-14.3	14.7	16.3
1776	Resveratrol	BRD-K80738081-001-07-0	-26.6	-39.0	12.9	12.5	-18.4	-15.6
1777	Ro 19-4605	BRD-K80778372-001-01-7	16.1	-9.5	14.0	13.9	19.1	20.1
1778	N-PHENYLANTHRANILIC ACID	BRD-K80863915-001-05-2	19.4	19.4	-7.8	11.7	8.2	-0.8
1779	TRIACETYLRESVERATROL	BRD-K80946661-001-03-6	6.3	4.9	-15.9	-40.1	2.7	2.7
1780	METHYLXANTHOXYLIN	BRD-K81120886-001-01-0	7.2	2.0	0.3	15.7	2.7	0.0
1781	SALICYLAMIDE	BRD-K81130846-001-12-5	15.3	8.3	33.1	60.1	4.6	16.4
1782	Cerivastatin	BRD-K81169441-236-04-1	-7.0	-8.8	17.7	-26.3	24.5	-8.7
1783	SCH 58261	BRD-K81225797-001-01-5	-24.1	24.4	12.1	-16.2	10.9	8.8
1784	Dantrolene, sodium salt	BRD-K81272440-236-06-9	-32.1	4.4	-38.0	-48.1	-9.4	-22.1
1785	CHRYSIN DIMETHYL ETHER	BRD-K81298036-001-06-2	-17.8	-10.1	-49.2	-50.2	-14.0	-15.7
1786	TCS 359	BRD-K81376179-001-01-4	6.2	5.6	29.1	28.6	-3.0	0.4
1787	SAHA	BRD-K81418486-001-18-6	14.4	-5.4	-5.4	0.3	-9.0	5.0
1788	TACRINE HYDROCHLORIDE	BRD-K81473089-003-15-4	-3.4	2.4	12.7	14.0	10.8	8.6
1789	DICYCLOHEXYLUREA	BRD-K81521265-001-02-8	-8.6	-25.8	9.8	8.8	22.2	28.5
1790	EIT hydrobromide	BRD-K81623406-004-03-4	2.5	2.5	1.6	4.9	10.3	8.5
1791	AQ-RA 741	BRD-K81729199-001-01-0	-3.5	-2.0	12.8	12.1	5.4	15.2

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1792	PRENYLETIN	BRD-K81750404-001-03-3	40.7	10.5	-12.6	-15.7	-18.3	-26.8
1793	PICROPODOPHYLLIN	BRD-K81829253-001-03-7	25.8	21.3	-17.1	1.0	-4.5	7.3
1794	CP 93129 dihydrochloride	BRD-K81876028-300-01-2	14.3	4.3	25.2	40.7	17.4	23.5
1795	1,3,5-TRIMETHOXYBENZENE	BRD-K81884069-001-03-6	0.0	2.8	-6.4	0.4	27.4	18.4
1796	TRICLABENDAZOLE	BRD-K81916719-001-05-5	46.6	21.2	17.4	23.9	27.8	47.0
1797		BRD-K81965037-001-03-2	-83.4	-84.6	-78.1	-77.6	-60.9	-65.9
1798	SERTRALINE HYDROCHLORIDE	BRD-K82036761-003-07-0	-44.0	-42.0	-64.2	-61.4	-49.4	-45.7
1799	BETAMIPRON	BRD-K82142815-001-12-6	38.2	6.5	8.9	22.7	18.9	2.1
1800	PYRITINOL	BRD-K82181219-001-01-9	5.9	10.7	0.1	11.6	4.1	15.4
1801	2',4'-DIHYDROXY-4-METHOXYCHALCONE	BRD-K82207906-001-01-0	27.8	2.5	-27.6	-14.8	8.5	2.7
1802	ISOSORBIDE MONONITRATE	BRD-K82225283-001-01-5	-3.1	-3.6	10.2	31.2	5.8	9.1
1803	N-METHYL (-)EPHEDRINE	BRD-K82236108-001-03-1	9.5	-6.1	-21.0	-12.7	3.8	2.8
1804	DICUMAROL	BRD-K82236179-001-06-8	-1.2	6.6	-42.8	-50.4	-4.5	-1.3
1805	PROPOFOL	BRD-K82255054-001-08-4	12.7	8.1	1.8	27.3	-2.0	3.4
1806	Carmoxirole hydrochloride	BRD-K82484965-003-02-7	29.2	16.7	20.3	26.0	38.6	30.9
1807	WHI-P180, Hydrochloride	BRD-K82708110-003-01-5	64.8	19.2	12.0	12.8	16.7	11.5
1808	Olomoucine	BRD-K82731415-001-05-4	20.1	-19.0	-1.5	26.5	12.8	12.7
1809	LORATADINE	BRD-K82795137-001-14-8	5.3	0.6	-40.8	-42.5	-4.6	-19.7
1810	Ro 15-4513	BRD-K82823076-001-01-8	8.7	7.7	15.9	7.5	16.8	24.6
1811	ROSUVASTATIN CALCIUM	BRD-K82941592-238-02-9	-0.3	-4.1	-6.7	1.6	5.8	17.0
1812	GR 135531	BRD-K83023055-001-01-9	-5.1	-5.8	3.7	18.0	6.0	10.0
1813	SALICYLANILIDE	BRD-K83036479-001-04-3	15.7	42.8	-13.4	-3.4	-0.5	-1.7
1814	RS 102895 hydrochloride	BRD-K83063356-003-01-7	2.8	-2.5	-23.2	-37.1	-2.9	-7.3
1815	Etofylline	BRD-K83064458-001-05-7	-7.6	-3.7	6.5	-4.9	0.1	-3.0
1816	(S)-(+)-Dimethindene maleate	BRD-K83192048-050-01-9	-15.2	-24.3	-4.9	-7.2	8.3	-1.7
1817	CHLOROPYRAMINE HYDROCHLORIDE	BRD-K83257731-003-14-4	-12.5	-10.4	-45.9	-55.5	-24.9	-14.9
1818	Protopine	BRD-K83302049-003-01-2	-4.9	-20.6	41.6	19.2	19.4	20.5
1819	L-693,403 maleate	BRD-K83322645-103-01-6	2.7	-17.4	23.9	15.0	10.8	13.9
1820	BARBITAL	BRD-K83359602-001-01-5	13.7	-8.4	-2.3	-6.6	5.6	-7.7
1821	SINOMENINE	BRD-K83459933-001-03-9	-6.6	-2.0	-6.7	-0.1	-18.4	-25.0
1822	FK 888	BRD-K83508485-001-01-9	-18.1	-22.6	-35.7	-32.7	-14.8	-19.9
1823	PARGYLINE HYDROCHLORIDE	BRD-K83597974-003-15-6	37.3	14.5	-0.7	14.2	4.2	-1.9
1824	SANT-1	BRD-K83637872-001-01-7	22.0	31.1	38.1	29.9	-1.0	12.9
1825	7-Chlorokynurenic acid	BRD-K84214706-001-04-0	-0.7	-0.6	15.8	24.9	15.0	11.9
1826	BRL 50481	BRD-K84266862-001-01-6	27.2	15.1	11.3	16.6	15.6	15.4
1827	2'-METHOXYFORMONETIN	BRD-K84390227-001-03-0	-17.6	-21.0	-1.1	-3.0	3.5	11.1
1828	R(+)-SKF-81297	BRD-K84421793-001-01-1	7.0	5.3	28.2	26.2	-8.0	-11.6
1829	3,4-DIMETHOXYDALBERGIONE	BRD-K84463716-001-02-5	31.2	25.2	-18.3	11.0	-34.0	-35.1
1830	NATEGLINIDE	BRD-K84658672-001-03-0	7.4	11.4	-8.2	-6.9	-5.6	-9.4
1831	Trequinsin hydrochloride	BRD-K84663978-001-03-1	-1.1	1.2	-36.6	-29.5	-1.6	-3.6
1832	Caffeic acid phenethyl ester	BRD-K84709232-001-02-6	-9.2	-15.4	-84.7	-86.2	-67.8	-65.3
1833	TANSHINONE IIA SULFONATE SODIUM	BRD-K84798689-236-01-1	16.1	16.8	13.0	17.0	31.6	30.7
1834	SINENSETIN	BRD-K84996949-001-01-5	-5.5	0.1	35.3	33.7	-18.8	-29.3
1835	AURAPTENE	BRD-K85013741-001-05-9	20.3	21.9	82.1	89.4	30.5	21.5
1836	NNC 05-2090 hydrochloride	BRD-K85015012-003-01-1	-18.0	-20.7	-96.6	-93.1	-70.0	-67.0
1837	4'-HYDROXYCHALCONE	BRD-K85068298-001-03-5	2.0	6.0	-43.4	-49.7	-7.3	-12.9

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			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1838	PILOCARPINE NITRATE	BRD-K85090592-008-15-1	15.5	-2.6	8.0	-9.2	4.7	4.2
1839	3-ACETAMIDOCOUMARIN	BRD-K85104575-001-07-3	-7.1	15.5	21.3	31.6	24.1	27.5
1840	TOLBUTAMIDE	BRD-K85119730-001-17-2	-0.2	5.4	13.6	5.1	3.9	6.6
1841	DNQX disodium salt	BRD-K85266041-304-01-7	-6.0	-17.1	-1.8	-20.8	13.2	7.3
1842	RAMIFENAZONE	BRD-K85333151-003-08-4	7.6	5.0	20.1	15.0	-18.6	-18.8
1843		BRD-K85555482-001-04-5	-19.4	5.1	-11.2	-2.9	5.2	8.6
1844	RESORCINOL MONOACETATE	BRD-K85603128-001-02-7	-12.5	17.1	9.5	14.7	-3.7	6.5
1845	IRIGENIN TRIMETHYL ETHER	BRD-K85880973-001-03-5	5.8	9.7	7.6	-3.1	5.2	4.7
1846		BRD-K85883481-001-08-3	1.7	1.8	12.0	24.7	23.2	24.9
1847	OBTUSAQUINONE	BRD-K85971060-001-03-6	58.6	73.9	7.0	53.8	6.7	11.8
1848	EMF-bca1-1	BRD-K85985071-001-16-5	7.4	14.6	-45.6	-50.7	-37.2	-52.6
1849	Eltoprazine hydrochloride	BRD-K86171477-003-01-9	2.4	-2.2	1.0	10.0	10.2	11.1
1850	DIPYRIDAMOLE	BRD-K86301799-001-19-9	25.4	20.5	8.5	26.5	-25.1	-20.0
1851	(R)-(-)-Deprenyl hydrochloride	BRD-K86434416-003-06-4	-10.9	-12.2	-2.4	0.4	15.6	9.2
1852	ISO-OLOMOUCINE	BRD-K86509404-001-03-8	-20.2	-8.0	-12.1	-5.7	11.8	13.1
1853	RS 79948 hydrochloride	BRD-K86600316-003-01-2	-3.8	-15.3	24.3	8.1	6.5	11.1
1854	Embelin	BRD-K86727142-001-06-6	-60.7	-69.4	-87.6	-86.9	-67.8	-71.0
1855	Olvanil	BRD-K86958018-001-01-9	21.0	13.8	49.6	41.1	-4.4	-2.3
1856	RS 102221 hydrochloride	BRD-K87048468-003-01-9	7.0	9.3	-35.6	-33.2	-43.1	-35.9
1857	Fusaric acid	BRD-K87049188-001-03-6	2.9	-1.9	36.9	28.0	25.1	32.4
1858	CARBIMAZOLE	BRD-K87156652-001-06-9	2.1	-17.6	-7.9	-0.6	-7.3	-6.6
1859	BENZAMIL HYDROCHLORIDE	BRD-K87158025-003-01-2	6.3	10.6	-12.9	-18.5	4.1	6.1
1860	?-CCB	BRD-K87349602-001-02-0	1.1	-0.2	32.4	20.5	10.8	5.3
1861	TrkA Inhibitor	BRD-K87484409-001-01-2	0.2	16.8	15.2	-2.8	17.4	13.3
1862	SULFAMETER	BRD-K87492696-001-09-0	8.8	-3.9	4.1	23.8	22.1	26.9
1863	RS 504393	BRD-K87510569-001-01-0	18.6	6.3	-12.2	-10.3	-0.9	-6.0
1864	MPMQ hydrochloride	BRD-K87696786-003-01-0	0.3	-4.6	0.1	-16.1	0.1	-1.7
1865	CETYLPYRIDINIUM CHLORIDE	BRD-K87700323-003-03-6	-93.8	-94.0	-83.5	-82.2	-79.5	-77.1
1866	DUARTIN, DIMETHYL ETHER	BRD-K87798455-001-03-4	-4.7	-2.2	-15.4	-19.6	9.8	-3.9
1867	AG-825	BRD-K87919739-001-04-2	-1.4	-6.5	-4.7	-1.8	-21.1	-5.1
1868	PIMETHIXENE MALEATE	BRD-K88090157-050-06-6	-6.5	0.4	-61.9	-57.4	-39.4	-44.5
1869	ASARYLALDEHYDE	BRD-K88219015-001-05-8	-7.8	27.7	11.5	18.9	4.5	7.4
1870	WIN 55,212-2 mesylate	BRD-K88282786-066-04-9	23.7	15.5	-58.9	-59.3	7.7	4.5
1871	2,5-DI-t-BUTYL-4-HYDROXYANISOLE	BRD-K88329126-001-01-0	-10.2	-15.2	-45.9	-29.6	-22.0	-41.0
1872	Xaliproden hydrochloride	BRD-K88358234-003-01-4	-1.9	-10.1	10.7	-1.4	6.9	8.3
1873	TRIMETAZIDINE DIHYDROCHLORIDE	BRD-K88366685-300-04-5	-8.3	-2.4	3.8	13.5	20.1	7.1
1874	THONZYLAMINE HYDROCHLORIDE	BRD-K88405679-003-02-3	9.5	5.2	-0.1	9.2	9.2	-2.5
1875	PYRIMETHAMINE	BRD-K88429204-001-18-7	16.9	-6.1	-25.8	-3.2	-13.8	-12.1
1876	IPRONIAZID SULFATE	BRD-K88568253-065-03-9	32.6	35.0	22.6	15.5	11.2	2.6
1877	ANIRACETAM	BRD-K88611939-001-13-3	16.5	2.0	13.9	18.9	28.1	21.8
1878	NONOXYNOL-9	BRD-K88625236-001-03-4	-104.8	-98.6	-112.6	-113.2	-77.3	-77.1
1879	ARECOLINE HYDROBROMIDE	BRD-K88646909-004-10-5	4.0	13.3	8.9	39.6	39.5	46.5
1880	PD 198306	BRD-K88677950-001-01-3	2.6	13.0	26.5	12.2	27.9	18.1
1881	CHLOROTHIAZIDE	BRD-K88682005-001-07-5	2.2	40.6	5.2	4.3	27.6	24.5
1882	Methyl 2,5-dihydroxycinnamate	BRD-K88741031-001-01-0	34.5	41.1	16.5	4.0	-42.5	-45.5
1883	EMD 66684	BRD-K88759641-003-01-0	2.7	-11.2	11.0	4.4	12.3	16.4

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			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1884	LOBARIC ACID	BRD-K88849294-001-08-8	-42.2	-54.4	-83.8	-79.9	-73.6	-74.0
1885	OBLIQUIN	BRD-K88954184-001-03-0	1.5	-1.3	25.1	40.8	10.5	4.2
1886	Cdk Inhibitor, p35	BRD-K88988070-001-01-9	7.7	-10.9	9.4	-6.0	11.4	21.3
1887	ALVERINE CITRATE	BRD-K89055274-048-14-4	12.7	16.0	-11.1	-8.4	-1.4	-8.8
1888	CHLOROCRESOL	BRD-K89056082-001-03-6	27.2	26.8	-0.5	13.8	-17.3	-19.9
1889	EMD 41000	BRD-K89271983-001-01-5	-22.7	-25.9	-10.0	7.1	-6.5	3.1
1890	NPPB	BRD-K89272762-001-07-7	12.3	2.1	-27.5	-39.4	-17.1	-14.5
1891	DMP 543	BRD-K89274813-001-01-5	-7.3	4.5	-9.7	-7.2	1.8	-5.3
1892	PIRENZEPINE HYDROCHLORIDE	BRD-K89375097-300-06-2	27.0	14.8	-11.5	15.6	-9.7	1.2
1893	L 655240	BRD-K89402695-001-01-5	-58.9	-41.5	-94.4	-92.2	-76.0	-68.2
1894	CHLORPHENIRAMINE (S) MALEATE	BRD-K89595132-050-03-0	-10.4	-8.7	-13.1	0.8	8.2	-1.8
1895	VINCAMINE	BRD-K89704198-001-08-1	2.5	36.9	19.9	27.4	11.6	11.2
1896	TRIFLUOPERAZINE HYDROCHLORIDE	BRD-K89732114-300-07-1	-80.3	-92.5	-94.8	-94.0	-88.6	-88.6
1897	AG 592	BRD-K89930444-001-01-9	58.5	58.3	-14.1	-24.0	-9.9	-8.4
1898	GALANGIN TRIMETHYL ETHER	BRD-K89975061-001-02-4	-9.5	7.5	-15.2	-14.1	-19.1	-31.5
1899	CHLORPROMAZINE	BRD-K89997465-001-05-3	-81.0	-78.3	-95.6	-96.0	-87.3	-86.5
1900	AMPROLIUM	BRD-K90027121-300-08-2	37.5	11.6	13.3	12.2	22.0	24.9
1901	5-Iodo-A-85380 dihydrochloride	BRD-K90065682-300-01-8	-9.2	-2.8	3.7	6.9	1.4	21.4
1902	DIMETHYL 4,4-o-PHENYLENE-BIS (3-THIOPHANATE)	BRD-K90168339-001-04-5	4.7	-2.7	27.0	25.9	21.0	8.6
1903		BRD-K90230846-001-04-9	17.8	31.0	37.7	35.2	-14.9	-3.2
1904	W-7 hydrochloride	BRD-K90259198-003-07-1	-38.3	-41.5	-70.3	-66.4	-42.2	-48.0
1905	MY-5445	BRD-K90524085-001-06-0	-6.5	4.9	-30.2	-32.3	4.5	-1.1
1906	2-Phenylbenzimidazole	BRD-K90551865-001-05-1	5.7	32.9	17.7	9.7	23.3	16.5
1907	Ipsapirone	BRD-K90574421-001-01-9	-16.5	-21.5	-7.2	-14.6	13.6	14.3
1908	EPIAFZELECHIN (2R,3R)(-)	BRD-K90607708-001-03-7	24.2	4.4	-2.6	-11.9	1.4	-4.2
1909	Nefazodone hydrochloride	BRD-K90789829-003-03-3	-0.6	-1.5	-52.2	-52.9	-31.9	-27.3
1910	SR 142948	BRD-K91243525-001-01-5	-1.9	5.2	19.5	19.5	9.9	13.6
1911	ANISOMYCIN	BRD-K91370081-001-17-8	27.0	19.7	-4.6	9.4	17.7	2.8
1912	PICEATANNOL	BRD-K91509126-001-04-6	47.4	44.5	-19.9	-17.6	-59.2	-58.3
1913	DIOSMIN	BRD-K91548452-001-03-0	95.3	109.4	20.3	27.7	8.4	12.6
1914	4-HQN	BRD-K91758890-001-03-5	-14.4	-10.0	4.8	-4.3	19.4	12.7
1915	3H-1,2-DITHIOLE-3-THIONE	BRD-K91781484-001-01-3	-11.0	-11.8	17.6	27.1	11.2	15.0
1916	2-[1-(4-Piperonyl)piperazinyl]benzothiazole	BRD-K91868854-001-02-8	-1.8	-10.7	8.5	3.6	4.5	-1.8
1917	SD 169	BRD-K91904471-001-01-6	-19.8	-30.2	23.9	24.5	11.9	20.3
1918	AM 251	BRD-K92000912-001-06-8	-9.4	-14.0	-24.9	-25.2	-8.3	-6.1
1919	GBR 12783	BRD-K92015269-001-01-6	0.9	-14.0	-32.0	-25.2	-14.4	-10.4
1920	TRIAMTERENE	BRD-K92049597-001-10-9	10.0	-4.8	81.8	89.1	-8.8	-30.2
1921	3-HYDROXY-3',4'-DIMETHOXYFLAVONE	BRD-K92171060-001-03-4	62.7	92.4	11.2	13.0	6.2	5.8
1922	5-Carboxamidotryptamine maleate	BRD-K92382976-103-01-8	-4.3	-13.7	33.4	-6.5	8.2	11.0
1923	MYCOPHENOLATE MOFETIL	BRD-K92428153-001-01-0	67.5	37.8	43.1	23.0	24.1	19.7
1924	LY255283	BRD-K92492521-001-01-1	-37.8	-36.8	-76.1	-84.7	-23.7	-34.1
1925	2-Chloro-11-(4-methylpiperazino)dibenz[b,f]oxepin maleate	BRD-K92588747-051-01-9	-23.7	-19.6	25.6	27.2	-34.5	-45.4
1926		BRD-K92723993-066-04-5	-28.7	-30.2	-40.9	-31.0	-27.9	-35.2
1927	PERINDOPRIL ERBUMINE	BRD-K92731339-227-03-1	-6.1	-8.0	-11.3	-6.4	-1.7	8.6
1928	MEFENAMIC ACID	BRD-K92778217-001-17-8	38.6	16.3	-5.4	10.5	-0.7	14.5
1929	(R)-(+)-Propranolol hydrochloride	BRD-K92830582-003-04-8	-2.0	-4.7	-18.0	2.3	-18.8	-4.0

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1930	2,4,5-TRICHLOROPHENOXYACETIC ACID	BRD-K92860374-001-03-3	-2.9	-3.2	-6.0	7.0	21.2	15.1
1931	Melperone hydrochloride	BRD-K92984783-003-02-4	-1.5	-10.0	-10.7	-3.7	8.9	11.2
1932	ARC 239 dihydrochloride	BRD-K93188295-300-01-4	23.7	16.0	17.4	43.5	2.0	-8.4
1933	PIMPINELLIN	BRD-K93197368-001-03-7	15.8	-24.2	-19.6	-19.0	7.1	-1.2
1934	ETHAMBUTOL HYDROCHLORIDE	BRD-K93231391-300-03-1	2.8	-6.7	-9.9	7.6	-1.0	3.0
1935	DINITOLMIDE	BRD-K93240442-001-04-3	47.3	22.5	14.4	39.1	14.7	26.3
1936	GW 9662	BRD-K93258693-001-05-8	-9.9	-3.8	21.4	15.7	29.3	18.4
1937	Lamotrigine isethionate	BRD-K93460210-071-01-6	24.6	-1.7	0.4	5.9	5.2	10.4
1938	BUSPIRONE HYDROCHLORIDE	BRD-K93461745-003-14-4	4.6	8.6	11.0	11.6	29.5	23.5
1939	SULFAMERAZINE	BRD-K93524252-001-15-5	11.5	17.5	24.6	28.5	22.1	23.0
1940	N-Chlorophenyl-N-hexylpiperazine	BRD-K93541117-001-01-4	5.6	-12.7	-20.3	-15.3	8.0	16.9
1941		BRD-K93568044-001-11-4	-9.6	-25.3	2.1	-3.4	17.3	13.4
1942	DIACETAMATE	BRD-K93611241-001-01-4	-14.2	-0.7	-12.8	-9.8	-14.4	-23.0
1943	TADALAFIL	BRD-K93645900-001-04-8	21.8	-5.0	-4.2	-8.6	-6.7	-12.8
1944	K-252c	BRD-K93879806-001-01-4	188.9	55.2	14.0	19.6	12.6	12.8
1945	DIETHYLTOLUAMIDE	BRD-K94080537-001-05-5	-1.0	7.8	-11.2	-4.6	16.8	13.5
1946	COTININE	BRD-K94144010-001-09-7	6.2	1.7	0.1	12.5	0.1	-7.4
1947	PAEONOL	BRD-K94239562-001-03-0	2.6	5.8	23.1	33.3	11.2	8.5
1948	RONIDAZOLE	BRD-K94266545-001-15-9	-2.3	0.5	5.7	8.1	18.6	22.2
1949	SCH 39166 hydrobromide	BRD-K94270326-004-01-0	0.8	6.4	-19.8	-7.7	-7.2	-10.0
1950	METAMECONINE	BRD-K94324294-001-03-5	-10.4	-7.5	-10.5	-11.2	3.9	14.8
1951	KINETIN RIBOSIDE	BRD-K94325918-001-05-3	12.9	5.9	36.5	16.1	16.0	17.7
1952	BML-190	BRD-K94379058-001-03-5	-10.2	-13.4	-23.4	-18.3	-17.8	-16.4
1953	Mevastatin	BRD-K94441233-001-03-1	26.9	-8.1	-36.4	-42.5	-7.2	-12.7
1954	AMI-193	BRD-K94512704-001-02-1	-6.2	6.7	-17.3	16.5	7.6	-1.0
1955	PINOCEMBRIN	BRD-K94689771-001-02-5	-5.9	-3.6	6.2	10.8	-1.2	-4.1
1956	CHROMOCARB	BRD-K94720315-001-05-4	6.4	-11.7	8.6	8.9	13.0	-0.6
1957	Y 134	BRD-K94832621-001-01-5	-16.4	-12.0	-53.2	-50.5	-40.8	-42.7
1958	(+)-Anabasine hydrochloride	BRD-K94837957-003-01-4	55.9	51.1	31.9	44.8	47.0	37.4
1959	1-(3-trifluoromethyl) phenylpiperazine monohydrochloride	BRD-K94887716-001-01-5	10.6	15.2	13.9	13.0	29.3	20.9
1960	DR 2313	BRD-K94920105-001-01-3	-7.5	-9.0	-2.7	0.1	5.5	10.9
1961	ISOBUTYLMETHYLXANTHINE	BRD-K94979336-001-09-3	8.1	7.8	14.6	12.3	17.9	15.9
1962	APOTOXICAROL	BRD-K95048371-001-01-9	23.3	20.4	-11.0	-0.7	7.0	1.0
1963	OCTISALATE	BRD-K95161686-001-01-0	20.4	15.3	-27.8	46.0	4.9	22.5
1964	PROBENECID	BRD-K95237249-001-15-8	-1.0	-23.5	9.6	15.1	7.1	-0.2
1965	DIENESTROL	BRD-K95309561-001-15-5	14.0	14.5	-67.6	-47.3	-22.7	-6.3
1966	PHA 665752	BRD-K95435023-001-01-0	-37.3	-19.4	-96.8	-92.0	-50.0	-56.4
1967	SINAPIC ACID	BRD-K95487349-001-04-2	-18.0	-7.8	55.5	94.8	-31.7	-32.3
1968	PICROTOXININ	BRD-K95554982-001-04-1	14.2	17.8	-3.8	25.6	15.1	16.1
1969	(S)-(-)-Pindolol	BRD-K95598440-001-03-6	2.5	-11.3	21.0	5.6	3.9	10.4
1970	BHQ	BRD-K95603879-001-06-7	45.3	51.4	34.3	28.9	15.4	16.8
1971	BMS 191011	BRD-K95609758-001-01-1	-17.0	-29.2	-70.2	-71.8	-49.2	-46.0
1972	Tetrabenazine	BRD-K95739795-001-01-1	-3.7	-3.4	14.8	14.5	-3.2	9.4
1973	Trapidil	BRD-K95763993-001-03-7	1.4	-12.7	13.1	-1.1	1.9	8.7
1974	CGP 13501	BRD-K95851186-001-02-9	12.9	-5.8	2.6	11.1	14.3	20.9
1975	HEXAMETHYLQUERCETAGETIN	BRD-K95885906-001-01-8	-14.8	-17.1	-20.9	-5.0	-18.8	-25.6

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
1976	LY 344864 hydrochloride	BRD-K95899059-003-01-0	-2.1	-24.9	-10.7	-15.1	1.2	0.1
1977	RESERPINE	BRD-K95921201-001-07-0	-8.1	-1.6	-16.5	2.6	-13.0	-10.6
1978	ISAXONINE	BRD-K95957366-001-01-8	33.2	5.5	4.0	25.3	12.0	12.6
1979	1-Acetyl-4-methylpiperazine hydrochloride	BRD-K96055017-003-01-9	7.7	36.7	-6.1	12.7	5.1	11.0
1980	SCOPOLETIN	BRD-K96163925-001-09-9	41.0	24.3	53.7	59.0	-9.8	-6.4
1981	CEPHARANTHINE	BRD-K96194081-001-06-0	-19.6	-10.7	-44.2	-34.6	-29.4	-33.6
1982	DIMETHYLCAFFEIC ACID	BRD-K96256403-001-05-0	-4.1	5.9	-1.5	-17.7	0.0	-1.4
1983	GW 7647	BRD-K96263742-001-02-3	-95.3	-97.0	-132.9	-131.0	-78.3	-82.8
1984	PHENTERMINE	BRD-K96319534-001-01-7	24.1	15.4	21.1	10.5	-1.1	7.2
1985	NIFEDIPINE	BRD-K96354014-001-10-4	120.8	119.2	27.8	24.8	-42.8	-44.8
1986	CHLORAMPHENICOL PALMITATE	BRD-K96424892-001-01-1	-1.1	30.2	1.1	43.0	8.8	14.5
1987	LEOIDIN	BRD-K96660256-001-03-6	-48.5	-47.9	-100.2	-100.4	-78.0	-77.6
1988	SR 49059	BRD-K96720755-001-01-8	-24.5	7.7	-4.1	-5.9	0.2	-11.1
1989	SKF 86002 dihydrochloride	BRD-K96809896-300-01-5	22.2	-19.9	-0.9	11.3	15.2	13.8
1990	Pirfenidone	BRD-K96862998-001-03-1	-3.2	-2.7	3.4	-2.6	8.4	9.4
1991	QUININE ETHYL CARBONATE	BRD-K97028990-001-03-6	2.9	4.6	6.1	-6.3	15.6	7.4
1992	TBB	BRD-K97118047-001-02-0	-60.2	-57.1	-94.6	-100.0	-44.3	-48.3
1993	3-METHOXYCATECHOL	BRD-K97139501-001-03-3	77.8	83.5	45.5	45.1	-58.9	-59.4
1994	DROPERIDOL	BRD-K97158071-001-08-2	-1.1	-3.8	-13.7	-2.8	17.4	13.7
1995	THIOTHIXENE	BRD-K97309399-001-05-2	-64.3	-59.6	-73.1	-73.0	-53.1	-52.2
1996	PI 828	BRD-K97365803-001-01-3	-5.9	-10.5	2.7	24.4	2.6	9.2
1997	QUERCETIN	BRD-K97399794-001-09-6	58.3	76.5	-16.7	8.0	-22.9	-42.0
1998	ACEDAPSONE	BRD-K97417064-001-01-6	-20.7	-22.7	-27.3	-17.8	4.0	-3.3
1999	coumestrol	BRD-K97509413-001-01-8	-3.7	-8.4	71.4	43.2	-37.2	-39.0
2000	MELATONIN	BRD-K97530723-001-11-8	-14.0	-0.5	30.4	40.8	21.2	9.3
2001	Mepyramine maleate	BRD-K97564742-103-01-9	42.4	24.5	12.3	9.0	4.4	2.0
2002	THYMOQUINONE	BRD-K97566842-001-03-5	26.1	23.6	-1.5	-1.9	30.4	11.7
2003	CHLORPROPAMIDE	BRD-K97746869-001-15-5	-1.7	10.0	9.9	19.8	15.7	26.8
2004	Nicorandil	BRD-K97752965-001-01-6	-4.4	-23.9	-2.2	0.2	7.1	7.2
2005	PDGF Receptor Tyrosine Kinase Inhibitor II	BRD-K97922702-001-01-3	-0.4	6.1	19.2	24.5	36.6	28.9
2006		BRD-K98039984-001-06-3	-9.7	14.0	-1.3	-4.3	2.7	8.1
2007	Compound W	BRD-K98143539-001-01-4	-60.1	-51.9	-92.9	-91.5	-35.0	-38.8
2008	SIB 1757	BRD-K98157055-001-04-2	59.6	30.3	53.3	31.4	27.0	28.3
2009	CHLORZOXAZONE	BRD-K98174813-001-08-1	9.3	7.1	6.2	17.6	12.5	9.5
2010	ANGOLENSIN (R)	BRD-K98281970-001-03-4	-3.9	-11.1	-51.3	-21.4	-21.4	-17.6
2011	N-Ethylmaleimide	BRD-K98297262-001-01-1	-5.2	-12.8	3.5	12.0	19.6	37.1
2012	AMSACRINE	BRD-K98490050-001-01-8	-74.8	-82.7	-99.3	-98.9	-84.7	-82.9
2013	CLONIDINE HYDROCHLORIDE	BRD-K98530306-003-07-6	66.3	59.8	19.6	17.3	13.0	8.3
2014	Parthenolide	BRD-K98548675-001-02-6	-39.1	-45.7	-79.0	-75.5	-53.8	-43.8
2015	4-HYDROXYINDOLE	BRD-K98735139-001-01-1	17.8	-3.9	-23.7	-16.4	-71.0	-68.2
2016	CHLOROACETOXYQUINOLINE	BRD-K98737600-001-02-5	8.3	16.1	15.9	31.9	-22.1	-25.1
2017	NIFLUMIC ACID	BRD-K98763141-001-17-5	9.4	27.2	-8.6	3.5	8.3	3.7
2018	FUMAZENIL	BRD-K98769987-001-12-0	17.1	-19.7	-6.3	6.5	13.2	14.3
2019	Felbamate	BRD-K99107520-001-09-2	-6.2	-20.0	-23.0	0.7	-2.2	0.2
2020	DIBUCAINE HYDROCHLORIDE	BRD-K99121711-003-12-2	-28.4	-16.1	-35.7	-29.2	-48.2	-41.0
2021	SB 203580, Sulfone	BRD-K99291625-001-02-3	-3.4	2.8	-6.2	-11.6	12.7	17.2

no.	Compound		Normalized scores					
	Name	Broad Institute ID	HPr+_DNA		CBA		Amplex Red_HRP	
			Plate 1	Plate 2	Plate 1	Plate 2	Plate 1	Plate 2
2022	ANTAZOLINE PHOSPHATE	BRD-K99300445-011-12-8	7.8	14.0	-20.6	19.4	-18.3	0.3
2023	TUBOCURARINE CHLORIDE	BRD-K99621550-003-03-4	2.5	15.3	8.3	28.6	7.8	7.9
2024	BUTACAINE	BRD-K99622919-001-15-6	13.3	4.1	21.1	23.8	10.3	-17.8
2025	HEXACHLOROPHENE	BRD-K99792991-001-18-2	-70.4	-66.2	-83.8	-83.5	-64.6	-64.3
2026	DPO-1	BRD-K99922388-001-01-2	29.5	17.6	2.0	11.6	16.0	13.7
2027	FLUNIXIN MEGLUMINE	BRD-K99984802-100-06-9	27.3	2.5	2.6	15.1	6.9	5.2
2028	Formoterol hemifumarate	BRD-M00539986-051-01-1	16.5	12.6	13.4	16.5	-3.9	-4.2
2029	4-Phenyl-1,2,3,4-tetrahydroisoquinoline hydrochloride	BRD-M10474530-001-02-3	-3.8	-19.9	-3.8	7.7	3.1	-6.7

Mitigation of NADPH Oxidase 2 Activity as a Strategy to Inhibit Peroxynitrite Formation

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