Supplementary Information (PDF)

A screening based approach to circumvent tumor microenvironment-driven intrinsic resistance to BCR-ABL+ inhibitors in Ph+ acute lymphoblastic leukemia

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This Supplementary Information (PDF) section comprises of table of contents; materials and methods for FACS assessment of viability; FACS assessment of cell cycle percentages; drug/cytokine washout and cytokine recovery studies; dasatinib re-challenge studies; detailed description of chemical library screened; HT drug screens - data processing, quality control and hit scoring criteria; cluster analysis of hits using therapeutic drug classes; Supplementary Figures S1-S11 with legends; Supplementary Table 1 and Supplementary References.

Table of contents for Supplementary Information (PDF):

Production and culture of murine leukemia initiating cells (LICs)

Replication-defective mouse stem cell virus (MSCV) retroviral vectors co-expressing either the wild-type (WT) allele of human $p185^{BCR-ABL}$ or mutant BCR-ABL alleles $p185^{T315I}$ or $p185^{F317L}$, and either green fluorescent protein (GFP) or luciferase, were packaged into replication-incompetent ecotropic virions[17,18,22]. Whole bone marrow cell suspensions from *Arf* $^{-/-}$ young adult mice were transduced to produce *Arf* $^{-/-}$ p185+ pre-B LICs [17,22]. After initial establishment on autologous stromal cell layers over 7 days, transformed pre-B cells were briefly expanded in the absence of a stromal layer for 2 days in liquid culture in BCM10 media (RPMI1640 supplemented with 10% Hyclone fetal calf serum, 4 mM glutamine, 100 Units/mL penicillin, 100 μg/mL streptomycin, and 55 μM beta-mercaptoethanol[18]), and cryopreserved. Prior to use in any assays, *Arf* $^{-/-}$ $p185^{WT}$ and *Arf* $^{-/-}$ $p185^{T315I}$ pre-B cells (BCR-ABL^{WT} LICs and BCR-ABL^{T315I} LICs, respectively) were thawed and allowed to recover and expand exponentially in BCM10 for 3 days.

In vivo adoptive leukemia transfer Ph+ ALL model

Mice were housed in an American Association of Laboratory Animal Care (AALAC)–accredited facility and treated on Institutional Animal Care and Use Committee (IACUC)–approved protocols in accordance with NIH guidelines. Adoptive cell transfers were performed by injecting LICs into tail veins of healthy, non-conditioned, immune-competent 10- to 12-week-old IL-$7^{+/+}$ or IL-$7^{-/-}$ C57Bl/6J mice (Jackson Labs, Bar Harbor, ME). Animals were observed daily and sacrificed when moribund (dehydration, ruffled fur, poor mobility, respiratory distress). Survival curves were generated using GraphPad Prism Version 5.0 (La Jolla, CA). The Mantel-Cox test was applied to pairwise comparisons of survival data.

FACS assessment of viability

Viability of LICs was estimated after counterstaining approximately 5 x 10^5 LICs (in 0.5 mL volume) with 35 µL of a propidium iodide (PI) solution (0.25 mg/mL in PBS). The percentage of viable cells was calculated by electronic gating on PI-negative cells on PI versus forward scatter dot plots, with forward scatter signals consistent with LICs, and comparison of this number with total cell number. Data were collected and analyzed on a BD Biosciences LSR II flow cytometer (San Jose, CA), using BD Biosciences FACS DiVa software.

FACS assessment of cell cycle percentages

For determination of percentages in cell cycle phases, 5 x 10^5 LICs were centrifuged, washed once with PBS, recentrifuged, and cell pellets were resuspended in 0.5 mL PI staining solution (0.05 mg/mL PI, 0.1% sodium citrate, 0.1% Triton X100), which lysed the cells and stained nuclear DNA with PI. Samples were then treated with DNAse-free RNAse (0.2 mg/mL in 10 M Tris-HCl/15 mM NaCl, pH 7.5) for 30 min at room temperature, filtered, and analyzed for red fluorescence from a PI-labeled DNA on BD Biosciences FACS Calibur flow cytometer (San Jose, CA) by using BD Biosciences CellQuest Pro software. The percentages of cells within each cell cycle phase were computed using the computer program ModFit (Verity Software House, Topsham, ME).**Drug/cytokine washout and cytokine recovery studies**

For washout studies, BCR-ABL^{WT} LICs were diluted to a density of 1 × 10^5 LICs/mL in BCM-10 containing no or 5 mg/mL IL7, and treatment with either dasatinib or 0.1% DMSO by volume (non-drug treated controls) was initiated at time 0 h in triplicate 100 mm petri dishes. Daily monitoring for expected drug-induced changes was performed by naked-eye microscopy from 0 to 72 h. At the 72 h time point, after harvesting under identical conditions, total LIC density and viability percentage for all samples were determined using Beckman Coulter Vi-cell (trypan

blue) in triplicates. Each sample was spun down in 50 mL BD Falcon™ tubes; the supernatant was discarded and LIC pellet resuspended in freshly prepared BCM-10 (not containing any cytokine or drug). This washing step was repeated 4 times to ensure complete removal of the drug and/or cytokine. After the last wash, each pellet was resuspended to 1×10^6 total LICs per mL master stocks. Aliquots from master stocks were taken for (i) flow assessment of viability and cell cycle percentages (as described above); (ii) manual CTG assay using 25 uL sample per well in 384-well microplates (in triplicates), as an independent determination for LIC growth. For assessment of extracellular cytokine on recovery of LICs that were previously challenged with dasatinib (0 to 72 h), washed master stocks were diluted to 5×10^5 total LICs per mL in BCM10 with or without 5 ng/mL IL7, plated in 6 well plates (10 cm^2 approx), and incubated at 37°C from 72 to 144 h for recovery, during which time daily naked-eye microscopic examinations were performed. At 144 h, for each sample total LIC density and viability percentage assessment by Beckman, viability and cell cycle percentages by flow assessment and independent CTG evaluations were performed as described for the 72 h time point. Cell growth trends by CTG readout corroborated the findings from trypan blue (Beckman) and DAPI staining (FACS). Key results are presented in **Supplementary Figure S6;** total viable LICs in a sample were calculated as a product of absolute LIC count determined by Beckman and absolute sample viability determined by FACS analysis. **Dasatinib re-challenge studies**

Further studies were performed to evaluate the possibility of a genetically drug-resistant subpopulation that could undergo selection with dasatinib/IL7 co-treatment during 0-72 h of dasatinib/cytokine washout studies above. To this aim, BCR-ABL^{WT} LICs were treated with 100 nM dasatinib or 0.1% DMSO in the absence or presence of 5 ng/mL IL7 in 100 mm dishes from 0-72 h, as described above; in addition, a dasatinib challenge (first-time challenge) across 6 log-

fold concentration in the presence or absence of 5 ng/mL IL7 was also performed using CTG assay during this time period (0-72 h). At 72 h, dasatinib/IL7 co-treated LICs from 100 mm dishes were washed (as described above) and immediately challenged (second challenge) from 72 to 144 h with six log-fold concentration range of dasatinib in 384-well microplates either in the presence or absence of 5 ng/mL IL7 using CTG assay. At 144 hrs, dasatinib showed similar potency against LICs in the absence of IL7, irrespective of previous dasatinib exposure. Furthermore, potency of dasatinib was blunted, to a similar extent, during both the first and second drug challenges only when extracellular IL7 was present (data not shown).

Detailed description of chemical library screened

The screening library consisted of 5600 (approximately 3200 unique) approved drugs and chemicals with known biological activity (bioactives). The library was assembled from 3 commercial suppliers: Microsource, Prestwick, and Sigma. The Microsource compounds included the following: (a) the Spectrum collection, which contains 2000 biologically active and structurally diverse compounds, including known drugs, experimental bioactives, and pure natural products(1, 2); (b) the US Drug Collection, which contains 1040 drugs that have reached clinical trials in the US and have been assigned USAN or US Pharmacopeia status; and (c) the Killer collection, which contains a reference set of 160 synthetic and natural toxic substances (http://www.msdiscovery.com/index.html). The Prestwick compounds include 1120 small molecules selected for high chemical and pharmacologic diversity. Ninety percent of the collection is composed of known marketed drugs, and the remainder includes bioactive alkaloids or related substances. Human bioavailability and human toxicity data are available for most compounds (http://www.prestwickchemical.fr/index.php?pa=26). The Sigma LOPAC1280 (Library of Pharmacologically Active Compounds) collection reflects the most commonly

screened targets in the drug discovery community, including marketed drugs, failed development candidates, and "gold standards" that have well-characterized activities (http://www.sigmaaldrich.com/chemistry/drug-discovery/validation-libraries.html).

Data processing, quality control and hit scoring criteria for HT drug screens

All data processing and visualization was performed using custom programs written in the Pipeline Pilot platform (Accelrys, v.7.5) and the R program 6.6(3, 4). The R drc package was used to fit sigmoidal curves(4). ROC statistics were computed using the ROCR package(5).

The quality of the primary drug-screening studies, performed in parallel against BCR-ABL^{WT} and BCR-ABL^{T315I} LICs, was evaluated by multiple methods including, but not limited to, identification of known antileukemic agents, identification of multiple compound replicates intentionally included in the 5600 collection, and *Z'* and other screening quality metrics (described in **Supplementary Figures S7 to S10**). In the screening experiments, all assay plates demonstrated attenuation of dasatinib potency in presence of IL7 or BCR-ABL mutation, similar to results described in **Figure 1a and 1b.** An empirically determined, statistically significant but liberal cut-off of >10% activity was chosen to include agents of relatively lower activity considering the high-risk nature of Ph+ ALL and the drug-rich nature of the library as well as to allow for a more complete structure-activity relationship and therapeutic class analysis after subsequent potency determination through secondary screening

The discriminatory power of the phenotypic assay was assessed using receiver operating characteristic (ROC) statistics. A total of 165 compounds were selected to sample the primary assay according to the distribution of observed activities. ROC curves are shown in **Supplementary Figure S10**. The assay has good discriminatory power; with similar AUCs of

approximately 0.83 and 0.85 against BCR-ABL^{WT} and BCR-ABL^{T315I} LICs, respectively (an ideal assay has an AUC of 1.0, whereas a random assay has an AUC of 0.5).

The activity class designations in the **Excel Supplement** were assigned based on the curve score and visual inspection of dose-response curves. The curve score is a 4 character code derived from the following heuristic:

- First character: letter (A,B,C or D) indicating curve quality
    - D = less than 2 points above the noise (defined as outliers from the negative control population)
    - C = $r^2 < 0.50$ or range > 200% or EC_{50} > maximum concentration tested
    - A = $r^2 > 0.80$ and difference between two last points < 10% (indicating saturation)
    - B = not A,C, or D
    - N prefix = activity decreases with increase concentration
- Second character: number (1-6) indicating potency
    - 1 = $EC_{50} < 0.1$ µM
    - 2 = 0.1 µM ≥ $EC_{50} < 1.0$ µM
    - 3 = 1.0 µM ≥ $EC_{50} < 10.0$ µM
    - 4 = $EC_{50} > 10.0$ µM
    - 5 = all C and D curves are assigned 5
- Third character: number (1-6) indicating efficacy
    - 1 = 75% ≥ range < 200%
    - 2 = 50% ≥ range < 75%
    - 3 = 25% ≥ range < 50
    - 4 = range < 25%

    - 5 = all C and D curves are assigned 5
- Fourth character: number (1-6) indicating hill slope
    - 1 = hill ≤ 2
    - 2 = $2 <$ hill ≤ 4
    - 3 = $4 <$ hill ≤ 8
    - 4 = hill > 8
    - 5 = all C and D curves are assigned 5

A complete list of all compounds evaluated in the secondary drug-screening experiments with their structure, supplier information, synonyms, EC_{50} values, and therapeutic classification is reported in the **Excel Supplement**.**Cluster analysis of hits using therapeutic classes**

The therapeutic cluster graph was generated by first assigning each compound an Anatomical Therapeutic Chemical Classification System (ATC). This classification system groups drugs into a 5 level hierarchy according to therapeutic indication and chemical properties. The first level indicates anatomical main group and consists of 1 letter; the second level indicates therapeutic main group and consists of 2 digits; the third level indicates therapeutic or pharmacological subgroup and consists of 1 letter; the fourth level indicates chemical, therapeutic or pharmacological subgroup and consists of one letter; and the fifth level indicates the chemical substance and consists of 2 digits. The resulting 7 characters constitute an ATC code, and a compound can be assigned multiple ATC codes. ATC codes can be depicted as a network graph by defining a node to represent each level in the ATC code and then connecting nodes according to parent-child relationships (e.g., first-level node A is the parent of second level nodes A01, A02, etc.). Compounds without an ATC code were assigned based on similarity to known agents, or were assigned to custom codes located under the parent V99

(labeled as “Not defined in ATC” in Figure 2). See Supplementary Figure 10 for the frequency of ATC Level 1 and Level 2 codes among the 706 compounds submitted to dose-response analysis.

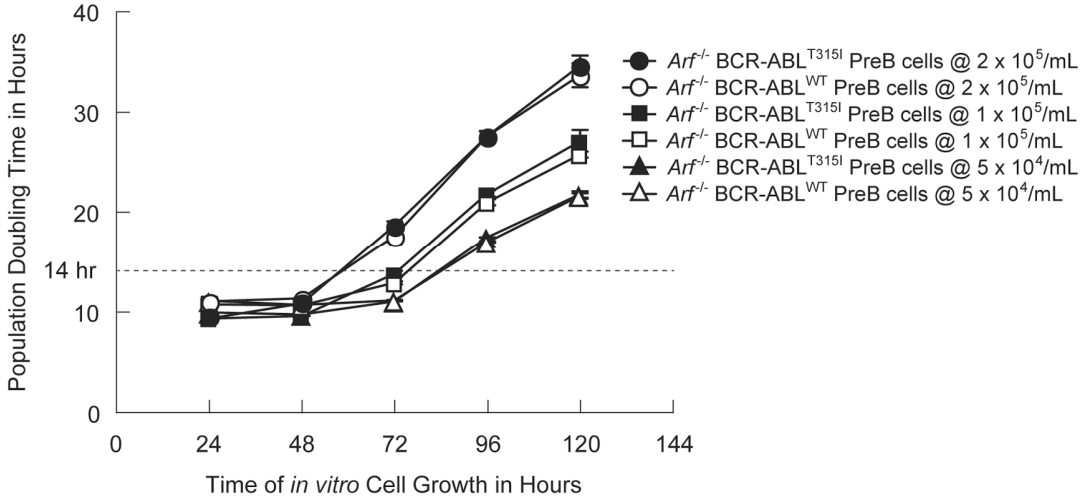
The resulting network was visualized in Cytoscape (v 2.8.1) using the yFiles circular layout algorithm(6). The cytoscape file for this network is available for download as part of this supplement.

In vivo preclinical therapeutic studies

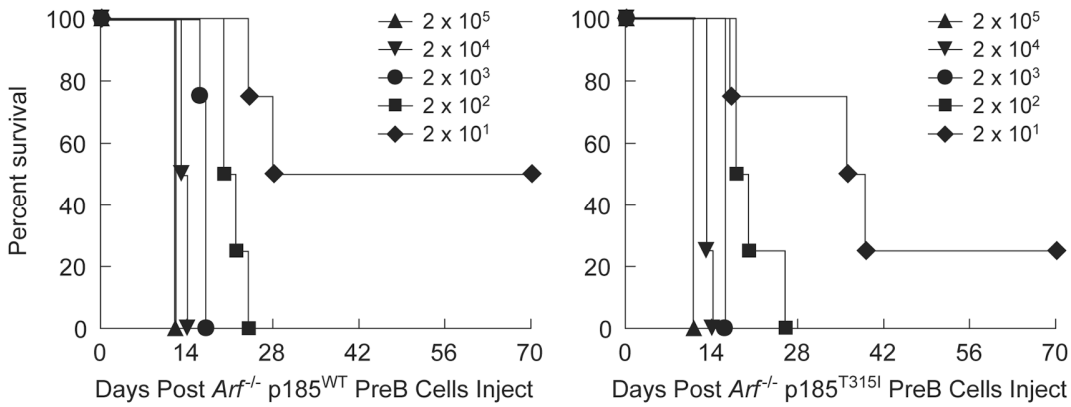
For *in vivo* use, dasatinib (LC Labs, Woburn, MA) in citric acid (pH 3.1) [25], and DHA (Avachem, San Antonio, TX) in 0.5% carboxy-methylcellulose/0.5% Tween 80/0.5% benzyl alcohol, were administered by oral gavage. In toxicity studies (data not shown), DHA was ranged up to 300 mg/kg as a single or split dose for 5 days/week over a six week time period. Repeated single doses of 300 mg/kg (5 days/week) were determined to induce no significant weight loss, lethargy, seizures or deaths [26]. During therapeutic studies, animal weights were monitored daily to ensure no significant body weight reductions.

Bioluminescent imaging and evaluation of cures

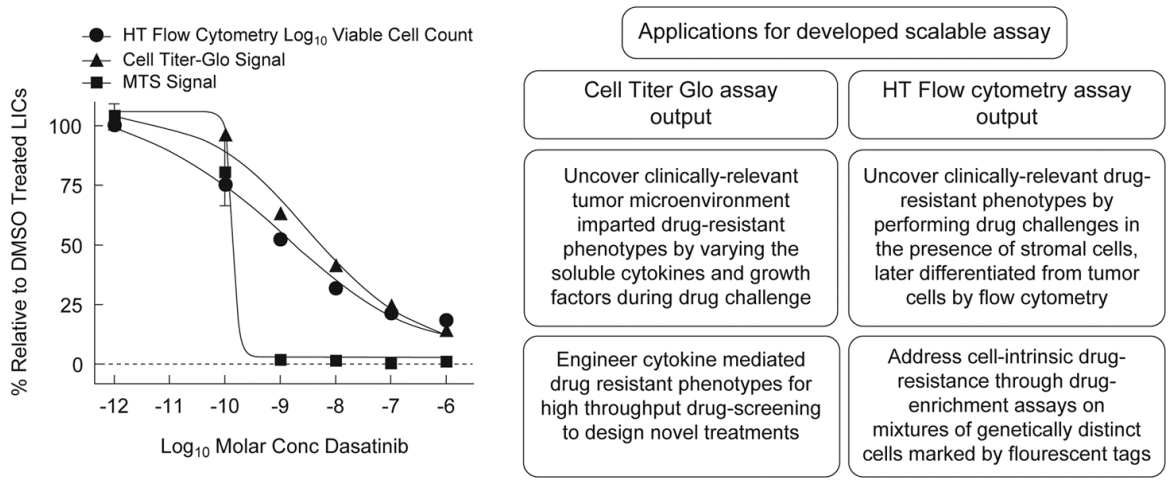
Bioluminescent imaging and analysis were performed using a Xenogen IVIS-200 system and Living Image software 3.01 (Caliper Life Sciences, Hopkinton, MA)[17]. Total bioluminescent flux measurements (photons/second) were quantified over the whole animal body. Recipient mice that remained clinically healthy 12 months after terminating therapy and had no detectable bioluminescent signal *in vivo* were designated “long-term survivors.”



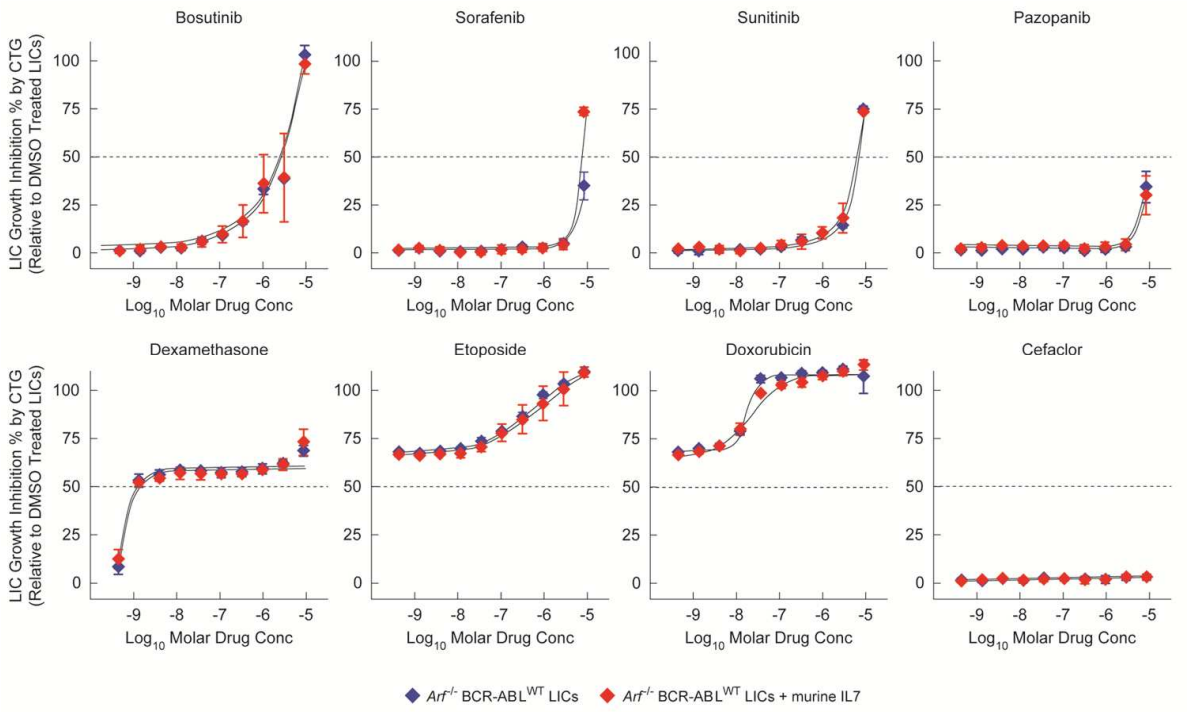
Supplementary Figure S1: ***Comparison of the growth properties of Arf$^{-/-}$ p185^{WT} (filled symbols) and Arf$^{-/-}$ p185 ^{T315I} preB (empty symbols) populations during in vitro cell culture.*** *Both cell types were plated at multiple cell dilutions (n=3 for each condition, time=0 h) in 6-well plates and serially followed daily for 5 days to evaluate absolute viable cell count, total viability, doubling times, and total population doublings, using the Beckman Coulter cell counter (trypan blue staining) and fluorescence-activated cell sorting (FACS) analysis in parallel. Both cell types had identical growth properties. Only the comparison for population doubling time in hours (+/- sd) for 3 relevant plating densities is presented. FACS cell-cycle analysis confirmed that a population doubling time less than 14 h was sufficient to maintain cells in exponential growth (>50% cells in S-phase).*



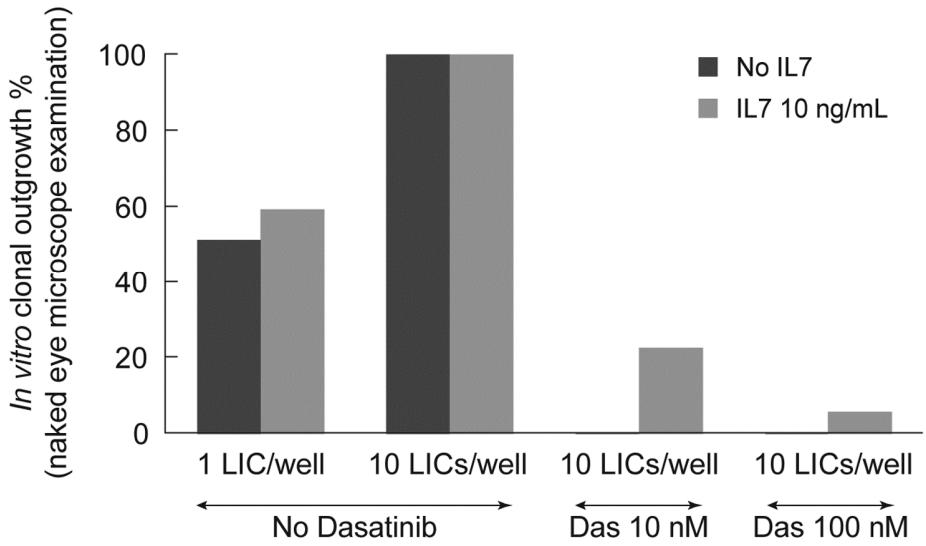
Supplementary Figure S2: ***Leukemia stem cell function (LSC) function assay by serial dilution and implantation comparing the in vivo leukemia initiating capacity of Arf$^{-/-}$ p185^{WT} (left) and Arf$^{-/-}$ p185^{T315I} preB (right) populations.*** *Kaplan-Meier curves represent the overall survival of nonconditioned immunocompetent* C57Bl/6J *recipient mice that received serial log-fold dilutions (n=4 per arm) of LIC-number (as indicated in the inset legend) on day 0. Arf$^{-/-}$ p185-transformed preB murine cells are hereafter referred as LICs.*



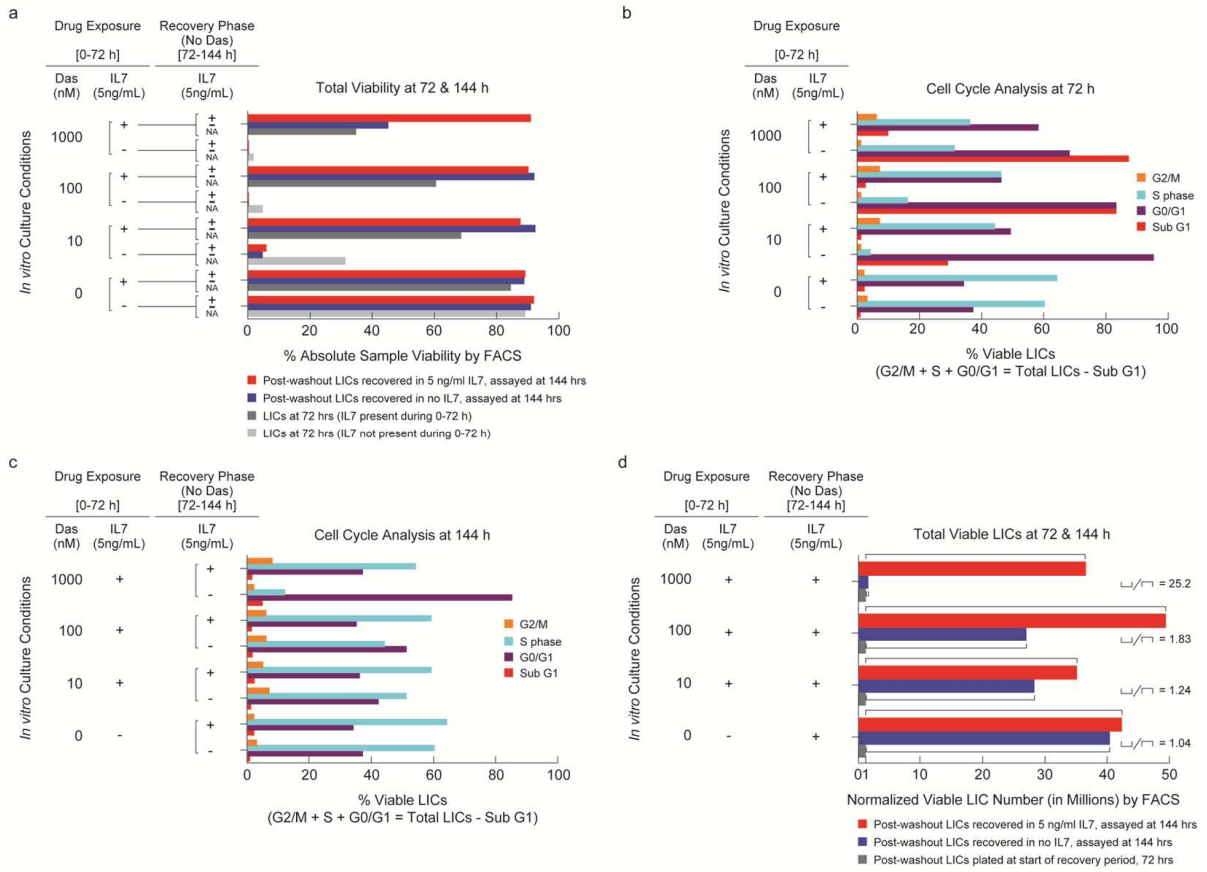
Supplementary Figure S3: ***Optimization of the high-throughput LIC-based phenotypic assay.*** *BCR-ABL^{WT} LICs plated at 5 × 10^4 per mL were challenged with 6 log-fold concentration range of dasatinib or DMSO in 384-well microplates. After a 72 h drug challenge, LIC growth was measured by 3 cellular readouts: CellTiter-Glo (CTG) assay (ATP content), MTS assay (viability), and high-throughput flow cytometry (total viability and viable cell counts by DAPI exclusion). Measured assay readouts at various drug concentrations (x-axis) were normalized to DMSO-treated LICs and graphed (+/- sd) on y-axis. Total viable LIC counts were determined by FACS, reflecting dasatinib-induced phenotypic changes across a 6 log-fold drug-concentration, were closely paralleled by the CTG cellular assay output but not by the commonly used MTS assay.*



Supplementary Figure 4: ***Comparative evaluation of IL7-mediated protection conferred against non-BCR-ABL–specific targeting drugs (top panel) and conventional cytotoxic antileukemic clinical drugs (bottom panel).*** *BCR-ABL^{WT} LICs were treated with indicated drugs or DMSO (no drug) for 72 h in the absence (blue) or presence (red) of high (10 ng/mL) murine IL7, in triplicates. The antibiotic drug Cefaclor (often used in leukemia clinics) was used as a non-antileukemic drug control. For each drug concentration, LIC growth was measured by the CTG assay and average values were normalized to DMSO-treated LICs and graphed (+/- sd).*

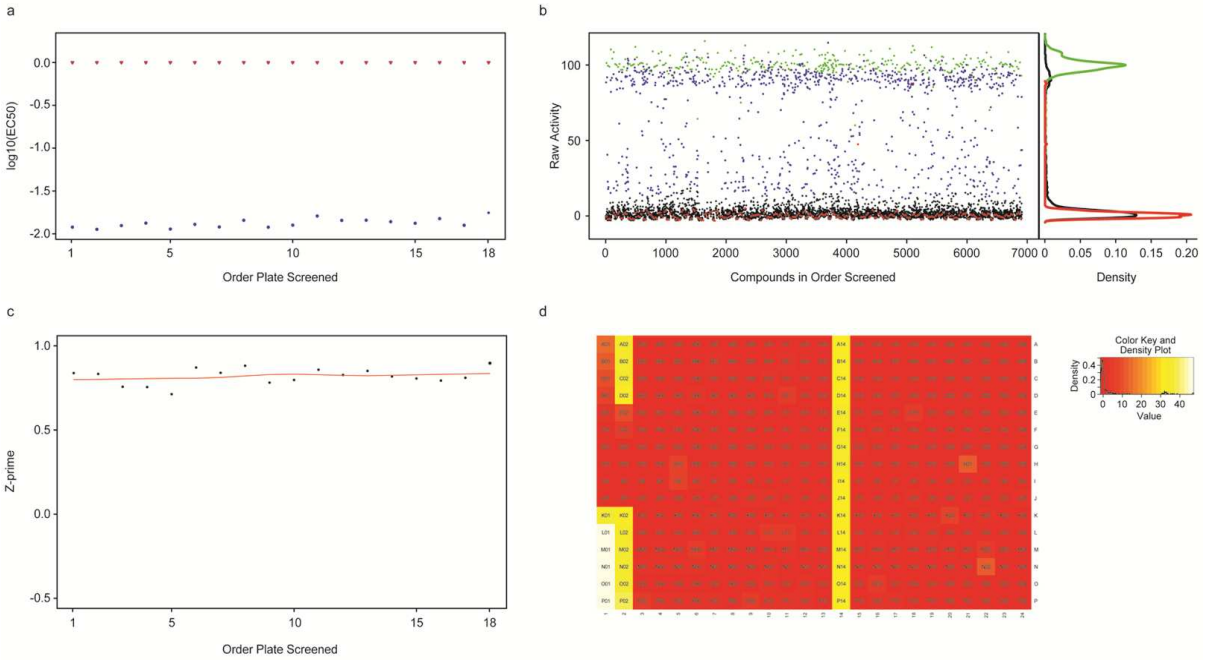


Supplementary Figure 5: ***In vitro leukemia clonal outgrowth efficiency assays.*** *Either 1 or 10 viable BCR-ABL^{WT} LICs per well sorted by single-cell flow cytometry into 3 clear-bottom 384-well plates for each condition (n=1152) were treated (t=0) with DMSO (0.1 % by volume) or dasatinib in the absence (black) or presence (grey) of IL7 (10 ng/mL). After 8 days of incubation, naked-eye microscopic examination was performed. Wells showing significant positive growth (approximately ≥50 LICs per well) were scored positive and percentage of positive wells for each condition indicated on the x-axis was calculated.*

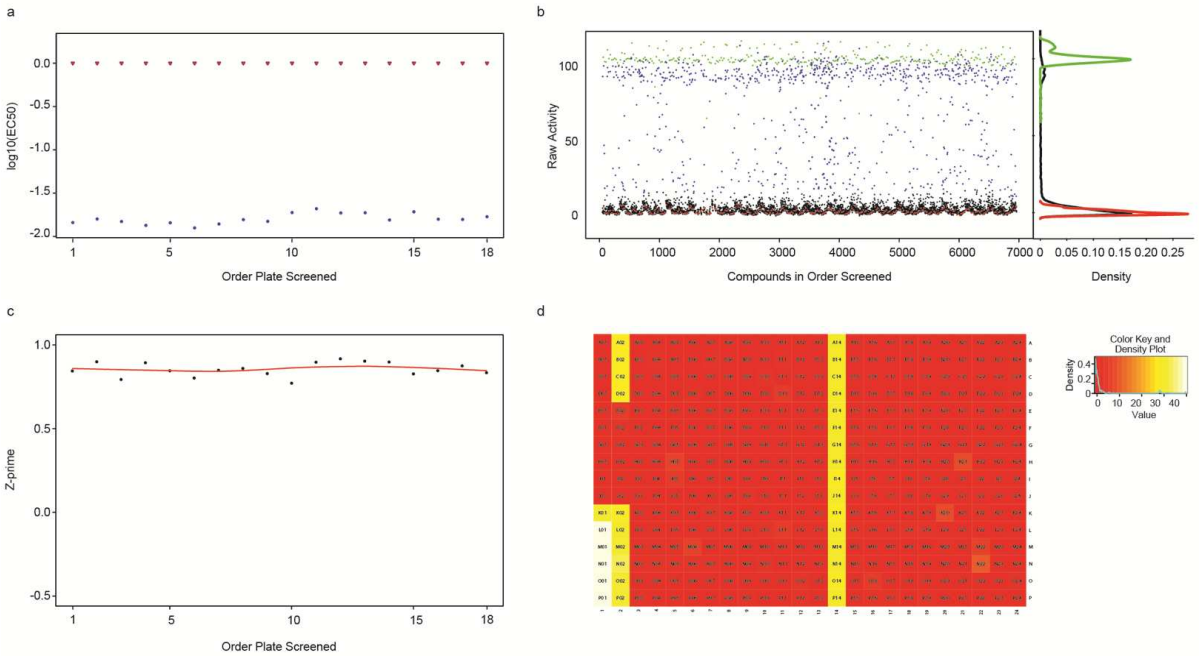


Supplementary Figure 6: ***Protection of BCR-ABL^{WT} LICs by IL7 during dasatinib exposures (0 to 72 h) and in the post-exposure recovery period (72 to 144 h, no dasatinib).*** *See Supplementary Methods above for details. (**a**) Total sample viabilities (DAPI staining, FACS) at the end of exposure period (dark gray=IL7; light gray=No IL7) and recovery period (red=IL7; blue=No IL7). Light gray vs. dark gray comparison depicts significant IL7 protection during dasatinib exposures. Few LICs surviving dasatinib exposures in the absence of IL7 (light gray), later deteriorated and died during recovery period, irrespective of IL7, confirming that BCR-ABL inhibitor exposures commit BCR-ABL+ cells to death(7). IL7 significantly improved recovery of dasatinib/IL7 co-treated LICs (red vs blue), clearly evident at 1000 nM but not at 100 nM and 10 nM dasatinib concentration because of over-confluent growth in presence of IL7*

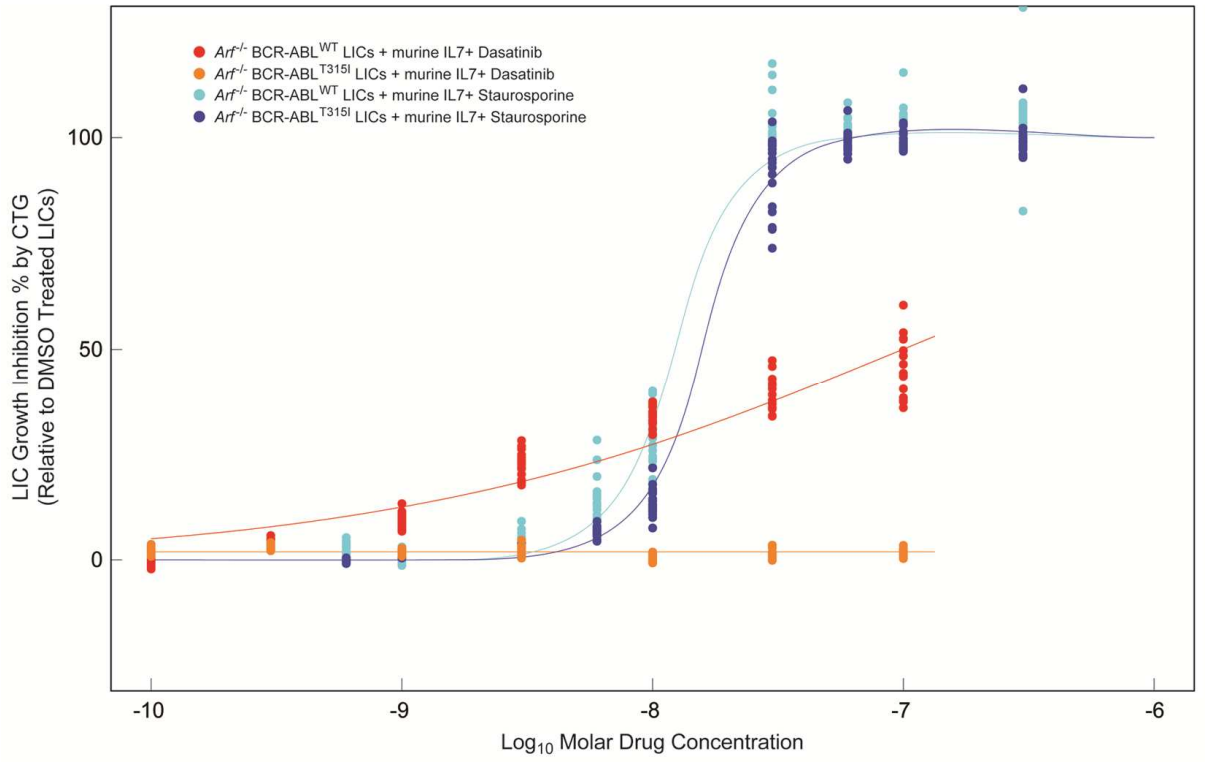
*(see Methods, (c) and (d)). (**b**) Cell cycle changes (FACS) at the end of exposure period (corresponding to light and gray bars in (a)). Incremental dasatinib doses (which cause incremental BCR-ABL inhibition(8)) induced cell cycle arrest and apoptosis; IL7 significantly protected LICs from these changes (**c**) Cell cycle analysis at the end of recovery period (corresponding to blue and red in (a)). (**d**) Conditions showing positive LIC growth during recovery period, normalized for equal number of LICs plated at start of recovery (dark grey). Ratio of fold LIC-change in presence (face-down bracket) to that in absence (face-up bracket) of IL7 increased in LICs with higher previous BCR-ABL inhibition from higher dasatinib concentrations during exposure period.*



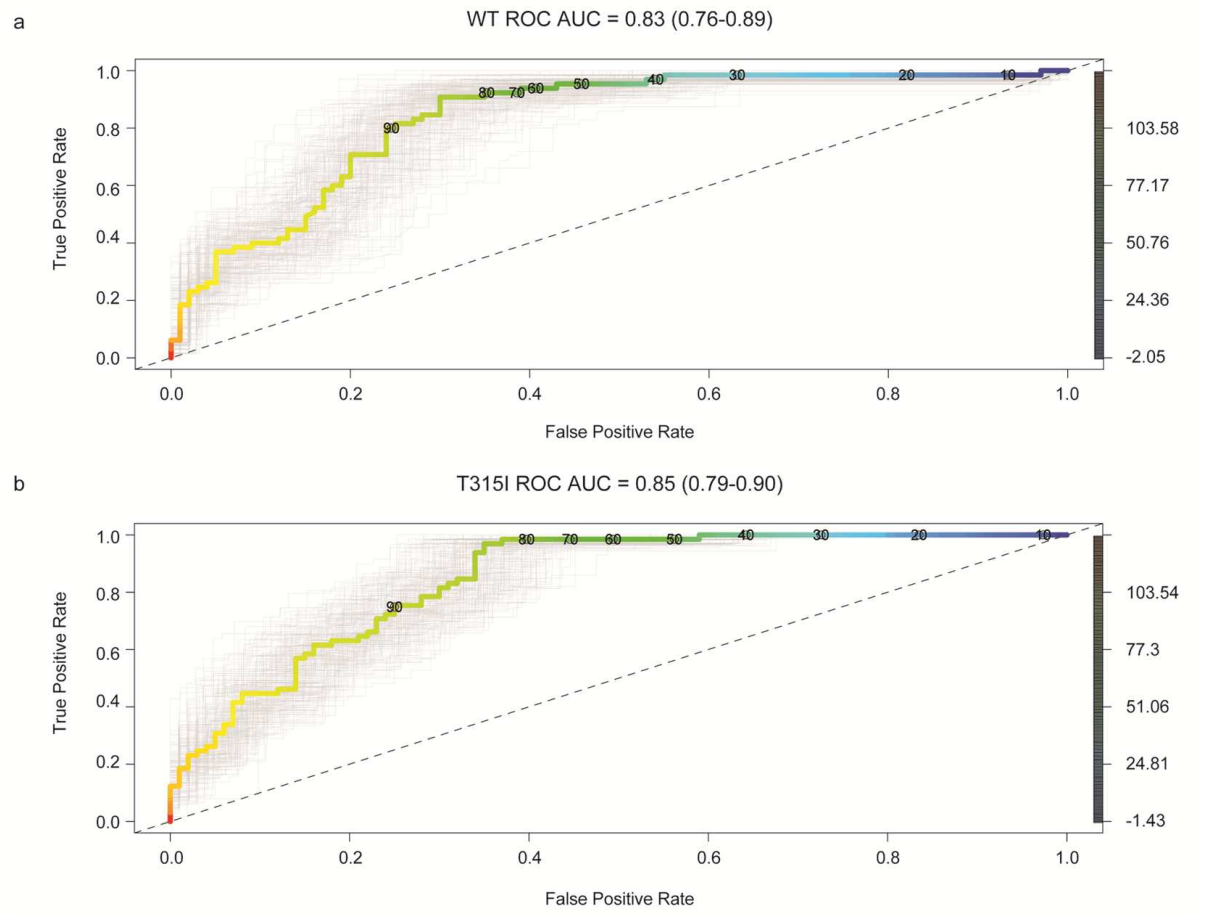
Supplementary Figure S7: ***Quality control for the primary screen of 5600 agents against BCR-ABL^{WT} LICs performed in the presence of 0.85 ng/mL IL7.*** *See Supplementary table1 for well locations. (**a**) Distribution of EC_{50} of non-BCR-ABL–inhibiting reference compound staurosporine (calculated from wells 2A-2J in (d)). (**b**) Scatter plot of percent activity of the test compounds relative to controls. Good separation is seen between negative controls (red, DMSO-treated. max signal, column 13 in (d)) and positive controls (green, 300 nM staurosporine, min signal, column 14 in (d)). Test compounds showing statistically significant activity relative to background noise (negative controls, red) are depicted in blue and inactive test compounds in black. Densities for positive, negative, and test compounds are shown on the right. (**c**) Distribution of Z' values for each plate in the primary screen. All Z' values throughout the run – average=0.82, lowest=0.71 and highest=0.9 (**d**) Heat map comparison of well activity averaged across all plates. Wells 1A-1J and 2A-2J show serial dilutions of dasatinib and staurosporine. In presence of IL7, average LIC growth inhibition of approx. 45% was achieved by 100 nM dasatinib (well 1A), the later approaching maximum concentration achieved in human plasma.*



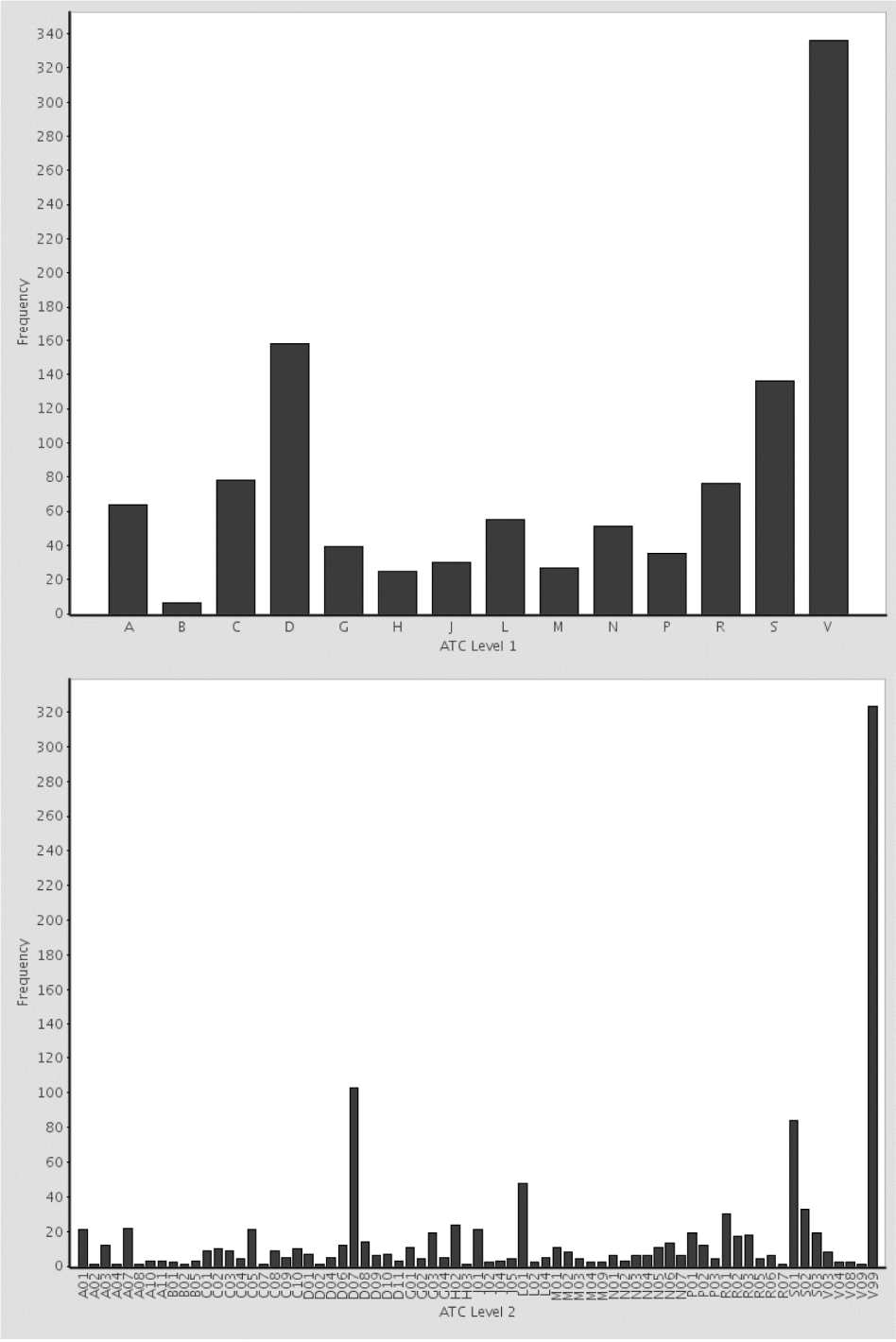
Supplementary Figure S8: ***Quality control for primary screen of 5600 agents against BCR-ABL^{T315I} LICs performed in the presence of 0.85 ng/mL IL7.*** *(**a**) Distribution of EC_{50} of non-BCR-ABL–inhibiting reference compound staurosporine (calculated from wells 2A-2J in (d)). (**b**) Scatterplot of percent activity of the test compounds relative to controls. Good separation is seen between negative controls (red, DMSO-treated, max signal, column 13 in (d)) and positive controls (green, 300 nM staurosporine, min signal, column 14 in (d)). Test compounds showing statistically significant activity relative to background noise (negative controls, red) are depicted in blue; inactive test compounds are black. (**c**) Distribution of Z' values for each plate in the primary screen. All Z' values throughout the run – average=0.85, lowest=0.77, and highest=0.92 (**d**) Heat map comparison of well activity averaged across all plates. Wells 1A-1J and 2A-2J show serial dilutions of dasatinib and staurosporine tested against BCR-ABL^{T315I} LICs. Although 100 nM dasatinib (Well 1A) was totally ineffective, well 2A with highest staurosporine concentration (300 nM) showed average LIC growth inhibition of approximately 100%.*



Supplementary Figure S9: ***Primary high-throughput drug screening experiments capture BCR-ABL-KI drug-resistant phenotypes with high accuracy.*** *Distributions of independent dose response curves of dasatinib and staurosporine against BCR-ABL^{WT} and BCR-ABL^{T315I} LICs in the presence of 0.85 ng/mL IL7 calculated separately from all assay plates (wells 1A-1J and 2A-2J) of primary drug screening experiments (also see Supplementary Fig. S7d and S8d) are presented. Both IL7-imparted dastinib–resistant phenotype in BCR-ABL^{WT} LICs (EC_{50} in nM: 95%CI = 86-116, average >100) and BCR-ABL-mutation-imparted BCR-ABL-KI–resistant phenotype in BCR-ABL^{T315I} LICs, similar to* ***Figure 1b,*** *were consistently captured across all plates. Low interplate variability in calculated EC_{50} values was observed for the non-BCR-ABL-targeting reference compound staurosporine (95%CI for EC_{50} in nM: WT = 11-12, T315I = 15-16) and majority of the validated hits (refer the* ***Excel Supplement****).*



Supplementary Figure S10: ***Receiver Operating Characteristic (ROC) analysis demonstrates that both (a) BCR-ABL^{WT} and (b) BCR-ABL^{T315I} LIC-based assays have high discriminatory power (AUC 0.83 and 0.85, respectively).*** *The ROC curve is plotted as a function of % activity, and is color coded according to the right Y-axis. The ROC curves in gray are calculated from 200 bootstrap simulations. The dashed line corresponds to a random assay.*



Supplementary Figure S11: ***Frequency of ATC Level 1 (top) and ATC Level 2 (bottom) compounds for the 706 compounds submitted to secondary analysis.***

Supplementary Table 1: *Steps in optimized high-throughput screening assay (CTG readout)*

Step	*Parameter*	*Value*	*Description*
1	Plate cells	25 µL	Plate LICs 5 x 10^4 per mL (25 µl/well) in BCM10 + 0.85 ng/mL IL7 into 384-well opaque bottom white microplates using Wellmate (Matrix)
2	Primary drug screening controls in columns 1-2 and 13-14	25 nL	1A-1I: Nine dasatinib concentrations (100 nM, 30 nM, 10nM, 3 nM, 1 nM, 0.3 nM, 0.1 nM, 0.03 nM and 0.01 nM) – control for IL7- and BCR-ABL mutation-imparted resistance against BCR-ABL-KIs 2A-2I: Nine staurosporine concentrations (300 nM, 100 nM, 60 nM, 30 nM, 10 nM, 6 nM, 3 nM, 1 nM, 0.6 nM)– non-BCR-ABL-specific reference control in the presence of IL7 13A-13P, 1J, 2J: DMSO 0.1% (Max Signal OR Negative Control); 14A-14P: staurosporine at 300 nM (Min Signal OR Positive Control); 1K-1P, 2K-2P: 40 µM dasatinib
	Secondary drug screening controls in columns 21-24	25 nL	21A-21P: DMSO 0.1% (Max Signal); 22A-22P, 23K-24P, 24K-24P: staurosporine at 300 nM (Min Signal) 23A-23J: Staurosporine – 10 log-fold dilutions (3 µM to 0.3 pM) - non-BCR-ABL–specific reference control in the presence of IL7 24A-24J: Dasatinib – 10 log-fold dilutions (1 µM to 0.1 pM) – control for IL7- and BCR-ABL mutation-imparted BCR-ABL–KI drug-resistance
3	Add test compounds in columns 3-12 and 15-24 in primary; columns 1-20 in secondary screen	25 nL	Primary screening: Single final drug concentration of 10 µM Secondary screening: Triplicate ten half-log serial dilutions (5 µM to 2 nM final concentration) of primary screening hits to determine their half-maximal inhibitory concentrations (IC_{50}) against LICs 384-well master drug-stock plates prepared at 1000X in DMSO. Drug delivered to assay plates by pin transfer (using V&P Scientific pin tool, 10H pins), giving a final drug concentration of 1× and 0.1% DMSO in all control and test wells of assay plates
4	Incubation 1	72 h	Liconics incubator, 8%CO_2, 37°C (standard LIC culture conditions)
5	Incubation 2	20 min	Room temp, low light (instructions as per Promega)
6	Add reagent	25 µL	CellTiter Glo (Promega) pre-equilibrated to RT before use
7	Incubation 3	25 min	Room temp, low light (per Promega)
8	Assay readout	ATP levels	Envision, Luminescent mode – ATP levels as a measure of LIC number and viable growth in 72 h – Signal measured in RLUs
9	Data processing	Pipeline Pilot	% inhibition by test compound = 100 * (Log_{10}Test Signal – Log_{10}Min Signal mean)/(Log_{10}Min Signal mean – Log_{10}Max Signal mean) Z-prime (Z') = 1-[(3*stdev of Log_{10} Max Signal + 3*stdev of Log_{10} Min Signal)/(Log_{10}Max Signal mean - Log_{10}Min Signal mean)] Z'is a dimensionless calculation

			to assess assay quality - for a good assay $Z' \geq 0.5$, and for a perfect assay $Z' = 1$

Supplementary References

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Worksheet	Description	Legend	Notes
Host Factors	The effect of 15 leukemia-microenvironment relevant cytokines on dasatinib potency (EC_{50}) against Arf-/-BCR-ABLWT LICs	* **hostFactor**: cytokine name * **conc**: cytokine concentration * **hill**: hill slope * **EC_{50}**: dasatinib EC_{50} (nM) * **EC_{50}CI**:= EC_{50} 95% confidence interval * **r^2**: r-squared of the non-linear regression	Triplicate measurements were pooled and fit to a single curve using a two parameter logistic model (bottom fixed to 0% and top fixed to 100%)
Structure	Structural information for 706 compounds	* **sample**: St. Jude registration number (regnumber + batch number) * **regnumber:** St. Jude registration root number * **supplier name**: name of the chemical supplier for this compounds * **supplier ID**: vendor unique identifier * **salt name**: name of any salt present * **salt eqs.**: number of salt equivalents * **solvate name**: name of any solvate present * **solvate eqs.**: number of solvate equivalents * **formula weight**: total molecular weight of all species present in the sample * **molsmiles**: molecular SMILES * **synonym**: alternate names for this compound	
Screen Summary (1)	List of 15 clinically-used conventional anti-leukemic agents validated during dose-response screening experiments	* **Name of clinical anti-leukemic agent** * **WT_EC_{50}**: mouse wild-type BCR-ABL B-cell EC_{50} (μM) * **WT_EC_{50}CI**: WT EC_{50} 95% confidence interval * **WT_actclass**: WT activity classification * **WT_curveScore**: grade for quality of the WT dose-response curve (see Supplemental for details) * **T315I_EC_{50}**: mouse T315I BCR-ABL B-cell EC_{50} (μM) * **T315I_EC50CI**: T315I EC50 95% confidence interval * **T315I_actclass**: T315I activity classification * **T315I_curveScore**: grade for quality of the T315I dose-response curve (see Supplemental for details)	Conventional anti-leukemic agents - Cladribine, Clofarabine, Decitabine, Fludarabine, Nelarabine and Pentostatin, all of which are nucleoside analogs/antimetabolites, were originally not present among agents tested; many agents with similar MOA were validated. Other clincal anti-leukemic agents which belong to categories - antibody, growth factors, enzymes or oligonucleotides, are not compatible to HTS and were not present in the tested compound library.
Screen Summary (2)	Complete dose-response screening data for 706 compounds	* **WT_EC_{50}**: mouse wild-type BCR-ABL B-cell EC_{50} (μM) * **WT_EC_{50}CI**: WT EC_{50} 95% confidence interval * **WT_actclass**: WT activity classification * **WT_curveScore**: grade for quality of the WT dose-response curve (see Supplemental for details) * **T315I_EC_{50}**: mouse T315I BCR-ABL B-cell EC_{50} (μM) * **T315I_EC50CI**: T315I EC50 95% confidence interval * **T315I_actclass**: T315I activity classification * **T315I_curveScore**: grade for quality of the T315I dose-response curve (see Supplemental for details) * **comment**: comments on - observed differential activity	A few compounds showed differential activity between WT and T315I. Most of these are annotated with "Differential activity within experimental error", indicating that there was sufficient uncertainty in the curve fit or that the differences are a result of the hard cutoffs applied for activity classification and are not significant.

ATC Classification	ATC classification for 706 compounds	* **ATC_L1**: Anatomical Therapeutic Chemical (ATC) Classification System first level (anatomical main group) * **ATC_L2**: Anatomical Therapeutic Chemical (ATC) Classification System second level (therapeutic main group) * **ATC_L3**: Anatomical Therapeutic Chemical (ATC) Classification System third level (therapeutic/pharmacological subgroup) * **ATC_L4**: Anatomical Therapeutic Chemical (ATC) Classification System fourth level (chemical/therapeutic/pharmacological subgroup)

hostFactor	conc	hill	EC_{50}	EC_{50}CI	r^2
IL3	0.0 ng/ml	0.5391	5.1118	3.8724 - 6.7479	0.987
IL3	0.01 ng/mL	0.4619	7.5159	5.4628 - 10.3405	0.983
IL3	0.1 ng/mL	0.3164	22.1664	12.1764 - 40.3525	0.944
IL3	1 ng/mL	0.3553	23.3197	14.1087 - 38.5443	0.958
IL3	10 ng/mL	0.3911	22.5621	14.9315 - 34.0924	0.971
IL3	100 ng/mL	0.4276	21.5773	15.2841 - 30.4619	0.979
IL15	0.0 ng/ml	0.5374	4.5252	3.4241 - 5.9805	0.987
IL15	0.01 ng/mL	0.5456	4.7956	3.6317 - 6.3325	0.987
IL15	0.1 ng/mL	0.5223	5.1369	3.9508 - 6.6792	0.988
IL15	1 ng/mL	0.5639	4.6853	3.4341 - 6.3924	0.984
IL15	10 ng/mL	0.5474	4.8593	3.7109 - 6.3630	0.987
IL15	100 ng/mL	0.5803	4.2075	3.2656 - 5.4211	0.989
IL6	0.0 ng/ml	0.5269	4.5635	3.2798 - 6.3497	0.982
IL6	0.01 ng/mL	0.5395	4.6483	3.4190 - 6.3197	0.984
IL6	0.1 ng/mL	0.5771	4.2131	3.1209 - 5.6876	0.984
IL6	1 ng/mL	0.5312	4.645	3.4403 - 6.2716	0.984
IL6	10 ng/mL	0.5605	4.494	3.4060 - 5.9295	0.986
IL6	100 ng/mL	0.5772	4.4834	3.4583 - 5.8123	0.988
SCF	0.0 ng/ml	0.5433	5.0496	3.8776 - 6.5759	0.988
SCF	0.01 ng/mL	0.5206	5.1184	3.7436 - 6.9982	0.984
SCF	0.1 ng/mL	0.5289	4.7638	3.5384 - 6.4137	0.985
SCF	1 ng/mL	0.5263	4.9426	3.7637 - 6.4909	0.987
SCF	10 ng/mL	0.5293	4.9611	3.5256 - 6.9812	0.98
SCF	100 ng/mL	0.5473	4.8079	3.7504 - 6.1636	0.989
FLT3	0.0 ng/ml	0.5785	4.0982	2.9655 - 5.6635	0.982
FLT3	0.01 ng/mL	0.5549	3.251	2.3904 - 4.4215	0.984
FLT3	0.1 ng/mL	0.5837	4.0456	3.1306 - 5.2282	0.988
FLT3	1 ng/mL	0.5677	4.1235	2.9621 - 5.7402	0.981
FLT3	10 ng/mL	0.567	3.6648	2.7944 - 4.8065	0.987
FLT3	100 ng/mL	0.6116	3.9157	2.9477 - 5.2015	0.986
IL4	0.0 ng/ml	0.494	6.2811	4.3841 - 8.9990	0.979
IL4	0.01 ng/mL	0.4721	7.6786	5.1536 - 11.4406	0.974
IL4	0.1 ng/mL	0.4582	10.607	7.3974 - 15.2093	0.978
IL4	1 ng/mL	0.4529	11.2471	7.8367 - 16.1418	0.978
IL4	10 ng/mL	0.4687	10.4343	7.1849 - 15.1533	0.977
IL4	100 ng/mL	0.4579	11.1402	7.6311 - 16.2629	0.976
TSLP	0.0 ng/ml	0.5017	4.9482	3.5263 - 6.9434	0.981
TSLP	0.01 ng/mL	0.4805	5.692	3.8453 - 8.4256	0.975
TSLP	0.1 ng/mL	0.5043	8.314	6.0702 - 11.3872	0.983
TSLP	1 ng/mL	0.456	13.35	10.1901 - 17.4896	0.987
TSLP	10 ng/mL	0.4007	18.4296	12.8535 - 26.4247	0.978
TSLP	100 ng/mL	0.4177	17.6412	11.9235 - 26.1008	0.974
MCSF	0.0 ng/ml	0.5307	4.8682	3.5748 - 6.6296	0.984
MCSF	0.01 ng/mL	0.5375	4.803	3.0670 - 7.5216	0.968
MCSF	0.1 ng/mL	0.5247	5.4838	3.8284 - 7.8550	0.979
MCSF	1 ng/mL	0.5357	4.6983	3.2180 - 6.8595	0.977
MCSF	10 ng/mL	0.517	4.6896	3.2354 - 6.7975	0.978
MCSF	100 ng/mL	0.5489	4.943	3.4050 - 7.1756	0.978
IL9	0.0 ng/ml	0.5582	4.2149	2.9368 - 6.0491	0.979
IL9	0.01 ng/mL	0.5585	4.3679	3.0111 - 6.3359	0.977
IL9	0.1 ng/mL	0.5698	4.0533	2.8653 - 5.7341	0.98
IL9	1 ng/mL	0.538	4.6609	3.1394 - 6.9198	0.975
IL9	10 ng/mL	0.5789	4.4575	2.8883 - 6.8792	0.97
IL9	100 ng/mL	0.5306	5.3572	3.5917 - 7.9905	0.975
GMCSF	0.0 ng/ml	0.4922	4.9682	3.4753 - 7.1024	0.979
GMCSF	0.01 ng/mL	0.5195	4.4331	3.1515 - 6.2359	0.981
GMCSF	0.1 ng/mL	0.4903	5.2002	3.7301 - 7.2496	0.982
GMCSF	1 ng/mL	0.5287	5.0754	3.5354 - 7.2862	0.978
GMCSF	10 ng/mL	0.4985	5.1825	3.6136 - 7.4324	0.979
GMCSF	100 ng/mL	0.5077	5.2664	3.9156 - 7.0832	0.985
CXCL12	0.0 ng/ml	0.5302	4.2517	3.0049 - 6.0157	0.98
CXCL12	0.01 ng/mL	0.5506	4.02	2.8966 - 5.5790	0.982
CXCL12	0.1 ng/mL	0.555	4.3428	3.0724 - 6.1384	0.98
CXCL12	1 ng/mL	0.5543	4.9481	3.5552 - 6.8868	0.982
CXCL12	10 ng/mL	0.5257	6.341	4.6141 - 8.7143	0.983
CXCL12	100 ng/mL	0.5626	7.7776	5.4588 - 11.0814	0.979
GCSF	0.0 ng/ml	0.4859	5.3848	3.8070 - 7.6163	0.98
GCSF	0.01 ng/mL	0.4888	5.6829	4.1379 - 7.8048	0.983
GCSF	0.1 ng/mL	0.4995	5.2436	3.5467 - 7.7522	0.975
GCSF	1 ng/mL	0.5238	4.4557	2.9858 - 6.6491	0.974
GCSF	10 ng/mL	0.5082	5.5333	3.8070 - 8.0422	0.977
GCSF	100 ng/mL	0.5071	5.5916	3.8599 - 8.1003	0.978
TGFb	0.0 ng/ml	0.5196	4.4138	3.1588 - 6.1674	0.981
TGFb	0.01 ng/mL	0.8345	2.0792	1.3877 - 3.1152	0.972
TGFb	0.1 ng/mL	1.3386	1.0712	0.6824 - 1.6815	0.943
TGFb	1 ng/mL	1.1768	1.2921	0.8022 - 2.0810	0.949
TGFb	10 ng/mL	1.0645	1.4597	0.8969 - 2.3756	0.954
TGFb	100 ng/mL	1.258	1.4057	0.8535 - 2.3151	0.947
IL2	0.0 ng/ml	0.5186	4.3969	3.0447 - 6.3495	0.978
IL2	0.01 ng/mL	0.4837	4.8218	3.3902 - 6.8578	0.98

IL2	0.1 ng/mL	0.4856	4.531	3.0037 - 6.8346	0.974
IL2	1 ng/mL	0.51	4.4851	3.1998 - 6.2866	0.981
IL2	10 ng/mL	0.5181	4.753	3.2444 - 6.9630	0.977
IL2	100 ng/mL	0.507	4.6062	3.3039 - 6.4219	0.982
IL7	0.0 ng/ml	0.4659	7.0902	5.2763 - 9.5276	0.985
IL7	0.01 ng/mL	0.3318	61.9094	41.1312 - 93.1840	0.971
IL7	0.1 ng/mL	0.3661	251.4246	157.6730 - 400.9203	0.958
IL7	1 ng/mL	0.3761	281.2124	165.0664 - 479.0824	0.947
IL7	10 ng/mL	0.383	286.5185	173.4620 - 473.2615	0.95
IL7	100 ng/mL	0.352	448.189	245.0635 - 819.6787	0.938

sample	regnumber	supplier name	supplier ID	salt name	salt eqs	solvate name	solvate eqs	formula weight	molsmiles	synonym
SJ000000250-8	SJ000000250	SIGMA	P 9708	CHLORIDE	1	NO_SOLVATE	0	376.9439	CCCNC[C@H](O)COc1ccccc1C(=O)CCc2ccccc2	PROPAFENONE
SJ000000854-6	SJ000000854	SIGMA	Q 0125	NO_SALT	0	NO_SOLVATE	0	302.2357	OC1=C(Oc2cc(O)cc(O)c2C1=O)c3ccc(O)c(O)c3	QUERCETIN
SJ000113084-4	SJ000113084	SIGMA	D 9815	METHANESULFONATE	1	NO_SOLVATE	0	546.5751	Oc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)C4COc5ccccc5	DOXAZOSIN
SJ000126662-3	SJ000126662	SIGMA	861669	NO_SALT	0	NO_SOLVATE	0	434.4264	2ccc(cc2)[N+](=O)[O-])c3ncn([C@@H]4O[C@H](CO)[C@H](	NBTGR
SJ000285182-2	SJ000285182	MICROSOURCE	1501107	NO_SALT	0	NO_SOLVATE	0	292.2839	[C@H]2OC(=O)[C@@H]1[C@]3(O)C[C@H]4O[C@]45C(=O)	PICROTOXININ
SJ000285183-2	SJ000285183	MICROSOURCE	1500169	CHLORIDE	1	NO_SOLVATE	0	340.0325	CCCCCCCCCCCCCCCC[n+]1ccccc1	CETYLPYRIDINIUM CHLORIDE
SJ000285185-4	SJ000285185	PRESTWICK	548	PHOSPHATE	2	NO_SOLVATE	0	509	CCN(CC)CCCC(C)Nc1ccnc2cc(Cl)ccc12	CHLOROQUINE DIPHOSPHATE
SJ000285188-6	SJ000285188	SIGMA	C 6645	CHLORIDE	1	NO_SOLVATE	0	278.7166	=NC(=O)N(C=C1)[C@@H]2O[C@H](CO)[C@@H](O)[C@@	CYTARABINE
SJ000285190-2	SJ000285190	MICROSOURCE	1500305	NO_SALT	0	NO_SOLVATE	0	130.0772	Oc1ncc(F)c(O)n1	FLUOROURACIL
SJ000285193-1	SJ000285193	MICROSOURCE	1500375	NO_SALT	0	NO_SOLVATE	0	156.0535	CN(CCCl)CCCl	CHLORMETHINE
SJ000285194-2	SJ000285194	MICROSOURCE	1500382	NO_SALT	0	NO_SOLVATE	0	305.2002	N[C@@H](Cc1ccc(cc1)N(CCCl)CCCl)C(=O)O	MELPHALAN
SJ000285194-4	SJ000285194	SIGMA	M 2011	NO_SALT	0	NO_SOLVATE	0	305.2002	NC(Cc1ccc(cc1)N(CCCl)CCCl)C(=O)O	MELPHALAN
SJ000285195-2	SJ000285195	MICROSOURCE	1500387	NO_SALT	0	NO_SOLVATE	0	152.177	Sc1[nH]cnc2ncnc12	MERCAPTOPURINE
SJ000285196-2	SJ000285196	MICROSOURCE	1500398	NO_SALT	0	NO_SOLVATE	0	454.4392	cnc2nc(N)nc(N)c2n1)c3ccc(cc3)C(=O)N[C@@H](CCC(=O)O)	METHOTREXATE
SJ000285197-1	SJ000285197	MICROSOURCE	1500674	NO_SALT	0	NO_SOLVATE	0	320.3371	COc1c(C)c2COC(=O)c2c(O)c1C\C=C(/C)\CCC(=O)O	MYCOPHENOLIC ACID
SJ000285200-6	SJ000285200	SIGMA	P 0547	DROXYETHANESULFON	2	NO_SOLVATE	0	590.4194	NC(=N)c1ccc(OCCCCCOc2ccc(cc2)C(=N)N)cc1	PENTAMIDINE ISETHIONATE
SJ000285202-2	SJ000285202	MICROSOURCE	1500522	CHLORIDE	2	NO_SOLVATE	0	470.9568	CCN(CC)CCCC(C)Nc1c2ccc(Cl)cc2nc3ccc(OC)cc13	QUINACRINE
SJ000285203-5	SJ000285203	SIGMA	R 8875	NO_SALT	0	NO_SOLVATE	0	394.4171	2OC[C@H]3Oc4c5C[C@@H](Oc5ccc4C(=O)[C@H]3c2cc1OC	ROTENONE
SJ000285206-2	SJ000285206	MICROSOURCE	1500651	NO_SALT	0	NO_SOLVATE	0	334.4115	C2OCC=C3CN4CC[C@@]56C4C[C@@H]3[C@@H]2C5N1c7	STRYCHNINE
SJ000285207-1	SJ000285207	MICROSOURCE	1500572	SODIUM(I)	1	NO_SOLVATE	0	405.8295	CC[Hg]Sc1ccccc1C(=O)O	THIMEROSAL
SJ000285208-3	SJ000285208	MICROSOURCE	1500573	NO_SALT	0	NO_SOLVATE	0	167.1917	Nc1nc(S)c2[nH]cnc2n1	THIOGUANINE
SJ000285210-2	SJ000285210	MICROSOURCE	1500171	NO_SALT	0	NO_SOLVATE	0	304.2121	OC(=O)CCCc1ccc(cc1)N(CCCl)CCCl	CHLORAMBUCIL
SJ000285212-1	SJ000285212	MICROSOURCE	1501105	CHLORIDE	2	NO_SOLVATE	0	542.5095	(N)C(=O)N[C@@H]2[C@@H](CO)OC([C@@H]2O)n3cnc4c(	PUROMYCIN
SJ000285215-1	SJ000285215	MICROSOURCE	1500272	CHLORIDE	2	NO_SOLVATE	0	551.6389	1CN2CCc3cc(OC)c(OC)cc3C2C[C@@H]1CC4NCCc5cc(OC)	EMETINE
SJ000285215-6	SJ000285215	SIGMA	E 2375	CHLORIDE	2	NO_SOLVATE	0	551.6389	Cc3cc(OC)c(OC)cc3[C@@H]2C[C@@H]1C[C@H]4NCCc5c	EMETINE
SJ000285218-5	SJ000285218	SIGMA	C 7632	NO_SALT	0	NO_SOLVATE	0	196.1998	CC12C3CCC(O3)C1(C)C(=O)OC2=O	CANTHARIDIN
SJ000285219-2	SJ000285219	MICROSOURCE	1501189	NO_SALT	0	NO_SOLVATE	0	246.1924	C[C@H]1OC(C(O)[C@@H]1O)N2C=C(F)C(=O)NC2=O	FLUORO-5'-DEOXYURIDINE
SJ000285219-5	SJ000285219	SIGMA	F 8791	NO_SALT	0	NO_SOLVATE	0	246.1924	C@H]1O[C@H]([C@H](O)[C@@H]1O)N2C=C(F)C(=O)NC2=	FLUORO-5'-DEOXYURIDINE
SJ000285220-5	SJ000285220	SIGMA	P 0667	NO_SALT	0	NO_SOLVATE	0	248.3175	=C\CC[C@@]2(C)O[C@@H]2[C@H]3OC(=O)C(=C)[C@@H]	PARTHENOLIDE
SJ000285221-4	SJ000285221	SIGMA	A 1784	NO_SALT	0	NO_SOLVATE	0	440.4127	1nc(N)c2nc(CNc3ccc(cc3)C(=O)NC(CCC(=O)O)C(=O)O)cnc2	AMINOPTERIN
SJ000285225-2	SJ000285225	MICROSOURCE	1502108	NO_SALT	0	NO_SOLVATE	0	534.5986	OC(=O)CC(C)C)[C@H](C)OC(=O)[C@@H](NC(=O)c2cccc(N	ANTIMYCIN A
SJ000285226-6	SJ000285226	SIGMA	A 2169	NO_SALT	0	NO_SOLVATE	0	267.2413	CN([C@H]2C[C@@H]([N-][N+]#N)[C@@H](CO)O2)C(=O)N	ZIDOVUDINE
SJ000285227-1	SJ000285227	MICROSOURCE	1502111	NO_SALT	0	NO_SOLVATE	0	244.2046	1=NC(=O)N(C=N1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H	AZACITIDINE
SJ000285228-4	SJ000285228	PRESTWICK	790	NO_SALT	0	NO_SOLVATE	0	281.3474	H]1C[C@H](C)C(=O)[C@@H](C1)[C@H](O)CC2CC(=O)NC(	CYCLOHEXIMIDE
SJ000285229-2	SJ000285229	MICROSOURCE	1502113	NO_SALT	0	NO_SOLVATE	0	173.1267	NC(COC(=O)[CH-][N+]#N)C(=O)O	AZASERINE
SJ000285231-2	SJ000285231	MICROSOURCE	1502117	POTASSIUM(I)	2	NO_SOLVATE	0	802.9918	C[C@@]45CC(CC[C@H]4[C@]3(C)C2)C(=C)[C@@H]5O)C(	ATRACTYLOSIDE
SJ000285232-1	SJ000285232	MICROSOURCE	2300332	NO_SALT	0	NO_SOLVATE	0	414.4052	C)c1OC)[C@H]2[C@@H]3[C@H](COC3=O)[C@@H](O)c4cc	PODOFILOX
SJ000285232-8	SJ000285232	SIGMA	P 4405	NO_SALT	0	NO_SOLVATE	0	414.4052	(OC)c1OC)[C@H]2[C@@H]3C(COC3=O)[C@@H](O)c4cc5C	PODOFILOX
SJ000285234-2	SJ000285234	MICROSOURCE	1503602	SODIUM(I)	1	NO_SOLVATE	0	773.9986	=O)[C@H](CC)[C@H]2OC3(O[C@@]4(CC[C@](C)(O4)[C@H	SALINOMYCIN
SJ000285235-3	SJ000285235	PRESTWICK	396	NO_SALT	0	NO_SOLVATE	0	588.5565	](COC3=O)[C@H](O[C@@H]4O[C@@H]5CO[C@@H](C)O[(	ETOPOSIDE
SJ000285238-3	SJ000285238	MICROSOURCE	1500205	NO_SALT	0	NO_SOLVATE	0	399.437	=CC=C2C(=CC1=O)[C@H](CCc3cc(OC)c(OC)c(OC)c23)NC	COLCHICINE
SJ000285241-3	SJ000285241	MICROSOURCE	1500133	NO_SALT	0	NO_SOLVATE	0	277.2625	Cn1cnc(c1Sc2[nH]cnc3ncnc23)[N+](=O)[O-]	AZATHIOPRINE
SJ000285242-3	SJ000285242	MICROSOURCE	1500138	CHLORIDE	1	NO_SOLVATE	0	448.1273	CC(C)(C)CC(C)(C)c1ccc(OCCOCC[N+](C)(C)Cc2ccccc2)cc1	BENZETHONIUM CHLORIDE
SJ000285243-2	SJ000285243	MICROSOURCE	330002	NO_SALT	0	NO_SOLVATE	0	334.3272	12[C@@H]3NC3CN1C4=C([C@@H]2COC(=O)N)C(=O)C(=C	MITOMYCIN
SJ000285244-3	SJ000285244	MICROSOURCE	1500319	NO_SALT	0	NO_SOLVATE	0	1141.4468	)C(Cc3ccccc3)NC(=O)C(CC(C)C)NC(=O)C(CCCN)NC(=O)C	GRAMICIDIN
SJ000285246-2	SJ000285246	MICROSOURCE	1500618	CHLORIDE	1	NO_SOLVATE	0	259.7805	C[n+]1c2cc(N)ccc2cc3ccc(N)cc13	ACRIFLAVINIUM
SJ000285249-1	SJ000285249	MICROSOURCE	330001	NO_SALT	0	NO_SOLVATE	0	1253.4409	)C(C(C)C)N(C)C(=O)CN(C)C(=O)C6CCCC6C(=O)C(NC5=C	DACTINOMYCIN
SJ000285256-3	SJ000285256	MICROSOURCE	200022	CHLORIDE	1	NO_SOLVATE	0	605.0996	C@@H]([C@H](O)[C@H](C)O2)N(C)C)c3c(O)c4C(=O)c5c(O	AKLAVINE HYDROCHLORIDE
SJ000285261-3	SJ000285261	MICROSOURCE	1500315	CHLORIDE	1	NO_SOLVATE	0	408.0252	N(C)c1ccc(cc1)C(=C2C=CC(=[N+](C)C)C=C2)c3ccc(cc3)N(C)	GENTIAN VIOLET
SJ000285262-1	SJ000285262	MICROSOURCE	1500122	NO_SALT	0	NO_SOLVATE	0	924.079	(O)C(C(C[C@@H](OC3OC(C)C(O)[C@@H](N)C3O)\C=C\C=	AMPHOTERICIN B
SJ000285263-2	SJ000285263	MICROSOURCE	1500324	NO_SALT	0	NO_SOLVATE	0	270.0899	OC(=O)c1ccc(cc1)S(=O)(=O)N(Cl)Cl	HALAZONE
SJ000285267-3	SJ000285267	MICROSOURCE	1503322	NO_SALT	0	NO_SOLVATE	0	240.4328	CN(C)C(=S)SSC(=S)N(C)C	THIRAM
SJ000285270-2	SJ000285270	MICROSOURCE	1503324	NO_SALT	0	NO_SOLVATE	0	189.2183	S=P(N1CC1)(N2CC2)N3CC3	THIOTEPA
SJ000285272-2	SJ000285272	MICROSOURCE	1503059	NO_SALT	0	NO_SOLVATE	0	246.1924	OC[C@H]1OC(C[C@H]1O)N2C=C(F)C(=O)NC2=O	FLOXURIDINE
SJ000285273-3	SJ000285273	MICROSOURCE	1500328	NO_SALT	0	NO_SOLVATE	0	406.9035	Oc1c(Cl)cc(Cl)c(Cl)c1Cc2c(O)c(Cl)cc(Cl)c2Cl	HEXACHLOROPHENE
SJ000285276-2	SJ000285276	MICROSOURCE	1503239	NO_SALT	0	NO_SOLVATE	0	356.4817	CCN(CC)CCNc1ccc(CO)c2Sc3ccccc3C(=O)c12	HYCANTHONE
SJ000285278-1	SJ000285278	MICROSOURCE	1503266	NO_SALT	0	NO_SOLVATE	0	301.3204	COC(=O)Nc1nc2cc(ccc2[nH]1)C(=O)c3cccs3	NOCODAZOLE
SJ000285279-2	SJ000285279	MICROSOURCE	2300219	CHLORIDE	1	NO_SOLVATE	0	201.7395	CC[N+](C)(C)c1cccc(O)c1	EDROPHONIUM
SJ000285285-3	SJ000285285	MICROSOURCE	1503065	NO_SALT	0	NO_SOLVATE	0	210.2794	CN(C)c1nc(nc(n1)N(C)C)N(C)C	ALTRETAMINE
SJ000285292-10	SJ000285292	SIGMA	C 3909	NO_SALT	0	NO_SOLVATE	0	102.0919	N[C@@H]1CONC1=O	CYCLOSERINE
SJ000285294-1	SJ000285294	MICROSOURCE	1500644	NO_SALT	0	NO_SOLVATE	0	336.7379	CC(=O)O[Hg]c1ccccc1	PHENYLMERCURIC ACETATE
SJ000285299-2	SJ000285299	MICROSOURCE	1503214	NO_SALT	0	NO_SOLVATE	0	256.2551	CCC1=CN(C2OCC(O)C2CO)C(=O)NC1=O	EDOXUDINE
SJ000285307-3	SJ000285307	MICROSOURCE	1503244	SODIUM(I)	1	NO_SOLVATE	0	613.7877	C)C2CC[C@](O)(CC)[C@H](C)O2)C(=O)C(C)[C@@H](O)[C	LASALOCID SODIUM
SJ000285308-1	SJ000285308	MICROSOURCE	1503127	CHLORIDE	2	NO_SOLVATE	0	527.6643	c1cc(N)c2ccccc2[n+]1CCCCCCCCCC[n+]3c(C)cc(N)c4cccc	DEQUALINIUM CHLORIDE
SJ000285313-3	SJ000285313	MICROSOURCE	1505337	NO_SALT	0	NO_SOLVATE	0	434.6126	CCCCCCCC\C=C\CCCCCCCCOP(=O)(O)OCC[N+](C)(C)C	ELAIDYLPHOSPHOCHOLINE
SJ000285315-2	SJ000285315	MICROSOURCE	1505317	NO_SALT	0	NO_SOLVATE	0	257.2614	CCCCCCNC(=O)N1C=C(F)C(=O)NC1=O	CARMOFUR
SJ000285316-4	SJ000285316	PRESTWICK	302	CHLORIDE	1	NO_SOLVATE	0	442.0373	)C1)C(=O)N[C@H]([C@@H](C)O)[C@H]2O[C@H](SC)[C@H	LINCOMYCIN
SJ000285317-2	SJ000285317	MICROSOURCE	1500456	NO_SALT	0	NO_SOLVATE	0	145.1579	Oc1cccc2cccnc12	OXYQUINOLINE
SJ000285318-7	SJ000285318	SIGMA	E 8375	NO_SALT	0	NO_SOLVATE	0	275.3461	CNC(=O)Oc1ccc2N(C)[C@H]3N(C)CC[C@@]3(C)c2c1	PHYSOSTIGMINE SALICYLATE
SJ000285319-1	SJ000285319	MICROSOURCE	1503074	CHLORIDE	2	NO_SOLVATE	0	579.7898	C(CC)CN=C(N)N=C(N)NCCCCCCNC(=NC(=NCC(CC)CCC	ALEXIDINE HYDROCHLORIDE
SJ000285321-4	SJ000285321	PRESTWICK	385	CHLORIDE	2	NO_SOLVATE	0	515.4809	CCNCCNc1ccc(NCCNCCO)c2C(=O)c3c(O)ccc(O)c3C(=O)c1	MITOXANTRONE
SJ000285323-3	SJ000285323	MICROSOURCE	1500637	SODIUM(I)	2	NO_SOLVATE	0	752.6878	]c1c(O)c(Br)cc2C(=C3C=C(Br)C(=O)C=C3Oc12)c4ccccc4C(	MERBROMIN
SJ000285327-1	SJ000285327	MICROSOURCE	310035	SULFATE	1	NO_SOLVATE	0	428.4289	C[n+]1cc2c3OCOc3ccc2c4ccc5cc6OCOc6cc5c14	SANGUINARINE SULFATE
SJ000285332-1	SJ000285332	MICROSOURCE	1500260	NO_SALT	0	NO_SOLVATE	0	318.7101	S=C1CC=CC=[N+]1O[Zn]ON2C=CC=CC2=S	PYRITHIONE ZINC
SJ000285334-4	SJ000285334	PRESTWICK	152	PHOSPHATE	1	NO_SOLVATE	0	782.8583	[C@H]3O)N(C)C)[C@@H](C)C[C@@]4(CO4)C(=O)[C@H](	OLEANDOMYCIN PHOSPHATE
SJ000285335-1	SJ000285335	MICROSOURCE	1500611	SULFATE	1	NO_SOLVATE	0	907.0741	C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](OC(=O	VINBLASTINE
SJ000285335-4	SJ000285335	SIGMA	V 1377	SULFATE	1	NO_SOLVATE	0	907.0741	C(=O)OC)c5cc6c(cc5OC)N(C)C7[C@](O)([C@H](OC(=O)C)[	VINBLASTINE
SJ000285337-5	SJ000285337	PRESTWICK	256	NO_SALT	0	NO_SOLVATE	0	300.4351	C\C(=C\C(=O)O)\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C	ISOTRETINOIN
SJ000285337-8	SJ000285337	SIGMA	R 2625	NO_SALT	0	NO_SOLVATE	0	300.4351	C\C(=C/C=C/C(=C/C(=O)O)/C)\C=C\C1=C(C)CCCC1(C)C	TRETINOIN
SJ000285338-3	SJ000285338	PRESTWICK	143	NO_SALT	0	NO_SOLVATE	0	505.4466	ccc(NC(=N)NC(=N)NCCCCCCNC(=N)NC(=N)Nc2ccc(Cl)cc2	CHLORHEXIDINE
SJ000285343-2	SJ000285343	MICROSOURCE	1502025	NO_SALT	0	NO_SOLVATE	0	355.3894	OC(=O)CCC(=O)Nc1ccc(cc1)S(=O)(=O)Nc2nccs2	SUCCINYLSULFATHIAZOLE
SJ000285358-5	SJ000285358	SIGMA	H 4001	NO_SALT	0	NO_SOLVATE	0	362.4599	=C1CC[C@H]3[C@@H]4CC[C@](O)(C(=O)CO)[C@@]4(C)(	HYDROCORTISONE
SJ000285363-5	SJ000285363	SIGMA	M-149	METHANESULFONATE	1	NO_SOLVATE	0	451.6479	CSc1ccc2Sc3ccccc3CC(N4CCN(C)CC4)c2c1	METITEPINE
SJ000285364-2	SJ000285364	PRESTWICK	134	CHLORIDE	1	NO_SOLVATE	0	450.0178	ccc(cc1)[C@@H]2Sc3ccccc3N(CCN(C)C)C(=O)[C@@H]2OC	DILTIAZEM
SJ000285365-1	SJ000285365	MICROSOURCE	1502258	SODIUM(I)	1	NO_SOLVATE	0	691.898	2)[C@]3(CC)CC[C@@H](O3)[C@]4(C)CCC5(C[C@H](O)[C@	MONENSIN SODIUM SALT
SJ000285368-3	SJ000285368	PRESTWICK	710	NO_SALT	0	NO_SOLVATE	0	404.4965	H](CC[C@]4(O)C[C@@H](O)CC[C@]34C=O)[C@@]1(O)CC	STROPHANTHIDIN
SJ000285369-1	SJ000285369	MICROSOURCE	210515	NO_SALT	0	NO_SOLVATE	0	204.1788	OC1=CC=Cc2ccc(O)c(O)c2C1=O	PYROGALLIN
SJ000285373-9	SJ000285373	SIGMA	A 0257	SULFATE	0.5	NO_SOLVATE	0	337.4194	CN1C2CCC1CC(C2)OC(=O)C(CO)c3ccccc3	ATROPINE
SJ000285375-2	SJ000285375	MICROSOURCE	1504174	CHLORIDE	1	NO_SOLVATE	0	275.2411	CC(NC(C)(C)C)C(=O)c1cccc(Cl)c1	BUPROPION
SJ000285382-3	SJ000285382	PRESTWICK	730	NO_SALT	0	NO_SOLVATE	0	430.6199	[C@H]4[C@@H]5CC[C@H]6C[C@@H](O)CC[C@]6(C)[C@	HECOGENIN
SJ000285383-1	SJ000285383	MICROSOURCE	1501114	FUMARATE	1	NO_SOLVATE	0	407.5258	CN1CCC(=C2c3ccccc3Sc4ccccc24)CC1	PIMETHIXENE MALEATE
SJ000285387-8	SJ000285387	SIGMA	E 3250	SULFATE	0.5	NO_SOLVATE	0	213.2822	CN[C@@H](C)[C@H](O)c1ccccc1	PSEUDOEPHEDRINE HYDROCHLORIDE
SJ000285396-2	SJ000285396	MICROSOURCE	1502162	NO_SALT	0	NO_SOLVATE	0	199.6342	NC(Cc1ccc(Cl)cc1)C(=O)O	CHLOROPHENYLALANINE
SJ000285400-2	SJ000285400	MICROSOURCE	310010	NO_SALT	0	NO_SOLVATE	0	232.3181	C[C@H]1CCC[C@]2(C)C[C@H]3OC(=O)C(=C)[C@H]3C=C12	HELENINE
SJ000285410-5	SJ000285410	SIGMA	C 9911	NO_SALT	0	NO_SOLVATE	0	348.352	[C@@]1(O)C(=O)OCC2=C1C=C3N(Cc4cc5ccccc5nc34)C2=	CAMPTOTHECIN
SJ000285413-1	SJ000285413	MICROSOURCE	1505235	NO_SALT	0	NO_SOLVATE	0	324.4549	CC(=O)OCC(O)CC(=O)CCCCCCCCCCCC#C	AVOCADYNONE ACETATE
SJ000285423-2	SJ000285423	MICROSOURCE	1504181	NO_SALT	0	NO_SOLVATE	0	464.6362	2(C)CC[C@]3(C)C4=CC=C5C(=C(O)C(=O)C=C5[C@]4(C)CC	PRISTIMERIN
SJ000285426-2	SJ000285426	MICROSOURCE	1502177	ACETATE	1	NO_SOLVATE	0	468.5428	CSCCC(N)C(=O)NC(CC(C)C)C(=O)NC(Cc1ccccc1)C(=O)O	HIONYL-LEUCYLPHENYLALANINE ACETATE
SJ000285431-2	SJ000285431	MICROSOURCE	310028	NO_SALT	0	NO_SOLVATE	0	388.4541	H]2C[C@H]3OC(=O)C[C@H]4C(=C(OC)C(=O)C([C@@]34C)	QUASSIN
SJ000285433-1	SJ000285433	MICROSOURCE	1505230	NO_SALT	0	NO_SOLVATE	0	369.4606	O=C1CCc2cc(OCCCCc3nnnn3C4CCCCC4)ccc2N1	CILOSTAZOL
SJ000285436-3	SJ000285436	PRESTWICK	498	NO_SALT	0	NO_SOLVATE	0	282.3321	@H]2[C@@H](C)C(=O)O[C@@H]3O[C@@]4(C)CC[C@@H	ARTEMISININ
SJ000285439-2	SJ000285439	MICROSOURCE	1500603	NO_SALT	0	NO_SOLVATE	0	1272.4458	)C(CCC(=O)O)NC(=O)C(CC(=O)O)NC(=O)C(Cc3ccccc3)NC(	TYROTHRICIN
SJ000285440-2	SJ000285440	MICROSOURCE	1504240	NO_SALT	0	NO_SOLVATE	0	158.1534	O=C1C=CC(=O)c2ccccc12	1,4-NAPHTHOQUINONE
SJ000285442-1	SJ000285442	MICROSOURCE	1505345	NO_SALT	0	NO_SOLVATE	0	368.3799	COc1cc(\C=C\C(=CC(=O)\C=C\c2ccc(O)c(OC)c2)O)ccc1O	CURCUMIN
SJ000285443-2	SJ000285443	MICROSOURCE	1500762	NO_SALT	0	NO_SOLVATE	0	290.3126	Oc1ccc(cc1)C(=C2C=CC(=O)C=C2)c3ccc(O)cc3	ROSOLIC ACID
SJ000285445-2	SJ000285445	MICROSOURCE	1500775	NO_SALT	0	NO_SOLVATE	0	747.8288	OC(=O)Cc1cc(I)c(Oc2cc(I)c(O)c(I)c2)c(I)c1	TETRAC
SJ000285450-2	SJ000285450	MICROSOURCE	1500810	NO_SALT	0	NO_SOLVATE	0	194.2319	Nc1c2ccccc2nc3ccccc13	9-AMINOACRIDINE
SJ000285451-3	SJ000285451	PRESTWICK	586	CHLORIDE	1	NO_SOLVATE	0	371.8606	COc1ccc2cc3c4cc5OCOc5cc4CC[n+]3cc2c1OC	BERBERINE CHLORIDE
SJ000285452-1	SJ000285452	MICROSOURCE	1500813	NO_SALT	0	NO_SOLVATE	0	430.5338	2CC3C4CCC5=CC(=O)C=CC5(C)C4[C@@H](O)CC3(C)[C@	BUDESONIDE
SJ000285452-5	SJ000285452	SIGMA	B 7777	NO_SALT	0	NO_SOLVATE	0	430.5338	@@H]4CCC5=CC(=O)C=C[C@]5(C)[C@H]4[C@@H](O)C[(	BUDESONIDE
SJ000285453-3	SJ000285453	PRESTWICK	148	POTASSIUM(I)	1	NO_SOLVATE	0	397.5712	C=C1C=C[C@@H]3[C@@H]2CC[C@@]4(C)[C@H]3CC[C@	POTASSIUM CANRENOATE
SJ000285454-2	SJ000285454	MICROSOURCE	1500836	SODIUM(I)	1	NO_SOLVATE	0	438.4182	OCC1=C(N2C(SC1)[C@H](NC(=O)CCCC(N)C(=O)O)C2=O)	CEPHALOSPORIN C SODIUM
SJ000285460-1	SJ000285460	MICROSOURCE	1502030	NO_SALT	0	NO_SOLVATE	0	261.2301	CCN1C=C(C(=O)O)C(=O)c2cc3OCOc3cc12	OXOLINIC ACID
SJ000285461-1	SJ000285461	MICROSOURCE	1501117	CHLORIDE	1	NO_SOLVATE	0	465.0491	CCN(CCCCOC(=O)c1ccc(OC)c(OC)c1)C(C)Cc2ccc(OC)cc2	MEBEVERINE HYDROCHLORIDE
SJ000285462-2	SJ000285462	MICROSOURCE	1501118	OXY-5-SULFONATOBEN	1	NO_SOLVATE	0	693.0637	@H](O)[C@@H]3C(=C)c4c(Cl)ccc(O)c4C(=C3C(=O)[C@]2(	MECLOCYCLINE SULFOSALICYLATE
SJ000285465-2	SJ000285465	MICROSOURCE	1501121	CHLORIDE	1	NO_SOLVATE	0	214.8018	CC12CC3CC(C)(C1)CC(N)(C3)C2	MEMANTINE
SJ000285466-4	SJ000285466	SIGMA	A 4147	SODIUM(I)	1	NO_SOLVATE	0	161.166	NCCCS(=O)(=O)[O-]	HOMOTAURINE
SJ000285484-2	SJ000285484	MICROSOURCE	1500639	CHLORIDE	1	NO_SOLVATE	0	188.6784	NCC(O)c1ccc(O)cc1	OCTOPAMINE HYDROCHLORIDE
SJ000285487-3	SJ000285487	PRESTWICK	874	NO_SALT	0	NO_SOLVATE	0	180.164	CN1C(=O)NC(=O)c2c1ncn2C	THEOBROMINE
SJ000285490-1	SJ000285490	MICROSOURCE	201524	NO_SALT	0	NO_SOLVATE	0	630.767	(C)C)c3OC45C6CC(C=C4C(=O)c3c(O)c2C=C1)C(O)C5(C\C	DIHYDROGAMBOGIC ACID
SJ000285502-5	SJ000285502	SIGMA	A 8423	CHLORIDE	1	NO_SOLVATE	0	680.8116	CCCCc1oc2ccccc2c1C(=O)c3cc(I)c(OCCN(CC)CC)c(I)c3	AMIODARONE
SJ000285504-2	SJ000285504	MICROSOURCE	1503270	CHLORIDE	1	NO_SOLVATE	0	255.8107	CCCNC(C)C(=O)Nc1ccccc1C	PRILOCAINE
SJ000285506-2	SJ000285506	MICROSOURCE	2300009	NO_SALT	0	NO_SOLVATE	0	410.549	CCN(CC)CCOc1ccc2c(c1)C(=O)c3cc(OCCN(CC)CC)ccc23	TILORONE
SJ000285508-1	SJ000285508	MICROSOURCE	1503908	NO_SALT	0	NO_SOLVATE	0	853.9061	OC(=O)C)C2[C@H](OC(=O)c4ccccc4)[C@]5(O)C[C@H](OC(	PACLITAXEL
SJ000285512-1	SJ000285512	MICROSOURCE	300037	NO_SALT	0	NO_SOLVATE	0	376.4864	))OC1C\C(=C\CC\C(=C\CC[C@](C)(O)C2CC1C(=C)C(=O)O2	CRASSIN ACETATE
SJ000285522-3	SJ000285522	MICROSOURCE	2300253	NO_SALT	0	NO_SOLVATE	0	151.2056	C[C@@H](N)[C@@H](O)c1ccccc1	EPHEDRINE
SJ000285526-3	SJ000285526	PRESTWICK	950	NO_SALT	0	NO_SOLVATE	0	129.157	OC(=O)C1CCCNC1	NIPECOTIC ACID
SJ000285536-1	SJ000285536	MICROSOURCE	1500487	NITRATE	1	NO_SOLVATE	0	270.2569	CC[C@H]1[C@@H](Cc2cncn2C)COC1=O	PILOCARPINE
SJ000285540-4	SJ000285540	SIGMA	P 7791	CHLORIDE	1	NO_SOLVATE	0	418.9011	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)c4occc4	PRAZOSIN
SJ000285541-3	SJ000285541	PRESTWICK	274	NO_SALT	0	NO_SOLVATE	0	360.444	)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@]34C)[C@@H]1C(	PREDNISOLONE
SJ000285542-2	SJ000285542	MICROSOURCE	1500497	NO_SALT	0	NO_SOLVATE	0	402.4807	=O)[C@@]1(O)CCC2C3CCC4=CC(=O)C=CC4(C)C3[C@@H]	PREDNISOLONE ACETATE
SJ000285543-1	SJ000285543	MICROSOURCE	1500499	NO_SALT	0	NO_SOLVATE	0	358.4281	2CC(=O)C3C(CCC4=CC(=O)C=C[C@]34C)C1CC[C@]2(O)C	PREDNISONE
SJ000285544-3	SJ000285544	PRESTWICK	476	PHOSPHATE	2	NO_SOLVATE	0	449.3467	COc1cc(NC(C)CCCN)c2ncccc2c1	PRIMAQUINE
SJ000285547-5	SJ000285547	SIGMA	P 9391	CHLORIDE	1	NO_SOLVATE	0	270.8253	CCN(CC)CCNC(=O)c1ccc(N)cc1	PROCAINAMIDE
SJ000285549-5	SJ000285549	SIGMA	P 9178	FUMARATE	2	NO_SOLVATE	0	602.1426	CN1CCN(CCCN2c3ccccc3Sc4ccc(Cl)cc24)CC1	PROCHLORPERAZINE
SJ000285551-2	SJ000285551	MICROSOURCE	1500508	NO_SALT	0	NO_SOLVATE	0	314.4617	(=O)[C@H]1CCC2C3CCC4=CC(=O)CC[C@]4(C)C3CC[C@]1	PROGESTERONE
SJ000285554-2	SJ000285554	MICROSOURCE	201580	NO_SALT	0	NO_SOLVATE	0	420.4544	CCc1c(O)c2C(=O)C(=COc2c3C=CC(C)(C)Oc13)c4ccc(O)c(O	POMIFERIN
SJ000285564-2	SJ000285564	MICROSOURCE	1500476	SULFATE	1	NO_SOLVATE	0	232.2942	NNCCc1ccccc1	PHENELZINE
SJ000285569-2	SJ000285569	MICROSOURCE	1500490	NO_SALT	0	NO_SOLVATE	0	86.1356	C1CNCCN1	PIPERAZINE
SJ000285572-3	SJ000285572	MICROSOURCE	1500523	GLUCONATE	1	NO_SOLVATE	0	519.6167	ccc2nccc([C@H](O)[C@H]3C[C@@H]4CCN3C[C@@H]4C=C	QUININE SULFATE
SJ000285572-4	SJ000285572	PRESTWICK	280	CHLORIDE	1	H2O	1	377	ccc2nccc([C@H](O)[C@H]3C[C@@H]4CCN3C[C@@H]4C=C	QUININE SULFATE
SJ000285574-1	SJ000285574	MICROSOURCE	1500531	NO_SALT	0	NO_SOLVATE	0	124.1372	OCc1ccccc1O	SALICYL ALCOHOL
SJ000285577-2	SJ000285577	MICROSOURCE	1500539	NO_SALT	0	NO_SOLVATE	0	416.5734	=CC(=O)CC[C@]2(C)[C@H]3CC[C@@]4(C)[C@@H](CC[C	SPIRONOLACTONE
SJ000285584-1	SJ000285584	MICROSOURCE	1500759	NO_SALT	0	NO_SOLVATE	0	272.2097	Oc1ccc2C(=O)c3c(O)ccc(O)c3C(=O)c2c1O	QUINALIZARIN
SJ000285586-2	SJ000285586	MICROSOURCE	107108	NO_SALT	0	NO_SOLVATE	0	288.4244	C@]12CCC(=O)C[C@@H]1CCC3C2CC[C@@]4(C)C3CCC4	5-ALPHA-ANDROSTAN-3,17-DIONE
SJ000285587-1	SJ000285587	MICROSOURCE	200007	NO_SALT	0	NO_SOLVATE	0	628.7511	(C)C)c3OC45C6CC(C=C4C(=O)c3c(O)c2C=C1)C(=O)C5(C\C	GAMBOGIC ACID
SJ000285588-1	SJ000285588	MICROSOURCE	200789	NO_SALT	0	NO_SOLVATE	0	254.2375	Oc1ccc(cc1)C2=COc3cc(O)ccc3C2=O	DAIDZEIN
SJ000285591-1	SJ000285591	MICROSOURCE	1500455	NO_SALT	0	NO_SOLVATE	0	324.3737	CCCCC1C(=O)N(N(C1=O)c2ccc(O)cc2)c3ccccc3	OXYPHENBUTAZONE
SJ000285592-5	SJ000285592	SIGMA	T 9262	CITRATE	1	NO_SOLVATE	0	560.6145	CC\C(=C(/c1ccccc1)\c2ccc(OCCN(C)C)cc2)\c3ccccc3	TAMOXIFEN
SJ000285606-5	SJ000285606	SIGMA	T 7508	CHLORIDE	1	NO_SOLVATE	0	299.8632	CCCCNc1ccc(cc1)C(=O)OCCN(C)C	TETRACAINE HYDROCHLORIDE
SJ000285608-2	SJ000285608	MICROSOURCE	1500576	NO_SALT	0	NO_SOLVATE	0	443.6252	N(C)S(=O)(=O)c1ccc2Sc3ccccc3\C(=C/CCN4CCN(C)CC4)\c2	THIOTHIXENE
SJ000285608-4	SJ000285608	SIGMA	T 0780	CHLORIDE	1	NO_SOLVATE	0	479.1252	N(C)S(=O)(=O)c1ccc2Sc3ccccc3\C(=C\CCN4CCN(C)CC4)\c2	THIOTHIXENE
SJ000285610-5	SJ000285610	SIGMA	T 9025	CHLORIDE	1	NO_SOLVATE	0	406.0745	CSc1ccc2Sc3ccccc3N(CCC4CCCCN4C)c2c1	THIORIDAZINE
SJ000285614-1	SJ000285614	MICROSOURCE	1500582	SODIUM(I)	1	NO_SOLVATE	0	280.2845	Cc1ccc(cc1)C(=O)c2ccc(CC(=O)O)n2C	TOLMETIN
SJ000285618-1	SJ000285618	MICROSOURCE	1500615	NO_SALT	0	NO_SOLVATE	0	291.7295	Cc1cc(CC(=O)O)n(C)c1C(=O)c2ccc(Cl)cc2	ZOMEPIRAC SODIUM
SJ000285619-2	SJ000285619	MICROSOURCE	1500621	NO_SALT	0	NO_SOLVATE	0	203.2404	CN1N(C(=O)C(=C1C)N)c2ccccc2	AMINOPHENAZONE
SJ000285625-5	SJ000285625	PRESTWICK	577	CHLORIDE	1	NO_SOLVATE	0	389.9427	H]1[C@@H](O)CC[C@@H]2CN3CCc4c([nH]c5ccccc45)[C@	YOHIMBINE HYDROCHLORIDE
SJ000285630-6	SJ000285630	SIGMA	I-106	NO_SALT	0	NO_SOLVATE	0	206.2808	CC(C)Cc1ccc(cc1)[C@H](C)C(=O)O	IBUPROFEN
SJ000285635-2	SJ000285635	MICROSOURCE	1500354	BROMIDE	1	NO_SOLVATE	0	412.3565	C)[N+]1(C)[C@@H]2CCC1C[C@@H](C2)OC(=O)C(CO)c3cc	IPRATROPIUM
SJ000285638-1	SJ000285638	MICROSOURCE	1500359	CHLORIDE	1	NO_SOLVATE	0	336.8801	C[C@H](COc1ccccc1)N[C@H](C)[C@H](O)c2ccc(O)cc2	ISOXSUPRINE HYDROCHLORIDE
SJ000285643-1	SJ000285643	MICROSOURCE	1500376	CHLORIDE	2	NO_SOLVATE	0	461.9482	Cc1cccc(CN2CCN(CC2)C(c3ccccc3)c4ccc(Cl)cc4)c1	MECLOZINE
SJ000285646-1	SJ000285646	MICROSOURCE	1500380	NO_SALT	0	NO_SOLVATE	0	344.4876	3CC[C@H](C(=O)C)[C@@]3(C)C[C@H](O)C2[C@@]4(C)C	MEDRYSONE
SJ000285651-2	SJ000285651	MICROSOURCE	1500396	NO_SALT	0	NO_SOLVATE	0	114.1688	Cn1ccnc1S	THIAMAZOLE
SJ000285652-2	SJ000285652	MICROSOURCE	1500397	NO_SALT	0	NO_SOLVATE	0	241.2405	COc1ccccc1OCC(O)COC(=O)N	METHOCARBAMOL
SJ000285655-1	SJ000285655	MICROSOURCE	1500403	NO_SALT	0	NO_SOLVATE	0	211.2145	C[C@](N)(Cc1ccc(O)c(O)c1)C(=O)O	METHYLDOPA
SJ000285657-1	SJ000285657	MICROSOURCE	1500406	NO_SALT	0	NO_SOLVATE	0	374.4706	CC[C@](O)(C(=O)CO)[C@@]3(C)C[C@H](O)C2[C@@]4(C)(	METHYLPREDNISOLONE
SJ000285659-2	SJ000285659	MICROSOURCE	1500414	CHLORIDE	1	NO_SOLVATE	0	492.9	]2C[C@@H]3Cc4c(ccc(O)c4C(=C3C(=O)[C@]2(O)C(=C(C(=	MINOCYCLINE
SJ000285664-3	SJ000285664	PRESTWICK	46	CHLORIDE	1	NO_SOLVATE	0	245.7743	C(C1=NCCN1)c2cccc3ccccc23	NAPHAZOLINE
SJ000285666-5	SJ000285666	SIGMA	N 7634	NO_SALT	0	NO_SOLVATE	0	346.3346	OC(=C1C(C(=C(C)N=C1C)C(=O)OC)c2ccccc2[N+](=O)[O-])(	NIFEDIPINE
SJ000285667-2	SJ000285667	MICROSOURCE	1500433	NO_SALT	0	NO_SOLVATE	0	238.157	[O-][N+](=O)c1oc(\C=N\N2CC(=O)NC2=O)cc1	NITROFURANTOIN
SJ000285668-3	SJ000285668	PRESTWICK	563	NO_SALT	0	NO_SOLVATE	0	413.4205	cc2[C@H](OC(=O)c2c1OC)[C@@H]3N(C)CCc4cc5OCOc5c(	NOSCAPINE HYDROCHLORIDE
SJ000285671-2	SJ000285671	MICROSOURCE	1500438	NO_SALT	0	NO_SOLVATE	0	340.4559	)O[C@]1(CCC2C3CCC4=CC(=O)CC[C@@H]4C3CC[C@]12	NORETHISTERONE ACETATE
SJ000285674-3	SJ000285674	PRESTWICK	773	NO_SALT	0	NO_SOLVATE	0	312.4458	[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C	NORGESTREL
SJ000285678-2	SJ000285678	MICROSOURCE	1500460	NO_SALT	0	NO_SOLVATE	0	128.5563	Oc1ccc(Cl)cc1	PARACHLOROPHENOL
SJ000285683-5	SJ000285683	SIGMA	P 3510	CHLORIDE	1	NO_SOLVATE	0	374.885	COc1ccc(Cc2nccc3cc(OC)c(OC)cc23)cc1OC	PAPAVERINE HYDROCHLORIDE
SJ000285684-2	SJ000285684	MICROSOURCE	1500451	NO_SALT	0	NO_SOLVATE	0	228.2432	COc1ccc(C(=O)c2ccccc2)c(O)c1	OXYBENZONE
SJ000285686-5	SJ000285686	SIGMA	B 5399	NO_SALT	0	NO_SOLVATE	0	213.6607	NCC(CC(=O)O)c1ccc(Cl)cc1	BACLOFEN
SJ000285687-2	SJ000285687	MICROSOURCE	1500146	CHLORIDE	1	NO_SOLVATE	0	196.7215	CC(C[N+](C)(C)C)OC(=O)N	BETHANECHOL
SJ000285688-2	SJ000285688	MICROSOURCE	1500137	CHLORIDE	1	NO_SOLVATE	0	292.7432	NC(CO)C(=O)NNCc1ccc(O)c(O)c1O	BENSERAZIDE HYDROCHLORIDE
SJ000285689-1	SJ000285689	MICROSOURCE	1500139	NO_SALT	0	NO_SOLVATE	0	165.1891	CCOC(=O)c1ccc(N)cc1	BENZOCAINE
SJ000285692-2	SJ000285692	MICROSOURCE	1500144	NO_SALT	0	NO_SOLVATE	0	392.461	C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[	BETAMETHASONE
SJ000285695-1	SJ000285695	MICROSOURCE	1500158	CHLORIDE	1	NO_SOLVATE	0	182.6949	C[N+](C)(C)CCOC(=O)N	CARBACHOL
SJ000285696-1	SJ000285696	MICROSOURCE	1500159	NO_SALT	0	NO_SOLVATE	0	236.2685	NC(=O)N1c2ccccc2C=Cc3ccccc13	CARBAMAZEPINE
SJ000285704-1	SJ000285704	MICROSOURCE	1500168	NO_SALT	0	NO_SOLVATE	0	349.4047	C(N2C(SC1)[C@H](NC(=O)[C@H](N)C3=CCC=CC3)C2=O)C	CEFRADINE
SJ000285710-2	SJ000285710	MICROSOURCE	1500189	HYDROXYETHANAMINIU	1	NO_SOLVATE	0	269.3688	CC1=CC(=O)N(O)C(=C1)C2CCCCC2	CICLOPIROX
SJ000285712-2	SJ000285712	MICROSOURCE	1500196	CITRATE	1	NO_SOLVATE	0	595.0596	CCN(CC)CCOc1ccc(cc1)\C(=C(/Cl)\c2ccccc2)\c3ccccc3	CLOMIPHENE
SJ000285713-5	SJ000285713	SIGMA	C 6019	NO_SALT	0	NO_SOLVATE	0	344.8367	Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4	CLOTRIMAZOLE
SJ000285715-2	SJ000285715	MICROSOURCE	1500202	NO_SALT	0	NO_SOLVATE	0	179.603	Oc1ccc(Cl)c2cccnc12	CLOXYQUIN
SJ000285718-2	SJ000285718	MICROSOURCE	1500218	NO_SALT	0	NO_SOLVATE	0	182.1832	CN(C)N=Nc1[nH]cnc1C(=O)N	DACARBAZINE
SJ000285725-3	SJ000285725	PRESTWICK	725	METHANESULFONATE	1	NO_SOLVATE	0	655.784	))CCCCCNC(=O)CCC(=O)N(O)CCCCCNC(=O)CCC(=O)N(C	DEFEROXAMINE
SJ000285727-5	SJ000285727	SIGMA	D 6140	CHLORIDE	1	NO_SOLVATE	0	500.353	C[C@@H]3[C@H](O)c4c(Cl)ccc(O)c4C(=C3C(=O)[C@]2(O)C	DEMECLOCYCLINE HYDROCHLORIDE
SJ000285728-2	SJ000285728	MICROSOURCE	1500231	NO_SALT	0	NO_SOLVATE	0	434.4977	=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@	DEXAMETHASONE ACETATE

Name of clinical anti-leukemic agent	sample	WT_EC_{50}	WT_EC_{50}CI	WT_curveScore	WT_actclass	T315I_EC_{50}	T315I_EC_{50}CI	T315I_curveScore	T315I_actclass
CYTARABINE	SJ000285188-6	0.0639	0.0425 - 0.0961	A113	HIGH	0.0603	0.0355 - 0.1023	A113	HIGH
MELPHALAN*	SJ000285194-4	>5	NA	C555	WEAK	3.9408	NA	C555	WEAK
MERCAPTOPURINE	SJ000285195-2	0.0211	0.0013 - 0.3518	A111	HIGH	0.0444	0.0342 - 0.0575	B110	HIGH
METHOTREXATE	SJ000285196-2	0.0225	0.0014 - 0.3699	A111	HIGH	0.0438	0.0316 - 0.0606	A112	HIGH
THIOGUANINE	SJ000285208-3	0.0441	0.0248 - 0.0786	B110	HIGH	0.0202	0.0010 - 0.4084	B110	HIGH
AMINOPTRINE	SJ000285221-4	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH
AZACITIDINE	SJ000285227-1	1.2936	0.9338 - 1.7920	B311	WEAK	1.2871	0.8082 - 2.0498	B311	WEAK
ETOPOSIDE	SJ000285235-3	0.1369	0.1148 - 0.1632	A212	MED	0.1368	0.1164 - 0.1608	A212	MED
MITOXANTRONE	SJ000285321-4	0.0433	0.0348 - 0.0539	A112	HIGH	0.044	0.0361 - 0.0536	A112	HIGH
HYDROCORTISONE	SJ000285358-5	0.1905	0.1782 - 0.2036	A212	MED	0.19	0.1788 - 0.2020	A212	MED
PREDNISOLONE	SJ000285541-3	0.1573	0.1495 - 0.1654	A212	MED	0.1541	0.1406 - 0.1689	A212	MED
DEXAMETHASONE	SJ000285729-2	<0.1	0.0039 - 4.1318	B110	HIGH	0.0374	0.0102 - 0.1371	B110	HIGH
AMSACRINE	SJ000285974-2	0.0861	0.0767 - 0.0967	A112	HIGH	0.0747	0.0627 - 0.0889	A112	HIGH
IDARUBICIN	SJ000287925-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH
VINCRISTINE	SJ000288244-2	0.1045	0.0914 - 0.1194	A213	MED	0.1311	0.0021 - 8.2851	A214	MED

*often performs poorly in HTS

sample	WT_EC50	WT_EC50CI	WT_curveScore	WT_actclass	T315I_EC50	T315I_EC50CI	T315I_curveScore	T315I_actclass	comment
SJ000000250-8	>5	NA	B241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000000854-6	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000113084-4	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000126662-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285182-2	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285183-2	0.2213	0.1535 - 0.3190	A211	MED	0.21	0.1479 - 0.2981	A212	MED	
SJ000285185-4	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285188-6	0.0639	0.0425 - 0.0961	A113	HIGH	0.0603	0.0355 - 0.1023	A113	HIGH	
SJ000285190-2	0.7932	0.7229 - 0.8703	A212	MED	0.7231	0.6469 - 0.8083	A212	MED	
SJ000285193-1	2.1027	2.0841 - 2.1214	B313	WEAK	2.285	2.2763 - 2.2937	B313	WEAK	
SJ000285194-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285194-4	>5	NA	C555	WEAK	3.9408	NA	C555	WEAK	
SJ000285195-2	0.0211	0.0013 - 0.3518	A111	HIGH	0.0444	0.0342 - 0.0575	B110	HIGH	
SJ000285196-2	0.0225	0.0014 - 0.3699	A111	HIGH	0.0438	0.0316 - 0.0606	A112	HIGH	
SJ000285197-1	0.1499	0.1248 - 0.1800	A212	MED	0.1542	0.1235 - 0.1926	A212	MED	
SJ000285200-6	1.2025	0.8162 - 1.7718	B311	WEAK	1.1389	0.8043 - 1.6128	B311	WEAK	
SJ000285202-2	1.8339	1.7982 - 1.8703	B313	WEAK	1.7597	1.6984 - 1.8232	A313	WEAK	
SJ000285203-5	<0.1	NA	B110	HIGH	0.0824	0.0695 - 0.0978	A111	HIGH	
SJ000285206-2	>5	NA	NC555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285207-1	0.4043	0.3822 - 0.4278	A213	MED	0.4118	0.3793 - 0.4471	A213	MED	
SJ000285208-3	0.0441	0.0248 - 0.0786	B110	HIGH	0.0202	0.0010 - 0.4084	B110	HIGH	
SJ000285210-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285212-1	1.6282	1.5516 - 1.7085	A313	WEAK	1.7678	1.7312 - 1.8052	B313	WEAK	
SJ000285215-1	1.0484	0.8816 - 1.2467	A313	WEAK	1.0426	0.8815 - 1.2333	A313	WEAK	
SJ000285215-6	0.0552	0.0513 - 0.0594	A113	HIGH	0.0527	0.0477 - 0.0583	A113	HIGH	
SJ000285218-5	>5	NA	B332	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285219-2	2.0837	2.0004 - 2.1703	B312	WEAK	1.7397	1.5755 - 1.9210	B312	WEAK	
SJ000285219-5	2.9391	2.8596 - 3.0208	B312	WEAK	2.8605	2.7902 - 2.9326	B312	WEAK	
SJ000285220-5	>5	NA	C555	WEAK	2.8062	0.5197 - 15.1529	B314	WEAK	
SJ000285221-4	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000285225-2	0.1607	0.1521 - 0.1698	A212	MED	0.1603	0.1544 - 0.1665	A213	MED	
SJ000285226-6	>5	NA	B130	INACTIVE	>5	NA	A231	INACTIVE	
SJ000285227-1	1.2936	0.9338 - 1.7920	B311	WEAK	1.2871	0.8082 - 2.0498	B311	WEAK	
SJ000285228-4	0.3344	0.3149 - 0.3551	A211	MED	0.4033	0.3922 - 0.4148	A211	MED	
SJ000285229-2	1.9757	1.9316 - 2.0207	B322	WEAK	1.9622	1.8651 - 2.0644	B322	WEAK	
SJ000285231-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285232-1	0.117	0.1002 - 0.1366	A213	MED	0.1133	0.0999 - 0.1285	A213	MED	
SJ000285232-8	0.0619	0.0351 - 0.1092	A114	HIGH	0.0566	0.0444 - 0.0721	A114	HIGH	
SJ000285234-2	0.3225	0.2286 - 0.4550	A211	MED	0.3737	0.3442 - 0.4058	A211	MED	
SJ000285235-3	0.1369	0.1148 - 0.1632	A212	MED	0.1368	0.1164 - 0.1608	A212	MED	
SJ000285238-3	0.1022	0.0880 - 0.1188	A213	MED	0.1214	0.0955 - 0.1542	A214	MED	
SJ000285241-3	0.1569	0.1188 - 0.2071	B110	MED	0.1024	0.0737 - 0.1421	A211	MED	
SJ000285242-3	4.4693	NA	C555	WEAK	>5	NA	C555	INACTIVE	Differential activity within experimental error
SJ000285243-2	0.48	0.4327 - 0.5325	A213	MED	0.4074	0.3682 - 0.4508	A213	MED	
SJ000285244-3	1.5123	1.4902 - 1.5347	A313	WEAK	1.7214	1.6838 - 1.7597	A313	WEAK	
SJ000285246-2	0.8225	0.6899 - 0.9806	A212	MED	0.9896	0.8088 - 1.2108	A212	MED	
SJ000285249-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000285256-3	0.3341	0.2737 - 0.4077	A212	MED	0.3286	0.2649 - 0.4076	A212	MED	
SJ000285261-3	0.2342	0.1932 - 0.2840	A213	MED	0.2457	0.1708 - 0.3535	A214	MED	
SJ000285262-1	>5	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000285263-2	>5	NA	D555	INACTIVE	>5	NA	A241	INACTIVE	
SJ000285267-3	0.0853	0.0560 - 0.1301	A112	HIGH	0.1561	0.1245 - 0.1956	A212	MED	Differential activity within experimental error
SJ000285270-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285272-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000285273-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285276-2	4.0523	NA	C555	WEAK	3.1302	2.9524 - 3.3187	B312	WEAK	
SJ000285278-1	<1.0	NA	C555	MED	<1.0	NA	C555	MED	
SJ000285279-2	>5	NA	NC555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285285-3	>5	NA	B141	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285292-10	>5	NA	D555	INACTIVE	>5	NA	NC555	INACTIVE	
SJ000285294-1	0.074	0.0659 - 0.0830	A113	HIGH	0.0742	0.0666 - 0.0828	A113	HIGH	
SJ000285299-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285307-3	>5	NA	B344	INACTIVE	>5	NA	B334	INACTIVE	
SJ000285308-1	0.5458	0.5060 - 0.5886	A213	MED	0.5062	0.4281 - 0.5985	A213	MED	
SJ000285313-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285315-2	1.0561	1.0324 - 1.0803	B312	WEAK	0.7384	0.6862 - 0.7946	A212	MED	Differential activity within experimental error
SJ000285316-4	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285317-2	>5	NA	NC555	INACTIVE	3.8254	NA	C555	WEAK	Differential activity within experimental error
SJ000285318-7	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285319-1	1.7406	1.6595 - 1.8256	A314	WEAK	2.0096	1.9300 - 2.0925	B314	WEAK	
SJ000285321-4	0.0433	0.0348 - 0.0539	A112	HIGH	0.044	0.0361 - 0.0536	A112	HIGH	
SJ000285323-3	>5	NA	B332	INACTIVE	>5	NA	B321	INACTIVE	
SJ000285327-1	1.6528	1.6211 - 1.6851	A313	WEAK	1.8204	1.7962 - 1.8449	B313	WEAK	
SJ000285332-1	0.1515	0.1256 - 0.1826	A212	MED	0.2075	0.1841 - 0.2338	A212	MED	
SJ000285334-4	>5	NA	C555	INACTIVE	0	NA	C555	INACTIVE	
SJ000285335-1	0.0666	0.0196 - 0.2261	A114	HIGH	0.0687	0.0028 - 1.6949	A114	HIGH	
SJ000285335-4	0.1386	0.0008 - 22.9222	A214	MED	0.1244	0.0676 - 0.2290	A214	MED	
SJ000285337-5	>5	NA	B342	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285337-8	>5	NA	B140	INACTIVE	>5	NA	A241	INACTIVE	
SJ000285338-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285343-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285358-5	0.1905	0.1782 - 0.2036	A212	MED	0.19	0.1788 - 0.2020	A212	MED	
SJ000285363-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285364-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285365-1	2.2925	1.1080 - 4.7433	B321	WEAK	>5	NA	B334	INACTIVE	
SJ000285368-3	>5	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000285369-1	>5	NA	C555	WEAK	3.9664	NA	B313	WEAK	
SJ000285373-9	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285375-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285382-3	>5	NA	C555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285383-1	>5	NA	D555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285387-8	>5	NA	NC555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285396-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285400-2	>5	NA	B342	INACTIVE	>5	NA	B344	INACTIVE	
SJ000285410-5	0.0303	0.0268 - 0.0342	A113	HIGH	0.0276	0.0238 - 0.0319	B110	HIGH	
SJ000285413-1	0.9636	0.8101 - 1.1461	A214	MED	2.5855	NA	C555	WEAK	Differential activity within experimental error
SJ000285423-2	0.9398	0.8608 - 1.0260	A212	MED	0.9064	0.7444 - 1.1035	A212	MED	
SJ000285426-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285431-2	>5	NA	D555	INACTIVE	>5	NA	NB142	INACTIVE	
SJ000285433-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285436-3	1.1776	1.1246-1.2303	A322	WEAK	1.183	1.1246-1.2445	A322	WEAK	ARTEMISININ
SJ000285439-2	>5	NA	C555	INACTIVE	>5	NA	B313	INACTIVE	
SJ000285440-2	2.6129	2.3056 - 2.9611	B312	WEAK	1.7108	1.0736 - 2.7263	B311	WEAK	
SJ000285442-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285443-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285445-2	>5	NA	C555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285450-2	>5	NA	C555	WEAK	>5	NA	C555	WEAK	Differential activity within experimental error
SJ000285451-3	1.5777	1.1606 - 2.1448	B321	WEAK	4.852	NA	C555	WEAK	
SJ000285452-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000285452-5	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000285453-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285454-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285460-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285461-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285462-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285465-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285466-4	0.1742	0.1186 - 0.2559	A211	MED	0.1286	0.0965 - 0.1716	B110	MED	
SJ000285484-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285487-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285490-1	1.5512	1.5019 - 1.6022	A313	WEAK	>5	NA	B333	INACTIVE	Significant shift in efficacy, not potency
SJ000285502-5	>5	NA	B342	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285504-2	>5	NA	C555	INACTIVE	>5	NA	A241	INACTIVE	
SJ000285506-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285508-1	0.2163	0.1969 - 0.2377	A213	MED	0.2332	0.2081 - 0.2613	A213	MED	
SJ000285512-1	3.5581	3.5015 - 3.6156	B313	WEAK	4.287	NA	C555	WEAK	
SJ000285522-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285526-3	>5	NA	A241	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285536-1	>5	NA	C555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285540-4	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285541-3	0.1573	0.1495 - 0.1654	A212	MED	0.1541	0.1406 - 0.1689	A212	MED	
SJ000285542-2	0.1346	0.1233 - 0.1468	A212	MED	0.1274	0.1191 - 0.1363	A212	MED	
SJ000285543-1	>5	NA	A242	INACTIVE	>5	NA	B331	INACTIVE	
SJ000285544-3	>5	NA	B241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285547-5	>5	NA	D555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285549-5	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285551-2	>5	NA	C555	INACTIVE	>5	NA	A242	INACTIVE	
SJ000285554-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	

SJ000285564-2	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285569-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285572-3	>5	NA	NC555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285572-4	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285574-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285577-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285584-1	>5	NA	C555	INACTIVE	>5	NA	B141	INACTIVE	
SJ000285586-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285587-1	0.2018	0.0239 - 1.7053	A211	MED	0.2793	0.0259 - 3.0073	A211	MED	
SJ000285588-1	>5	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000285591-1	>5	NA	C555	WEAK	3.2243	2.9841 - 3.4838	B312	WEAK	
SJ000285592-5	>5	NA	C555	INACTIVE	>5	NA	B344	INACTIVE	
SJ000285606-5	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285608-2	>5	NA	A241	INACTIVE	>5	NA	B341	INACTIVE	
SJ000285608-4	>5	NA	C555	INACTIVE	>5	NA	B341	INACTIVE	
SJ000285610-5	>5	NA	C555	INACTIVE	>5	NA	B344	INACTIVE	
SJ000285614-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285618-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285619-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285625-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285630-6	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285635-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285638-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285643-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285646-1	0.2119	0.1898 - 0.2367	A212	MED	0.1965	0.1746 - 0.2213	A212	MED	
SJ000285651-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285652-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285655-1	>5	NA	B243	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285657-1	0.1253	0.1140 - 0.1376	A212	MED	0.125	0.1179 - 0.1324	A212	MED	
SJ000285659-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285664-3	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285666-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285667-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285668-3	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285671-2	>5	NA	D555	INACTIVE	>5	NA	NC555	INACTIVE	
SJ000285674-3	>5	NA	A241	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285678-2	>5	NA	B141	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285683-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285684-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285686-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285687-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285688-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285689-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285692-2	0.0399	0.0322 - 0.0495	A112	HIGH	0.0358	0.0302 - 0.0424	A113	HIGH	
SJ000285695-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285696-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285704-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285710-2	1.4543	1.3330 - 1.5866	A312	WEAK	1.2069	1.1588 - 1.2569	A313	WEAK	
SJ000285712-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285713-5	>5	NA	C555	INACTIVE	>5	NA	B314	INACTIVE	
SJ000285715-2	>5	NA	D555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285718-2	2.9705	2.5382 - 3.4763	B322	WEAK	>5	NA	B322	INACTIVE	Differential activity within experimental error
SJ000285725-3	>5	NA	C555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285727-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285728-2	0.0349	0.0313 - 0.0390	B110	HIGH	0.0363	0.0314 - 0.0420	A112	HIGH	
SJ000285729-2	<0.1	0.0039 - 4.1318	B110	HIGH	0.0374	0.0102 - 0.1371	B110	HIGH	
SJ000285740-1	>5	NA	NC555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285742-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285745-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285747-3	0.1383	0.1316 - 0.1452	A213	MED	0.1465	0.1407 - 0.1526	A213	MED	
SJ000285748-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285750-1	>5	NA	B344	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285752-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285761-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285764-3	4.1895	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000285766-1	0.0442	0.0401 - 0.0487	B110	HIGH	0.046	0.0427 - 0.0495	A113	HIGH	
SJ000285767-2	0.0214	0.0184 - 0.0249	B110	HIGH	0.0255	0.0228 - 0.0285	A113	HIGH	
SJ000285768-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000285769-1	0.0406	0.0358 - 0.0459	A112	HIGH	0.0434	0.0403 - 0.0468	A113	HIGH	
SJ000285770-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285778-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285781-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285783-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285786-2	0.1307	0.0938 - 0.1821	A212	MED	0.1136	0.0838 - 0.1538	A213	MED	
SJ000285787-2	0.8184	0.7921 - 0.8455	A213	MED	0.8671	0.8509 - 0.8837	A213	MED	
SJ000285787-4	0.5572	0.5418 - 0.5729	A213	MED	0.5282	0.5051 - 0.5523	A213	MED	
SJ000285790-1	2.5093	2.4752 - 2.5439	B313	WEAK	2.9331	2.8664 - 3.0014	B313	WEAK	
SJ000285797-2	>5	NA	A243	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285801-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285812-1	>5	NA	B344	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285814-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285814-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285818-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285820-1	0.0416	0.0213 - 0.0814	A111	HIGH	0.0512	0.0395 - 0.0664	A112	HIGH	
SJ000285827-2	1.5678	1.1031 - 2.2285	B311	WEAK	>5	NA	C555	WEAK	
SJ000285831-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285834-1	>5	NA	B341	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285835-2	>5	NA	C555	INACTIVE	>5	NA	B244	INACTIVE	
SJ000285836-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285837-1	>5	NA	B313	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285838-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285840-2	0.9191	0.8184 - 1.0322	A214	MED	0.8819	0.8216 - 0.9466	A214	MED	
SJ000285842-2	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285845-5	>5	NA	B241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285849-3	0.4435	0.3978 - 0.4944	A212	MED	0.4338	0.3884 - 0.4846	A212	MED	
SJ000285858-5	>5	NA	NC555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285860-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285864-3	1.2127	1.1502 - 1.2785	A313	WEAK	1.3427	1.2789 - 1.4096	A313	WEAK	
SJ000285866-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285878-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285879-3	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285880-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000285881-1	3.1053	2.9783 - 3.2377	B312	WEAK	2.3759	2.3476 - 2.4045	B313	WEAK	
SJ000285882-2	>5	NA	A242	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285885-5	>5	NA	NA241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285887-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285888-1	>5	NA	C555	WEAK	>5	NA	B313	WEAK	
SJ000285890-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285892-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285903-2	>5	NA	D555	INACTIVE	>5	NA	NC555	INACTIVE	
SJ000285909-2	>5	NA	A242	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285920-5	>5	NA	C555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000285922-4	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285925-2	>5	NA	B241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285935-1	>5	NA	C555	INACTIVE	>5	NA	B344	INACTIVE	
SJ000285936-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285940-2	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285949-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285950-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285951-3	>5	NA	D555	INACTIVE	>5	NA	NC555	INACTIVE	
SJ000285958-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285959-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000285960-1	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285965-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285966-2	1.2967	0.7065 - 2.3798	A314	WEAK	2.0144	1.9973 - 2.0317	B312	WEAK	
SJ000285967-1	>5	NA	B241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285971-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285972-1	4.2077	NA	C555	WEAK	2.4586	2.4189 - 2.4989	B312	WEAK	
SJ000285973-2	0.1698	0.1572 - 0.1833	A212	MED	0.1623	0.1542 - 0.1709	A212	MED	
SJ000285974-2	0.0861	0.0767 - 0.0967	A112	HIGH	0.0747	0.0627 - 0.0889	A112	HIGH	
SJ000285978-2	0.2212	0.1336 - 0.3662	A211	MED	0.1961	0.1048 - 0.3669	A211	MED	
SJ000285980-3	4.2933	NA	C555	WEAK	3.3236	3.1759 - 3.4782	B312	WEAK	
SJ000285983-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285987-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285991-2	1.1053	0.7753 - 1.5756	B311	WEAK	0.7808	0.7463 - 0.8169	A212	MED	Differential activity within experimental error
SJ000285996-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000285998-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000285999-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	

SJ000286003-2	0.7272	0.2263 - 2.3376	A211	MED	0.3626	0.3272 - 0.4017	A211	MED	
SJ000286004-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286006-3	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000286007-1	1.0062	0.8964 - 1.1294	A313	WEAK	0.9628	0.8199 - 1.1308	A212	MED	Differential activity within experimental error
SJ000286008-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286018-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286024-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286025-1	>5	NA	C555	INACTIVE	>5	NA	B332	INACTIVE	
SJ000286030-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000286034-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000286035-1	>5	NA	D555	INACTIVE	>5	NA	B341	INACTIVE	
SJ000286036-1	>5	NA	B143	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286037-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286038-1	0.0931	0.0858 - 0.1010	A113	HIGH	0.0782	0.0723 - 0.0846	A113	HIGH	
SJ000286038-4	0.0508	0.0445 - 0.0581	A113	HIGH	0.0578	0.0515 - 0.0649	A113	HIGH	
SJ000286039-3	0.0238	0.0179 - 0.0317	B110	HIGH	0.021	0.0145 - 0.0303	B110	HIGH	
SJ000286041-1	>5	NA	B141	INACTIVE	>5	NA	B341	INACTIVE	
SJ000286044-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286046-7	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286046-9	>5	NA	C555	INACTIVE	>5	NA	A241	INACTIVE	
SJ000286052-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286053-3	>5	NA	B332	INACTIVE	>5	NA	B321	INACTIVE	
SJ000286056-4	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286057-2	>5	NA	C555	WEAK	2.4313	2.4033 - 2.4597	B312	WEAK	
SJ000286063-1	>5	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000286065-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286075-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286086-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286093-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286097-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286098-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286101-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286109-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286112-2	>5	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000286113-2	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286118-3	>5	NA	D555	INACTIVE	>5	NA	A344	INACTIVE	
SJ000286121-3	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286124-1	>5	NA	C555	INACTIVE	>5	NA	B341	INACTIVE	
SJ000286127-5	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286128-2	0.4695	0.3938 - 0.5597	A213	MED	0.4789	0.3911 - 0.5864	A213	MED	
SJ000286133-5	>5	NA	C555	INACTIVE	>5	NA	B343	INACTIVE	
SJ000286134-5	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286142-2	0.4718	0.4465 - 0.4984	A213	MED	0.4944	0.4672 - 0.5231	A212	MED	
SJ000286143-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286144-3	1.2315	1.1244 - 1.3489	B312	WEAK	1.1138	0.9772 - 1.2695	B312	WEAK	
SJ000286146-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286151-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286152-2	>5	NA	D555	INACTIVE	>5	NA	NC555	INACTIVE	
SJ000286154-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000286155-5	>5	NA	B344	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286156-2	1.0381	0.8985 - 1.1994	A313	WEAK	1.0097	0.8164 - 1.2487	A313	WEAK	
SJ000286159-2	0.2887	0.2448 - 0.3404	A212	MED	0.3018	0.2554 - 0.3567	A212	MED	
SJ000286160-1	0.4594	0.3777 - 0.5586	A211	MED	0.3036	0.2841 - 0.3245	A213	MED	
SJ000286162-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286166-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286172-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286174-2	>5	NA	NC555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286175-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286178-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286181-2	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286185-2	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286186-3	2.4152	2.3733 - 2.4579	B313	WEAK	2.4276	1.7583 - 3.3517	B314	WEAK	
SJ000286187-2	0.9432	0.8364 - 1.0635	A213	MED	0.9116	0.8686 - 0.9568	A213	MED	
SJ000286188-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286191-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286195-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286199-2	>5	NA	D555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000286204-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286205-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000286213-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286217-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286225-4	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286229-4	>5	NA	A242	INACTIVE	>5	NA	A241	INACTIVE	
SJ000286231-4	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286236-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286243-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286248-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286251-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286267-1	>5	NA	C555	WEAK	4.6918	NA	C555	WEAK	
SJ000286300-1	>5	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000286312-1	>5	NA	C555	INACTIVE	>5	NA	B344	INACTIVE	
SJ000286359-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286366-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286380-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286381-1	0.1792	0.1603 - 0.2003	A222	MED	0.329	0.0988 - 1.0953	A234	MED	
SJ000286382-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286387-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286389-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286393-1	4.6178	NA	C555	WEAK	>5	NA	C555	INACTIVE	Differential activity within experimental error
SJ000286395-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286396-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286398-1	2.0556	1.9918 - 2.1214	B313	WEAK	2.928	2.8242 - 3.0356	B312	WEAK	
SJ000286406-1	0.9532	0.9390 - 0.9676	A213	MED	1.0358	0.9951 - 1.0783	A312	MED	
SJ000286408-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286413-1	>5	NA	C555	WEAK	3.4496	3.4248 - 3.4745	B313	WEAK	
SJ000286415-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286419-1	>5	NA	B241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286421-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286423-1	2.0321	1.9745 - 2.0914	B314	WEAK	2.0036	1.9296 - 2.0805	B314	WEAK	
SJ000286424-1	0.314	0.1913 - 0.5154	A221	MED	0.7253	0.6854 - 0.7675	A212	MED	
SJ000286430-1	>5	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000286434-1	1.6319	1.6097 - 1.6545	B313	WEAK	1.4706	1.3664 - 1.5827	B312	WEAK	
SJ000286436-1	<0.1	NA	B110	HIGH	0.1213	0.1021 - 0.1440	B110	MED	Differential activity within experimental error
SJ000286438-1	>5	NA	B321	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286446-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286448-1	0.1447	0.1099 - 0.1906	A212	MED	0.1909	0.1448 - 0.2516	A212	MED	
SJ000286450-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286451-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286453-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286455-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286458-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286481-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286496-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286501-2	>5	NA	B314	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286511-1	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286515-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286515-2	0.0648	0.0536 - 0.0783	A113	HIGH	0.0651	0.0561 - 0.0754	A113	HIGH	
SJ000286516-4	>5	NA	C555	INACTIVE	>5	NA	B313	INACTIVE	
SJ000286520-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286522-1	4.0011	NA	C555	WEAK	2.834	2.6811 - 2.9956	B312	WEAK	
SJ000286525-1	>5	NA	B141	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286530-1	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286533-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286536-1	0.7071	0.6825 - 0.7325	A212	MED	0.6411	0.6184 - 0.6645	A212	MED	
SJ000286537-1	0.3082	0.2752 - 0.3452	A221	MED	0.9009	0.7435 - 1.0917	A222	MED	
SJ000286548-2	2.0459	1.9915 - 2.1018	B322	WEAK	2.2948	2.2635 - 2.3267	B312	WEAK	
SJ000286550-2	>5	NA	NB241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286552-1	0.0503	0.0427 - 0.0592	B110	HIGH	0.042	0.0353 - 0.0499	B110	HIGH	
SJ000286565-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286572-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286576-1	0.8303	0.7823 - 0.8814	A212	MED	0.7585	0.7253 - 0.7932	A212	MED	
SJ000286594-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286616-1	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286619-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286644-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286645-1	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286646-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286648-1	>5	NA	B141	INACTIVE	>5	NA	C555	INACTIVE	

SJ000286657-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286658-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286694-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286708-1	3.054	2.3308 - 4.0015	B313	WEAK	2.6085	2.1808 - 3.1201	B314	WEAK	
SJ000286710-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286711-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286715-2	1.9516	1.8621 - 2.0453	B312	WEAK	2.4069	2.3605 - 2.4543	B312	WEAK	
SJ000286728-1	0.2169	0.1313 - 0.3584	A211	MED	0.3591	0.3283 - 0.3927	A212	MED	
SJ000286729-1	>5	NA	D555	INACTIVE	>5	NA	B141	INACTIVE	
SJ000286749-1	3.0281	2.9392 - 3.1196	B312	WEAK	2.4661	2.4380 - 2.4945	B312	WEAK	
SJ000286751-1	0.2951	0.1510 - 0.5765	A212	MED	0.2616	0.1867 - 0.3665	A212	MED	
SJ000286753-1	0.721	0.6923 - 0.7509	A213	MED	0.808	0.7737 - 0.8438	A213	MED	
SJ000286767-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286769-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286772-1	>5	NA	B241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286775-1	>5	NA	B314	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286776-1	>5	NA	NC555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286780-1	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286781-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286782-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286783-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286797-1	>5	NA	C555	INACTIVE	>5	NA	B314	INACTIVE	
SJ000286800-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286801-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286802-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286804-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286809-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286813-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286816-1	1.1816	0.5135 - 2.7190	B311	WEAK	2.1215	1.3636 - 3.3006	B311	WEAK	
SJ000286821-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286829-2	>5	NA	B241	INACTIVE	>5	NA	A241	INACTIVE	
SJ000286830-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286847-1	0.3333	0.3014 - 0.3686	A232	WEAK	0.6878	0.5576 - 0.8483	A233	WEAK	
SJ000286853-1	>5	NA	B241	INACTIVE	>5	NA	A242	INACTIVE	
SJ000286865-1	>5	NA	D555	INACTIVE	>5	NA	NA141	INACTIVE	
SJ000286868-1	>5	NA	A241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286877-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286884-1	>5	NA	B141	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286890-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286899-6	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286902-2	0.1882	0.1689 - 0.2098	A212	MED	0.1934	0.1731 - 0.2160	A212	MED	
SJ000286904-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286906-1	>5	NA	A242	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286948-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000286950-4	2.7871	2.6267 - 2.9574	B312	WEAK	>5	NA	C555	INACTIVE	
SJ000286959-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286960-1	2.0573	2.0333 - 2.0817	B313	WEAK	1.9578	1.9446 - 1.9711	B313	WEAK	
SJ000286962-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000286963-1	>5	NA	C555	INACTIVE	>5	NA	B334	INACTIVE	
SJ000286965-1	<0.1	NA	C555	HIGH	<0.1	NA	C555	HIGH	
SJ000286983-2	0.0323	0.0238 - 0.0438	B110	HIGH	0.0213	0.0159 - 0.0287	B110	HIGH	
SJ000286986-1	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000286993-1	1.03	0.8297 - 1.2786	A312	WEAK	1.3651	1.1879 - 1.5686	B312	WEAK	
SJ000287007-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287016-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287020-1	>5	NA	D555	INACTIVE	>5	NA	NB141	INACTIVE	
SJ000287054-1	>5	NA	A241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287055-3	1.4999	1.3631 - 1.6505	B312	WEAK	1.291	0.7246 - 2.3002	A324	WEAK	
SJ000287058-1	>5	NA	B141	INACTIVE	>5	NA	A241	INACTIVE	
SJ000287059-1	0.3416	0.3018 - 0.3866	A221	MED	2.4681	1.2594 - 4.8369	B311	WEAK	Differential activity within experimental error
SJ000287062-1	>5	NA	C555	WEAK	2.3374	2.3101 - 2.3651	B313	WEAK	
SJ000287073-2	>5	NA	A241	INACTIVE	>5	NA	B244	INACTIVE	
SJ000287074-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287076-4	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287077-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287078-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287087-1	1.9311	1.8976 - 1.9652	B313	WEAK	1.9031	1.8028 - 2.0090	B313	WEAK	
SJ000287088-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287090-1	>5	NA	A233	INACTIVE	1.2339	0.8712 - 1.7477	A324	WEAK	Differential activity within experimental error
SJ000287092-1	0.1214	0.0807 - 0.1827	A213	MED	0.1039	0.0705 - 0.1531	A212	MED	
SJ000287098-4	>5	NA	B344	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287101-1	>5	NA	B341	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287102-1	0.0362	0.0314 - 0.0418	B110	HIGH	0.0365	0.0165 - 0.0806	B110	HIGH	
SJ000287131-1	>5	NA	NB144	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287132-2	>5	NA	A141	INACTIVE	>5	NA	A241	INACTIVE	
SJ000287133-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287134-1	1.4028	1.1796 - 1.6684	B312	WEAK	1.2957	1.1132 - 1.5081	B312	WEAK	
SJ000287136-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287138-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287139-1	>5	NA	C555	WEAK	>5	NA	C555	WEAK	
SJ000287147-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287149-1	<1.0	NA	C555	MED	<1.0	NA	C555	MED	
SJ000287150-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287152-1	0.3768	0.3328 - 0.4266	A212	MED	0.3899	0.3213 - 0.4731	A212	MED	
SJ000287155-1	0.078	0.0708 - 0.0858	A112	HIGH	0.0669	0.0607 - 0.0738	A113	HIGH	
SJ000287160-1	1.8786	1.8381 - 1.9199	B312	WEAK	2.2265	2.1794 - 2.2747	B312	WEAK	
SJ000287177-1	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287181-1	>5	NA	C555	INACTIVE	>5	NA	A241	INACTIVE	
SJ000287182-5	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287193-3	>5	NA	B314	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287195-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287203-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287206-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287209-1	1.754	1.6223 - 1.8964	B312	WEAK	2.295	2.1725 - 2.4243	B312	WEAK	
SJ000287215-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287222-1	0.0618	0.0510 - 0.0749	A112	HIGH	0.0575	0.0479 - 0.0689	A112	HIGH	
SJ000287228-1	2.055	2.0312 - 2.0791	B312	WEAK	>1.0	0.0010 - 699.2647	A214	WEAK	
SJ000287229-1	>5	NA	B241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287231-1	0.0909	0.0792 - 0.1044	A112	HIGH	0.0837	0.0727 - 0.0963	A112	HIGH	
SJ000287238-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287239-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287245-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287247-1	0.0671	0.0513 - 0.0878	B110	HIGH	0.0582	0.0412 - 0.0823	B110	HIGH	
SJ000287256-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287261-1	0.1832	0.1553 - 0.2162	A212	MED	0.1749	0.1482 - 0.2063	A212	MED	
SJ000287270-1	0.4073	0.3609 - 0.4595	A212	MED	0.3365	0.2582 - 0.4385	A212	MED	
SJ000287281-1	>5	NA	B343	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287282-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287283-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287295-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287300-3	>5	NA	B344	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287313-1	>5	NA	B241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287314-3	1.0237	NA	C555	WEAK	>5	NA	D555	INACTIVE	Differential activity within experimental error
SJ000287317-4	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287320-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287329-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287330-1	2.8722	2.6847 - 3.0727	B312	WEAK	2.0003	1.9539 - 2.0478	B312	WEAK	
SJ000287331-1	0.2183	0.1905 - 0.2501	A212	MED	0.1906	0.1602 - 0.2267	A213	MED	
SJ000287333-1	0.0532	0.0458 - 0.0619	A113	HIGH	0.0577	0.0502 - 0.0663	A112	HIGH	
SJ000287335-1	>5	NA	A241	INACTIVE	>5	NA	B241	INACTIVE	
SJ000287348-1	0.0807	0.0681 - 0.0956	A112	HIGH	0.0847	0.0705 - 0.1018	A112	HIGH	
SJ000287350-1	>5	NA	B342	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287365-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287368-1	1.0958	0.8387 - 1.4317	B311	WEAK	0.5999	0.5365 - 0.6708	A211	MED	Differential activity within experimental error
SJ000287384-1	1.0372	0.9357 - 1.1498	A322	WEAK	1.4013	1.3316 - 1.4747	B312	WEAK	
SJ000287393-1	0.0457	0.0382 - 0.0547	B110	HIGH	0.0452	0.0368 - 0.0554	B110	HIGH	
SJ000287394-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287395-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287397-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287398-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287400-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287409-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287413-2	>5	NA	B343	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287428-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287441-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287448-1	4.723	NA	C555	WEAK	>5	NA	C555	INACTIVE	Differential activity within experimental error
SJ000287450-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287457-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	

SJ000287461-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287462-1	>5	NA	B331	INACTIVE	>5	NA	B331	INACTIVE	
SJ000287467-3	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287484-1	>5	NA	B241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287488-1	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287490-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287493-3	>5	NA	C555	INACTIVE	>5	NA	B343	INACTIVE	
SJ000287506-1	>5	NA	B130	INACTIVE	>5	NA	B130	INACTIVE	
SJ000287508-1	0.0223	0.0176 - 0.0283	B110	HIGH	0.0249	0.0201 - 0.0308	B110	HIGH	
SJ000287523-1	0.088	0.0770 - 0.1006	B110	HIGH	0.0797	0.0702 - 0.0905	A112	HIGH	
SJ000287543-1	>5	NA	NA141	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287544-1	>5	NA	C555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000287545-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287547-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287561-1	>5	NA	D555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000287562-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287563-1	0.1431	0.1270 - 0.1612	A213	MED	0.1397	0.1150 - 0.1698	A213	MED	
SJ000287568-1	0.0102	0.0086 - 0.0121	B110	HIGH	0.0069	0.0018 - 0.0267	B110	HIGH	
SJ000287585-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287590-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287618-2	>5	NA	D555	INACTIVE	>5	NA	B341	INACTIVE	
SJ000287619-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287632-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287647-2	>5	NA	B334	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287648-2	>5	NA	A241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287657-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287660-2	0.0659	0.0514 - 0.0847	A112	HIGH	0.0578	0.0446 - 0.0751	A112	HIGH	
SJ000287663-2	2.6629	1.6576 - 4.2777	B314	WEAK	2.5982	2.5103 - 2.6892	B314	WEAK	
SJ000287667-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287668-2	>5	NA	C555	INACTIVE	>5	NA	A241	INACTIVE	
SJ000287676-2	1.7578	1.6958 - 1.8221	B313	WEAK	1.7042	1.6139 - 1.7996	B322	WEAK	
SJ000287677-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287680-3	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287682-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287686-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287690-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287692-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287693-3	>5	NA	A344	INACTIVE	>5	NA	B342	INACTIVE	
SJ000287697-2	>5	NA	B130	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287703-2	>5	NA	B343	INACTIVE	>5	NA	B343	INACTIVE	
SJ000287705-2	>5	NA	C555	INACTIVE	>5	NA	B333	INACTIVE	
SJ000287706-2	>5	NA	B334	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287714-2	1.0777	0.3018 - 3.8488	A314	WEAK	1.692	1.0254 - 2.7920	B311	WEAK	
SJ000287728-2	1.6312	1.5355 - 1.7329	B312	WEAK	1.6193	1.4530 - 1.8047	B312	WEAK	
SJ000287730-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287734-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287737-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287741-2	0.4672	0.3855 - 0.5661	A213	MED	0.4667	0.3819 - 0.5704	A213	MED	
SJ000287744-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287749-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287750-2	>5	NA	B344	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287752-2	>5	NA	B342	INACTIVE	>5	NA	B341	INACTIVE	
SJ000287758-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287762-2	>5	NA	B141	INACTIVE	>5	NA	B244	INACTIVE	
SJ000287767-2	>5	NA	D555	INACTIVE	>5	NA	B341	INACTIVE	
SJ000287768-2	0.4478	0.4035 - 0.4969	A214	MED	0.4379	0.3997 - 0.4798	A213	MED	
SJ000287769-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287778-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287799-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287810-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287813-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287814-2	>5	NA	B314	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287821-2	>5	NA	C555	INACTIVE	>5	NA	B313	INACTIVE	
SJ000287827-2	0.0471	0.0338 - 0.0657	B110	HIGH	0.0435	0.0345 - 0.0548	A112	HIGH	
SJ000287837-2	>5	NA	B341	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287841-2	>5	NA	B342	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287864-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287868-2	>5	NA	B332	INACTIVE	2.2448	2.1303 - 2.3655	B314	WEAK	Significant shift in efficacy, not potency
SJ000287873-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287875-2	>5	NA	NC555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287882-2	>5	NA	D555	INACTIVE	>5	NA	NC555	INACTIVE	
SJ000287889-2	>5	NA	B334	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287891-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287899-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287901-2	>5	NA	B342	INACTIVE	>5	NA	B332	INACTIVE	
SJ000287902-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287925-2	<0.1	NA	B110	HIGH	<0.1	NA	B110	HIGH	
SJ000287942-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000287955-2	>5	NA	B244	INACTIVE	>5	NA	A241	INACTIVE	
SJ000287956-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287970-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287972-2	>5	NA	C555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000287975-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000287985-2	>5	NA	C555	INACTIVE	>5	NA	B344	INACTIVE	
SJ000287990-2	2.2004	2.1724 - 2.2288	B313	WEAK	2.2877	2.2204 - 2.3570	B313	WEAK	
SJ000287995-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288002-2	2.0053	1.9724 - 2.0387	B313	WEAK	2.0943	2.0403 - 2.1498	B314	WEAK	
SJ000288007-2	>5	NA	C555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000288017-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288020-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288025-2	>5	NA	B342	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288026-2	>5	NA	NB241	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288030-2	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288031-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288034-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288037-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288041-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288052-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288058-2	>5	NA	NA141	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288059-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288063-2	1.202	1.0820 - 1.3352	B322	WEAK	>5	NA	A342	INACTIVE	Significant shift in efficacy, not potency
SJ000288073-2	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288074-2	>5	NA	A241	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288081-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288084-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288092-2	>5	NA	NB144	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288093-2	>5	NA	NB242	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288098-2	>5	NA	C555	INACTIVE	>5	NA	B342	INACTIVE	
SJ000288099-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288114-2	>5	NA	D555	INACTIVE	>5	NA	B241	INACTIVE	
SJ000288126-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288139-2	>5	NA	C555	WEAK	2.2411	2.2103 - 2.2723	B313	WEAK	
SJ000288140-2	>5	NA	C555	INACTIVE	>5	NA	B314	INACTIVE	
SJ000288147-2	1.0095	0.6912 - 1.4743	A314	WEAK	0.9875	0.7673 - 1.2708	A214	MED	Differential activity within experimental error
SJ000288150-2	>5	NA	B331	INACTIVE	>5	NA	B331	INACTIVE	
SJ000288156-2	>5	NA	C555	INACTIVE	>5	NA	B323	INACTIVE	
SJ000288159-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288163-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288173-2	>5	NA	C555	WEAK	1.4271	1.2596 - 1.6168	B311	WEAK	
SJ000288175-2	>5	NA	NC555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288176-2	>5	NA	C555	INACTIVE	>5	NA	B333	INACTIVE	
SJ000288181-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288182-2	>5	NA	B241	INACTIVE	>5	NA	A241	INACTIVE	
SJ000288186-2	>5	NA	A141	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288194-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288209-2	>5	NA	D555	INACTIVE	>5	NA	A241	INACTIVE	
SJ000288210-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288211-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288216-2	>5	NA	B141	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288219-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288224-2	>5	NA	C555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288226-2	>5	NA	C555	INACTIVE	>5	NA	B242	INACTIVE	
SJ000288238-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288244-2	0.1045	0.0914 - 0.1194	A213	MED	0.1311	0.0021 - 8.2851	A214	MED	
SJ000288246-2	>5	NA	NB141	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288249-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288262-2	>5	NA	C555	INACTIVE	4.0527	NA	C555	WEAK	Differential activity within experimental error
SJ000288270-2	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	

SJ000288274-2	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288278-2	0.0149	0.0104 - 0.0214	B110	HIGH	0.0159	0.0113 - 0.0225	B110	HIGH	
SJ000288284-2	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288304-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288306-1	0.306	0.1694 - 0.5530	A211	MED	0.171	0.0776 - 0.3768	A211	MED	
SJ000288308-1	>5	NA	B341	INACTIVE	>5	NA	B344	INACTIVE	
SJ000288312-1	>5	NA	D555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288313-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288316-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288318-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288320-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000288325-1	>5	NA	B333	INACTIVE	4.198	4.0769 - 4.3227	B313	WEAK	Differential activity within experimental error
SJ000288326-1	>5	NA	A241	INACTIVE	>5	NA	B341	INACTIVE	
SJ000288327-1	>5	NA	D555	INACTIVE	>5	NA	D555	INACTIVE	
SJ000288328-1	>5	NA	C555	INACTIVE	>5	NA	C555	INACTIVE	
SJ000518967-1	0.3177	0.2999-0.3357	A212	MED	0.3133	0.2964-0.3311	A212	MED	DIHYDROARTEMISININ
SJ000518972-1	0.3581	0.3459-0.3639	A212	MED	0.3311	0.3206-0.3428	A212	MED	ARTESUNATE

sample	ATC_L1	ATC_L2	ATC_L3	ATC_L4
SJ000000250-8	C Cardiovascular system	C01 Cardiac therapy	C01B Antiarrhythmics, class I and III	C01BC Antiarrhythmics, class Ic
SJ000000854-6	V Various	V99 Unassigned	V99M Natural products	V99ME Flavone
SJ000113084-4	C Cardiovascular system	C02 Antihypertensives	:02C Antiadrenergic agents, peripherally actin	C02CA Alpha-adrenoreceptor antagonists
SJ000126662-3	V Various	V99 Unassigned	V99N Neurotransmitter	V99NU Purinergic agonist
SJ000285182-2	V Various	V99 Unassigned	V99N Neurotransmitter	V99NJ GABA antagonist
SJ000285183-2	)d forming organs;#D Dermatologicals;#R Res	;#D08 Antiseptics and disinfectants;#D09 M	septics and disinfectants;#D09A Medicated c	monium compounds;#D09AA Medicated dressings with antiinfectives;#R02AA Antiseptics
SJ000285185-4	ntiparasitic products, insecticides, and repell	P01 Antiprotozoals	P01B Antimalarials	P01BA Aminoquinolines
SJ000285188-6	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BC Pyrimidine analogues
SJ000285190-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BC Pyrimidine analogues
SJ000285193-1	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01A Alkylating agents	L01AA Nitrogen mustard analogues
SJ000285194-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01A Alkylating agents	L01AA Nitrogen mustard analogues
SJ000285194-4	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01A Alkylating agents	L01AA Nitrogen mustard analogues
SJ000285195-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BB Purine analogues
SJ000285196-2	Antineoplastic and immunomodulating agent	Antineoplastics agents;#L04 Immunosuppres	1B Antimetabolites;#L04A Immunosuppressa	lic acid analogues;#L04AX Other immunosuppressants
SJ000285197-1	Antineoplastic and immunomodulating agent	L04 Immunosuppressants	L04A Immunosuppressants	L04AA Selective immunosuppressants
SJ000285200-6	ntiparasitic products, insecticides, and repell	P01 Antiprotozoals	Agents against leishmaniasis and trypanoso	other agents against leishmaniasis and trypanosomiasis
SJ000285202-2	ntiparasitic products, insecticides, and repell	P01 Antiprotozoals	ents against amoebiasis and other protozoal	r agents against amoebiasis and other protozoal diseases
SJ000285203-5	V Various	V99 Unassigned	V99S Oxidative phosphorylation	V99SA Respiratory chain inhibitors
SJ000285206-2	V Various	V99 Unassigned	V99A Agricultural/Industrial	V99AG Rodenticide
SJ000285207-1	D Dermatologicals	D08 Antiseptics and disinfectants	D08A Antiseptics and disinfectants	D08AK Mercurial products
SJ000285208-3	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BB Purine analogues
SJ000285210-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01A Alkylating agents	L01AA Nitrogen mustard analogues
SJ000285212-1	V Various	V99 Unassigned	V99W Protein synthesis inhibitors	V99WA Other
SJ000285215-1	ntiparasitic products, insecticides, and repell	P01 Antiprotozoals	ents against amoebiasis and other protozoal	r agents against amoebiasis and other protozoal diseases
SJ000285215-6	ntiparasitic products, insecticides, and repell	P01 Antiprotozoals	ents against amoebiasis and other protozoal	r agents against amoebiasis and other protozoal diseases
SJ000285218-5	V Various	V99 Unassigned	V99J Phosphatase	V99UB PPA2/PP1
SJ000285219-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BC Pyrimidine analogues
SJ000285219-5	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BC Pyrimidine analogues
SJ000285220-5	V Various	V99 Unassigned	V99M Natural products	V99ML Terpene
SJ000285221-4	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BA Folic acid analogues
SJ000285225-2	V Various	V99 Unassigned	V99S Oxidative phosphorylation	V99SA Respiratory chain inhibitors
SJ000285226-6	J Antiinfectives for systemic use	J05 Antivirals for systemic use	J05A Direct acting antiviral drugs	transcriptase inhibitors;#J05AR Antivirals for treatment of HIV infections, combinations
SJ000285227-1	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BC Pyrimidine analogues
SJ000285228-4	V Various	V99 Unassigned	V99W Protein synthesis inhibitors	V99WA Other
SJ000285229-2	V Various	V99 Unassigned	V99R Other	V99RA Various
SJ000285231-2	V Various	V99 Unassigned	V99S Oxidative phosphorylation	V99SD Transport inhibitors
SJ000285232-1	D Dermatologicals	ibiotics and chemotherapeutics for dermatolo	D06B Chemotherapeutics for topical use	D06BB Antivirals
SJ000285232-8	D Dermatologicals	ibiotics and chemotherapeutics for dermatolo	D06B Chemotherapeutics for topical use	D06BB Antivirals
SJ000285234-2	V Various	V99 Unassigned	V99J Ion	V99JE Ionophore
SJ000285235-3	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	01C Plant alkaloids and other natural product	L01CB Podophyllotoxin derivatives
SJ000285238-3	M Musculo-skeletal system	M04 Antigout preparations	M04A Antigout preparations	: Preparations with no effect on uric acid metabolism
SJ000285241-3	Antineoplastic and immunomodulating agent	L04 Immunosuppressants	L04A Immunosuppressants	L04AX Other immunosuppressants
SJ000285242-3	D Dermatologicals;#R Respiratory system	tiseptics and disinfectants;#R02 Throat prepa	septics and disinfectants;#R02A Throat preu	aternary ammonium compounds;#R02AA Antiseptics
SJ000285243-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	1D Cytotoxic antibiotics and related substanc	L01DC Other cytotoxic antibiotics
SJ000285244-3	R Respiratory system	R02 Throat preparations	R02A Throat preparations	R02AB Antibiotics
SJ000285246-2	R Respiratory system	R02 Throat preparations	R02A Throat preparations	R02AA Antiseptics
SJ000285249-1	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	1D Cytotoxic antibiotics and related substanc	L01DA Actinomycines
SJ000285256-3	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	1D Cytotoxic antibiotics and related substanc	01DB Anthracyclines and related substances
SJ000285261-3	V Various	V99 Unassigned	V99H Dermatological	V99HA Antiseptic
SJ000285262-1	:#G Genito-urinary system and sex hormones	mmatory/anti-infective agents;#G01 Gynecol	1A Antiinfectives and antiseptics, excluding c	for local oral treatment;#A07AA Antibiotics;#G01AA Antibiotics;#J02AA Antibiotics
SJ000285263-2	V Various	V99 Unassigned	V99A Agricultural/Industrial	V99AA Disinfectant
SJ000285267-3	ntiparasitic products, insecticides, and repell	esiticides, including scabicides, insecticides,	P03A Ectoparasiticides, including scabicides	P03AA Sulphur containing products
SJ000285270-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01A Alkylating agents	L01AC Ethylene imines
SJ000285272-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BC Pyrimidine analogues
SJ000285273-3	D Dermatologicals	D08 Antiseptics and disinfectants	D08A Antiseptics and disinfectants	D08AE Phenol and derivatives
SJ000285276-2	V Various	V99 Unassigned	V99C Antimicrobial	V99CA Antimicrobial
SJ000285278-1	V Various	V99 Unassigned	V99G Cytoskeletal	V99GB Inhibitors microtubule polymerization
SJ000285279-2	N Nervous system	N07 Other nervous system drugs	N07A Parasympathomimetics	N07AA Anticholinesterases
SJ000285285-3	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01X Other antineoplastic agents	L01XX Other antineoplastic agents
SJ000285292-10	J Antiinfectives for systemic use	J04 Antimycobacterials	J04A Drugs for treatment of tuberculosis	J04AB Antibiotics
SJ000285294-1	D Dermatologicals	D09 Medicated dressings	D09A Medicated dressings	)09AA Medicated dressings with antiinfectives
SJ000285299-2	D Dermatologicals	ibiotics and chemotherapeutics for dermatolo	D06B Chemotherapeutics for topical use	D06BB Antivirals
SJ000285307-3	V Various	V99 Unassigned	V99C Antimicrobial	V99CA Antimicrobial
SJ000285308-1	s Genito-urinary system and sex hormones;#;	#G01 Gynecological anti-infectives and anti	ectives and antiseptics, excluding combinatio	derivatives;#G01AC Quinoline derivatives;#R02AA Antiseptics
SJ000285313-3	V Various	V99 Unassigned	V99M Natural products	V99MF Lipid
SJ000285315-2	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01B Antimetabolites	L01BC Pyrimidine analogues
SJ000285316-4	J Antiinfectives for systemic use	J01 Antibacterials for systemic use	LF Macrolides, lincosamides and streptogram	J01FF Lincosamides
SJ000285317-2	Dermatologicals;#G Genito-urinary system an	and disinfectants;#G01 Gynecological anti-	irrits;#G01A Antiinfectives and antiseptics, excl	treatment;#D08AH Quinoline derivatives;#G01AC Quinoline derivatives;#R02AA Antiseptics
SJ000285318-7	S Sensory organics;#V Various	hthalmologicals;#V03 All other therapeutics	pa preparations and miotics;#V03A All other th	1EB Parasympathomimetics;#V03AB Antidotes
SJ000285319-1	nd blood forming organs;#D Dermatologicals	ctants;#D09 Medicated dressings;#R02 Thro	fectants;#D09A Medicated dressings;#R02A	amidines;#D09AA Medicated dressings with antiinfectives;#R02AA Antiseptics;#S01AX Other anti-infectives;#S02AA Anti-infectives;#S03A
SJ000285321-4	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	1D Cytotoxic antibiotics and related substanc	01DB Anthracyclines and related substances
SJ000285323-3	V Various	V99 Unassigned	V99H Dermatological	V99HA Antiseptic
SJ000285327-1	V Various	V99 Unassigned	V99M Natural products	V99MA Alkaloid
SJ000285332-1	D Dermatologicals	D11 ther dermatological preparations	D11A Other dermatological preparations	D11AX Other dermatologicals
SJ000285334-4	J Antiinfectives for systemic use	J01 Antibacterials for systemic use	LF Macrolides, lincosamides and streptogram	J01FA Macrolides
SJ000285335-1	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	01C Plant alkaloids and other natural product	L01CA Vinca alkaloids and analogues
SJ000285335-4	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	01C Plant alkaloids and other natural product	L01CA Vinca alkaloids and analogues
SJ000285337-5	D Dermatologicals	D10 Anti-acne preparations	ations for topical use;#D10B Anti-acne prepar	for topical use in acne;#D10BA Retinoids for treatment of acne
SJ000285337-8	ogicals;#L Antineoplastic and immunomodul	Anti-acne preparations;#L01 Antineoplastics	preparations for topical use;#L01X Other antin	for topical use in acne;#L01XX Other antineoplastic agents
SJ000285338-3	nd blood forming organs;#D Dermatologicals	ctants;#D09 Medicated dressings;#R02 Thro	fectants;#D09A Medicated dressings;#R02A	amidines;#D09AA Medicated dressings with antiinfectives;#R02AA Antiseptics;#S01AX Other anti-infectives;#S02AA Anti-infectives;#S03A
SJ000285343-2	A Alimentary tract and metabolism	rrheals, intestinal anti-inflammatory/anti-infec	A07A Intestinal anti-infectives	A07AB Sulfonamides
SJ000285358-5	als;#H Systemics hormonal preparations (excl	s, dermatological preparations;#H02 Cortico	combinations;#H02A Corticosteroids for syst	ombinations;#H02AB Glucocorticoids;#R01AD Corticosteroids;#S01BA Corticosteroids, plain;#S01BB Corticosteroids and mydriatics in com
SJ000285363-5	N Nervous system	N05 Psycholeptics	N05A Antipsychotics	Diazepines, oxazepines, thiazepines and oxepines
SJ000285364-2	C Cardiovascular system	C08 Calcium channel blockers	ctive calcium channel blockers with direct car	C08DB Benzothiazepine derivatives
SJ000285365-1	V Various	V99 Unassigned	V99J Ion	V99JE Ionophore
SJ000285368-3	V Various	V99 Unassigned	V99M Natural products	V99MJ Steroid
SJ000285369-1	V Various	V99 Unassigned	V99A Agricultural/Industrial	V99AA Disinfectant
SJ000285373-9	nentary tract and metabolism;#S Sensory org	functional gastrointestinal disorders;#S01 Op	3C Antispasmodics in combination with psycl	03CB Belladonna and derivatives in combination with psycholeptics;#S01FA Anticholinergics
SJ000285375-2	N Nervous system	N06 Psychoanaleptics	N06A Antidepressants	N06AX Other antidepressants
SJ000285382-3	V Various	V99 Unassigned	V99M Natural products	V99MJ Steroid
SJ000285383-1	R Respiratory system	R06 Antihistamines for systemic use	R06A Antihistamines for systemic use	R06AX Other antihistamines for systemic use
SJ000285387-8	R Respiratory system	R01 Nasal preparations	R01B Nasal decongestants for systemic use	R01BA Sympathomimetics
SJ000285396-2	V Various	V99 Unassigned	V99N Neurotransmitter	V99NX Serotonin antagonist
SJ000285400-2	V Various	V99 Unassigned	V99C Antimicrobial	V99CA Antimicrobial
SJ000285410-5	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	L01X Other antineoplastic agents	L01XX Other antineoplastic agents
SJ000285413-1	V Various	V99 Unassigned	V99M Natural products	V99MF Lipid
SJ000285423-2	V Various	V99 Unassigned	V99L Lipase	V99LA Monoacylglycerol lipase
SJ000285426-2	V Various	V99 Unassigned	V99R Other	V99RA Various
SJ000285431-2	ntiparasitic products, insecticides, and repell	esiticides, including scabicides, insecticides,	P03A Ectoparasiticides, including scabicides	AX Other ectoparasiticides, including scabicides
SJ000285433-1	B Blood and blood forming organs	B01 Antithrombotic agents	B01A Antithrombotic agents	C Platelet aggregation inhibitors excluding heparin
SJ000285436-3	ntiparasitic products, insecticides, and repell	P01 Antiprotozoals	P01B Antimalarials	P01BE Artemisinin and derivatives, plain
SJ000285439-2	ological;#R Respiratory system;#S Sensory	utics for dermatological use;#R02 Throat pre	or topical use;#R02A Throat preparations;#S	ibiotics for topical use;#R02AB Antibiotics;#S01AA Antibiotics
SJ000285440-2	V Various	V99 Unassigned	V99M Natural products	V99MH Quinone
SJ000285442-1	V Various	V99 Unassigned	V99D Antioxidant	V99DA Antioxidant
SJ000285443-2	V Various	V99 Unassigned	V99A Agricultural/Industrial	V99AB Dye
SJ000285445-2	V Various	V99 Unassigned	V99O Nuclear hormore receptor	V99OI TR antagonist
SJ000285450-2	D Dermatologicals	D08 Antiseptics and disinfectants	D08A Antiseptics and disinfectants	D08AA Acridine derivatives
SJ000285451-3	V Various	V99 Unassigned	V99M Natural products	V99MA Alkaloid
SJ000285452-1	:t and metabolism;#D Dermatologicals;#R Re	7 Corticosteroids, dermatological preparation	Decongestants and other nasal preparations	AC Corticosteroids, potent (group III);#R01AD Corticosteroids;#R03BA Glucocorticoids
SJ000285452-5	:t and metabolism;#D Dermatologicals;#R Re	7 Corticosteroids, dermatological preparation	Decongestants and other nasal preparations	AC Corticosteroids, potent (group III);#R01AD Corticosteroids;#R03BA Glucocorticoids
SJ000285453-3	C Cardiovascular system	C03 Diuretics	C03D Potassium-sparing agents	C03DA Aldosterone antagonists
SJ000285454-2	J Antiinfectives for systemic use	J01 Antibacterials for systemic use	J01D Other beta-lactam antibacterials	J01DB First-generation cephalosporins
SJ000285460-1	J Antiinfectives for systemic use	J01 Antibacterials for systemic use	J01M Quinolone antibacterials	J01MB Other quinolones
SJ000285461-1	A Alimentary tract and metabolism	3 Drugs for functional gastrointestinal disord	A03A Drugs for functional bowel disorders	nthetic anticholinergics, esters with tertiary amino group
SJ000285462-2	D Dermatologicals	D10 Anti-acne preparations	D10A Anti-acne preparations for topical use	D10AF Anti-infectives for treatment of acne
SJ000285465-2	N Nervous system	N06 Psychoanaleptics	N06D Anti-dementia drugs	N06DX Other anti-dementia drugs
SJ000285466-4	N Nervous system	N03 Antiepileptics	N03A Antiepileptics	N03AG Fatty acid derivatives
SJ000285484-2	C Cardiovascular system	C01 Cardiac therapy	C Cardiac stimulants excluding cardiac glyco	C01CA Adrenergic and dopaminergic agents
SJ000285487-3	Cardiovascular system;#R Respiratory syste	iuretics;#R03 Drugs for obstructive airway di	uding thiazides;#R03D Other systemic drugs	03BD Xanthine derivatives;#R03DA Xanthines
SJ000285490-1	V Various	V99 Unassigned	V99M Natural products	V99MM Xanthanoid
SJ000285502-5	C Cardiovascular system	C01 Cardiac therapy	C01B Antiarrhythmics, class I and III	C01BD Antiarrhythmics, class III
SJ000285504-2	N Nervous system	N01 Anesthetics	N01B Anesthetics, local	N01BB Amides
SJ000285506-2	V Various	V99 Unassigned	V99R Other	V99RA Various
SJ000285508-1	Antineoplastic and immunomodulating agent	L01 Antineoplastics agents	01C Plant alkaloids and other natural product	L01CD Taxanes
SJ000285512-1	V Various	V99 Unassigned	V99M Natural products	V99ML Terpene
SJ000285522-3	ism;#C Cardiovascular system;#R Respirato	diac therapy;#R01 Nasal preparations;#R03	cosides;#R01A Decongestants and other nas	B Sympathomimetics, combinations excluding corticosteroids;#R03CA Alpha- and beta-adrenoreceptor agonists;#S01FB Sympathomimetic
SJ000285526-3	V Various	V99 Unassigned	V99N Neurotransmitter	V99NK GABA reuptake inhibitor
SJ000285536-1	N Nervous system;#S Sensory organics	ther nervous system drugs;#S01 Ophthalmo	bathomimetics;#S01E Antiglaucoma preparatir	parasympathomimetics;#S01EB Parasympathomimetics
SJ000285540-4	C Cardiovascular system	C02 Antihypertensives	, peripherally acting;#C02L Antihypertensivesto	r antagonists;#C02LE Alpha-adrenoreceptor antagonists and diuretics
SJ000285541-3	Systemics hormonal preparations (excluding	preparations;#H02 Corticosteroids for system	07X Corticosteroids, other combinations;#H	D07XA Corticosteroids, weak, other combinations;#H02AB Glucocorticoids;#R01AD Corticosteroids;#S01BA Corticosteroids, plain;#S01BE
SJ000285542-2	Systemics hormonal preparations (excluding	preparations;#H02 Corticosteroids for system	07X Corticosteroids, other combinations;#H	D07XA Corticosteroids, weak, other combinations;#H02AB Glucocorticoids;#R01AD Corticosteroids;#S01BA Corticosteroids, plain;#S01BE
SJ000285543-1	n;#H Systemics hormonal preparations (excl	nti-inflammatory/anti-infective agents;#H02 C	nflammatory agents;#H02A Corticosteroids fc	Corticosteroids acting locally;#H02AB Glucocorticoids
SJ000285544-3	ntiparasitic products, insecticides, and repell	P01 Antiprotozoals	P01B Antimalarials	P01BA Aminoquinolines
SJ000285547-5	C Cardiovascular system	C01 Cardiac therapy	C01B Antiarrhythmics, class I and III	C01BA Antiarrhythmics, class Ia
SJ000285549-5	N Nervous system	N05 Psycholeptics	N05A Antipsychotics	05AB Phenothiazines with piperazine structure
SJ000285551-2	G Genito-urinary system and sex hormones	ex hormones and modulators of the genital	stogens;#G03F Progestogens and estrogens	ivatives;#G03FA Progestogens and estrogens, fixed combinations
SJ000285554-2	V Various	V99 Unassigned	V99M Natural products	V99ME Flavone
SJ000285564-2	N Nervous system	N06 Psychoanaleptics	N06A Antidepressants	3AF Monoamine oxidase inhibitors, non-selective
SJ000285569-2	ntiparasitic products, insecticides, and repell	P02 Antihelmintics	P02C Antinematodal agents	P02CB Piperazine and derivatives
SJ000285572-3	al system;#P Antiparasitic products, insecticid	disorders of the musculo-skeletal system;#o	disorders of the musculo-skeletal system;#	Quinine and derivatives;#P01BC Methanolquinolines
SJ000285572-4	al system;#P Antiparasitic products, insecticid	disorders of the musculo-skeletal system;#o	disorders of the musculo-skeletal system;#	Quinine and derivatives;#P01BC Methanolquinolines
SJ000285574-1	V Various	V99 Unassigned	V99H Dermatological	V99HC Local anesthetic
SJ000285577-2	C Cardiovascular system	C03 Diuretics	C03D Potassium-sparing agents	C03DA Aldosterone antagonists
SJ000285584-1	V Various	V99 Unassigned	V99K Kinase	V99KC CK2 inhibitor
SJ000285586-2	G Genito-urinary system and sex hormones	ex hormones and modulators of the genital s	G03B Androgens	G03BB 5-androstanon-(3) derivatives
SJ000285587-1	V Various	V99 Unassigned	V99M Natural products	V99MM Xanthanoid
SJ000285588-1	V Various	V99 Unassigned	V99M Natural products	V99ME Flavone
SJ000285591-1	Musculo-skeletal system;#S Sensory organics	products;#M02 Topical products for joint ar	non-steroids;#M02A Topical products for joint	ory preparations, non-steroids for topical use;#S01BC Anti-inflammatory agents, non-steroids