

## Supplementary Results, Figures and Tables for:

### Chemical interrogation of nuclear size identifies compounds with cancer cell line-specific effects on migration and invasion

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## Complementary analyses of nuclear size chemical screen data

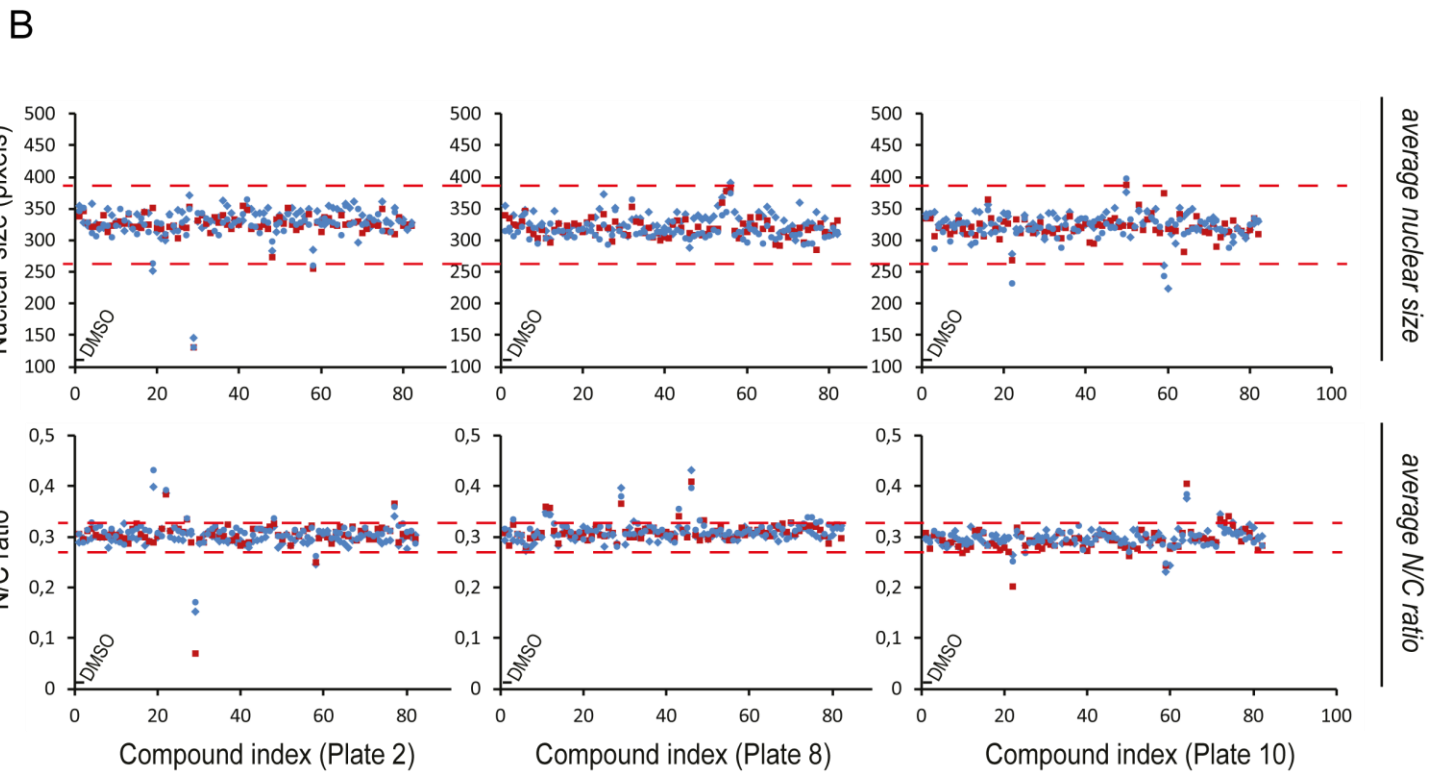
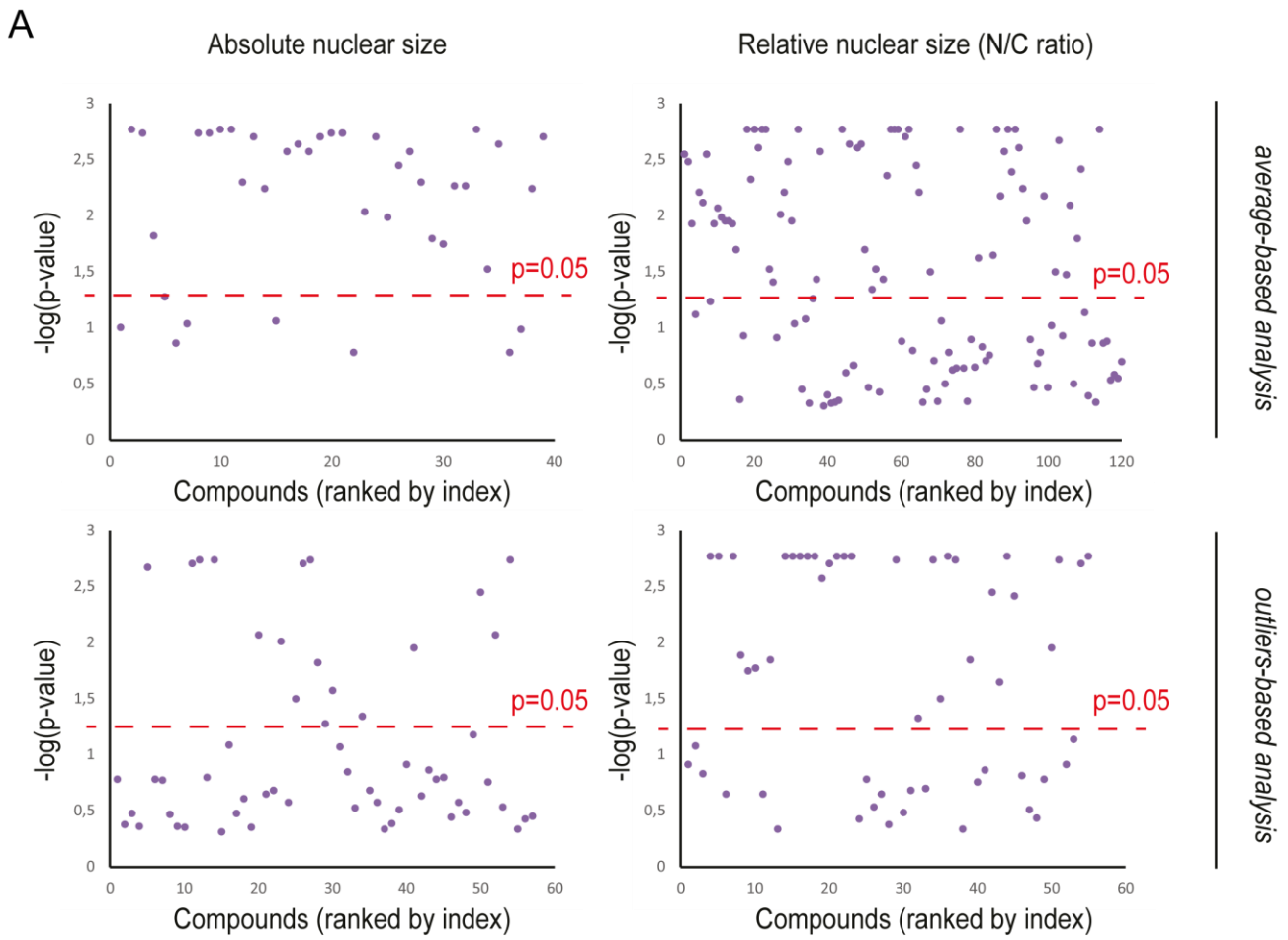
We calculated both the absolute nuclear size and the N/C ratio (nuclear-to-cytoplasm size ratio, i.e. relative nuclear size) from these data and then used two quantification strategies to analyze effects of compounds on both. These four analyses each yielded important insights that would have been missed if just one analysis approach had been undertaken. We first developed an average-based quantification strategy, as average nuclear size is traditionally used by cytologists to grade tumors. To implement this approach, the average values of the size metrics were determined across all imaged cells for each compound well and in-plate DMSO-treated controls. However, shifting the average metric values up or down does not obligatorily reflect loss of size regulation, but could reflect a change in the cell-regulated value to which the metric is set. Thus, to detect compounds that specifically disrupt nuclear size control by increasing the metric variance across a cell population, we also analyzed the same data using an outlier-based approach, which yields complementary information. We computed for each well the fractions of cells with abnormally large or small metric value (i.e., outlier cells). The outlier metric value refers to values beyond the outlier thresholds defined using standard procedures with respect to the distribution of metric values for all in-plate DMSO control wells (see Fig. 1B and Methods). For the average-based and outlier-based methods, respectively, the average metric values and the fractions of outlier cells from all wells were analyzed statistically to identify hit compounds that perturb the metric beyond the typical metric variability across the library. Hit compounds were confirmed using direct comparison with in-plate DMSO controls in Wilcoxon rank statistical tests.

There was a strong overlap between compound sets identified using average-based versus outlier-based analyses for absolute nuclear size although the outlier-based method tended to identify more hits (Supplementary Fig. S2a, Table 1, compare Supplementary Tables 2, 5). The general convergence of these fundamentally different analysis methods underscores the robustness of our data while the differences between them might be biologically relevant. For example, average-based only hits might alter the nuclear size set

point but not homeostatic control whereas outlier-based only hits might perturb homeostasis but not the nuclear size set point. Likewise, analysis of the N/C ratio, which normalizes nuclear size changes relative to overall cell size, (Supplementary Tables 4, 6), identifies compounds that disrupts the correct scaling of the nuclear size to the cell size, even in situations where the absolute nuclear size is unaffected.

The screen data was entirely analysed using the four analysis methods (Supplementary Tables 2, 4, 5, 6). In the main text, results were mostly discussed using the absolute nuclear size metric and the average analysis methodology because this metric/methodology association gave the most reproducible results in our triplicate pilot screen (Supplementary Fig. S1; Supplementary Table 1). However, we also discussed results obtained using the alternative, complementary analyses in particular to emphasize on particular signatures of compound classes across cell lines and time points. These results, presented on Figs. 4, S3, S4, S5, provide insight on the mechanisms and dynamics of nuclear size rectification.

## **Supplementary Figures:**

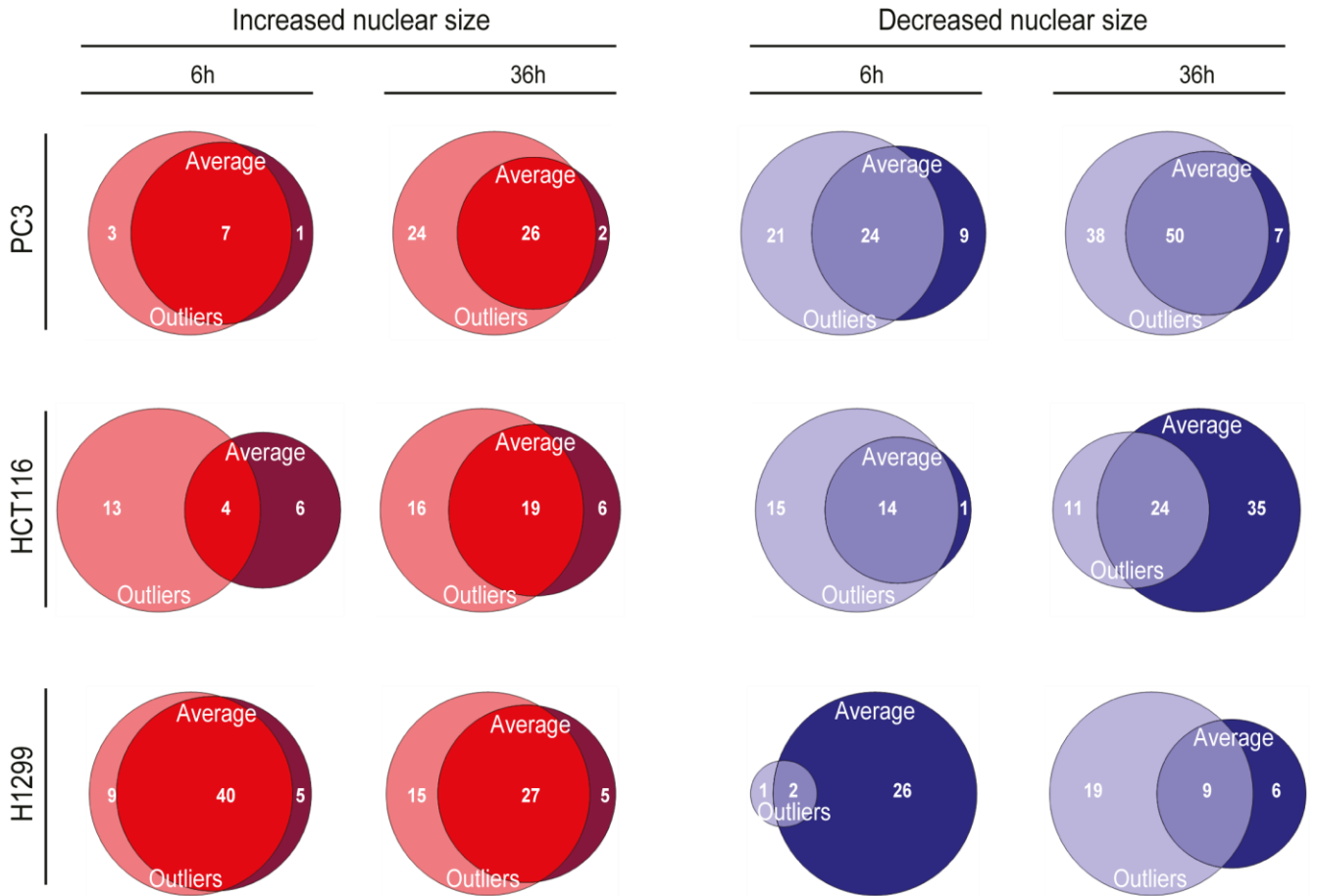


Tollis et al. Figure S1

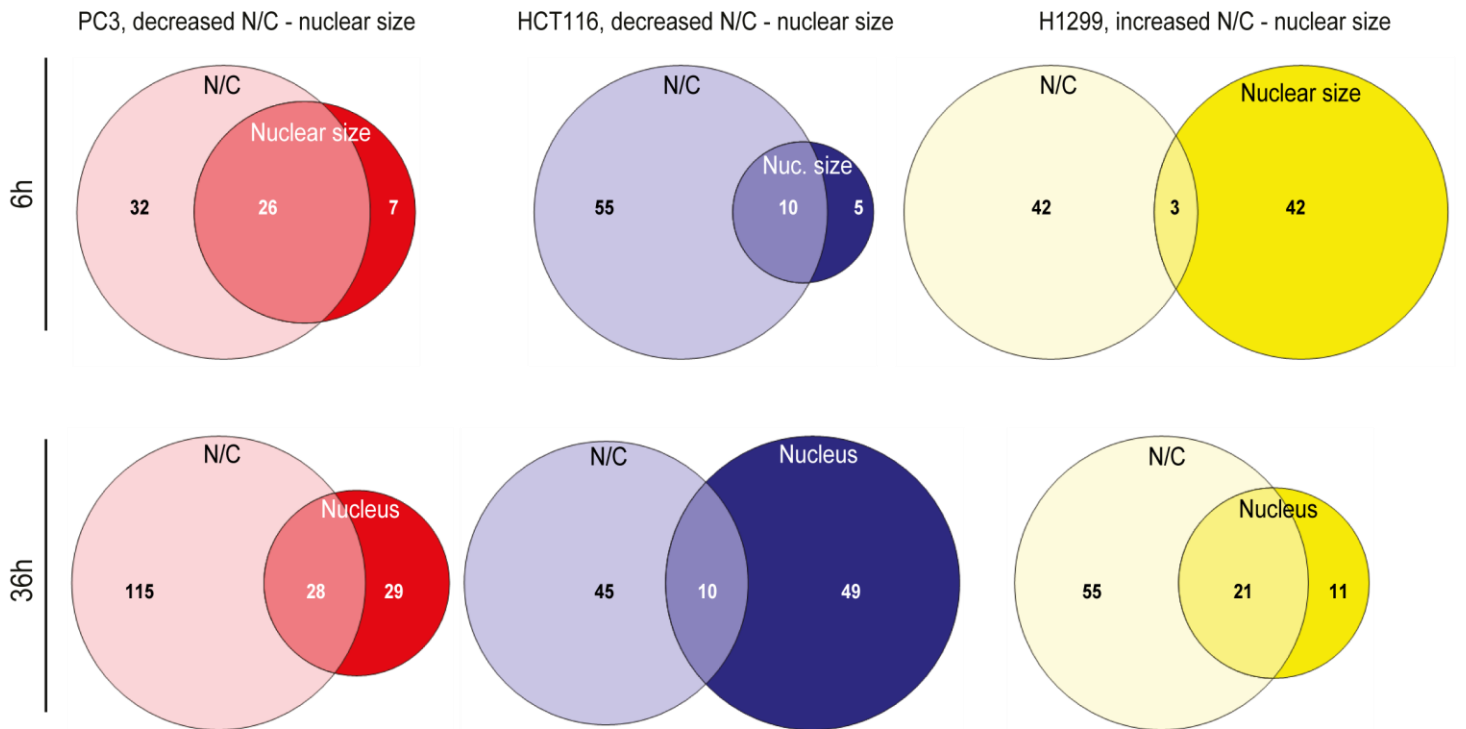
### **Supplementary Figure S1. Screen data reproducibility.**

A. Scatter plots showing the Wilcoxon rank tests p-values (log scale, vertical axis) for each “hit” compound (horizontal axis) compared with DMSO across all replicates (see Methods). Tests were performed from the average nuclear size (left scatters) and N/C ratio metrics (right scatters) data acquired on PC3 cells with 6h treatment (3 replicates), and using average-based (top scatters) and outliers-based (bottom scatters) analyses. The significance level ( $p=0.05$ ) is shown as red dashed lines. B. Examples of raw data scatter plots showing the average nuclear size (top scatters) and average N/C ratio (bottom scatters) as directly output by our Matlab analysis scripts for compound plate 2 (left), plate 8 (middle) and plate 10 (right). Blue circle, blue diamond and red squares represent the 3 replicates (PC3 cells, 6h treatment). For each plate/replicate/metric, the first 2 dots of the scatter represent the value metric averaged over all in-plate DMSO control wells (16 wells), and compounds are then listed from A2, A3 ... A11, B2 ... to H11. Dashed lines indicate the hit detection thresholds for each metric, as determined for PC3 cells, 6h treatment (see Methods).

A



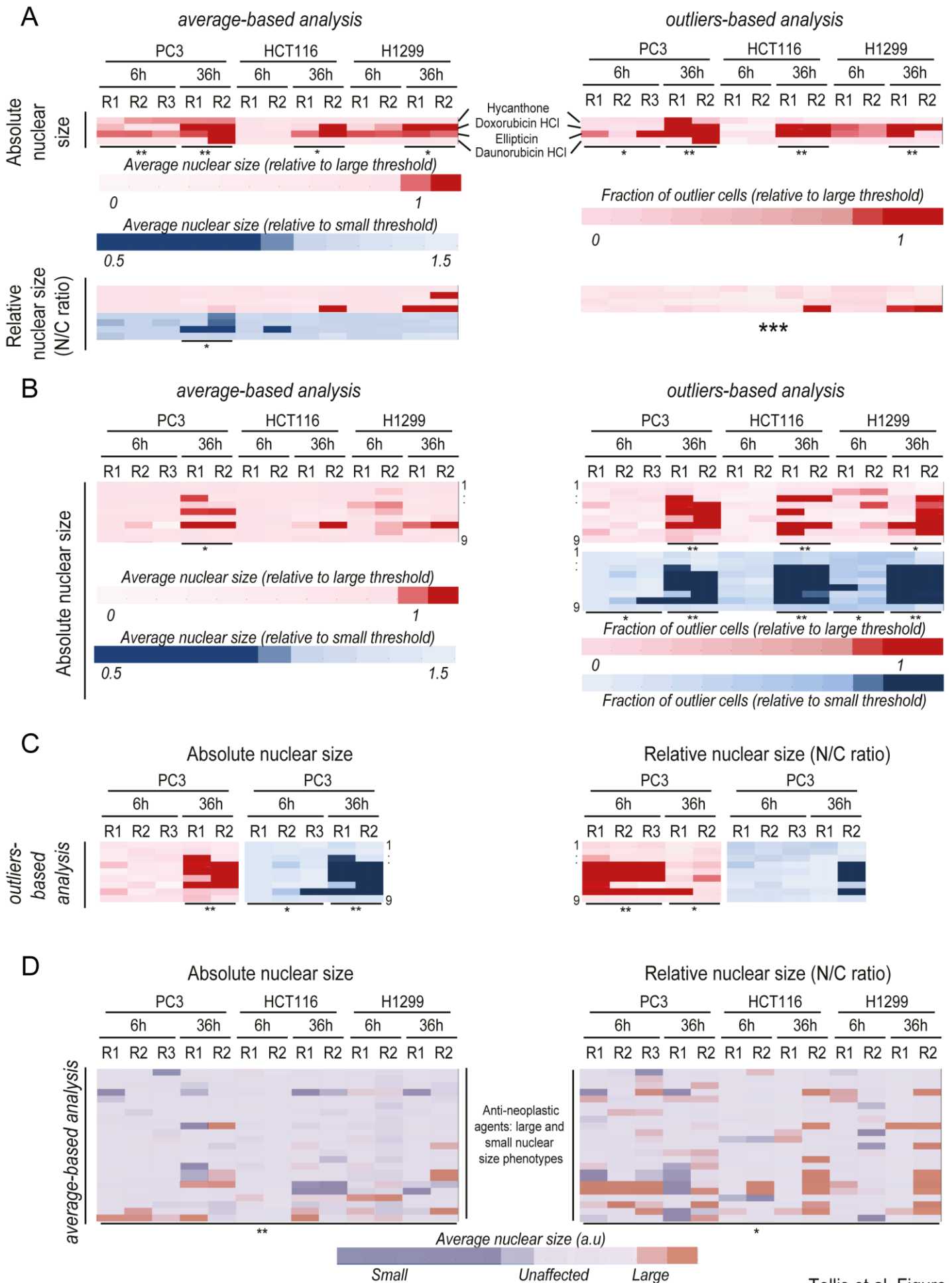
B



Tollis et al. Figure S2

**Supplementary Figure S2. Analysis methodology, but not the choice of metric, yielded overlapping results.**

A. Venn diagrams showing the overlap in compounds increasing (left diagrams, red) or reducing (right diagrams, blue) the absolute nuclear size, as determined by average-based (dark colours) or outlier-based (light colours) strategies as indicated. Overlaps in analysis methodologies were computed for PC3 (top), HCT116 (middle) and H1299 (bottom) cells treated for 6h or 36 h as indicated. B. Venn diagrams showing the overlap in compounds correcting cancer-related nuclear changes as determined using the average nuclear size (dark colours) vs average N/C ratio (light colours). Overlaps in hits determined using the two metrics were computed separately for PC3 (red), HCT116 (blue) and H1299 (yellow) cells treated for 6h (top row) or 36 h (bottom row) as indicated.



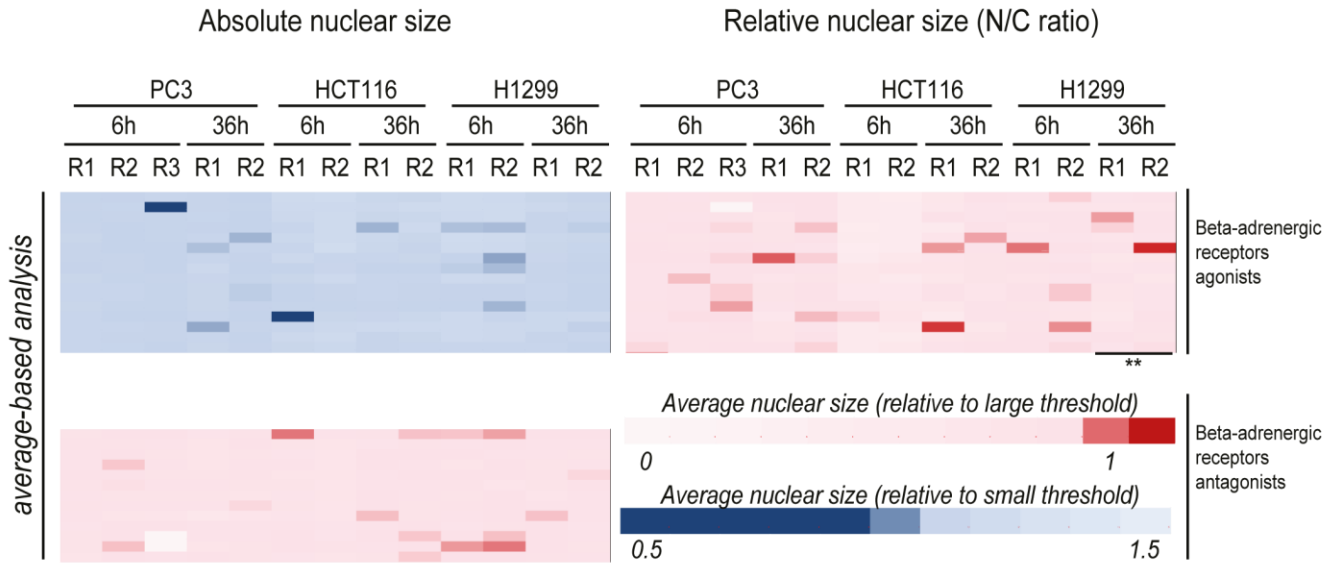


**Supplementary Figure S3. Comparison of absolute and relative nuclear size responses to different treatment duration informs on compound mechanism of action.**

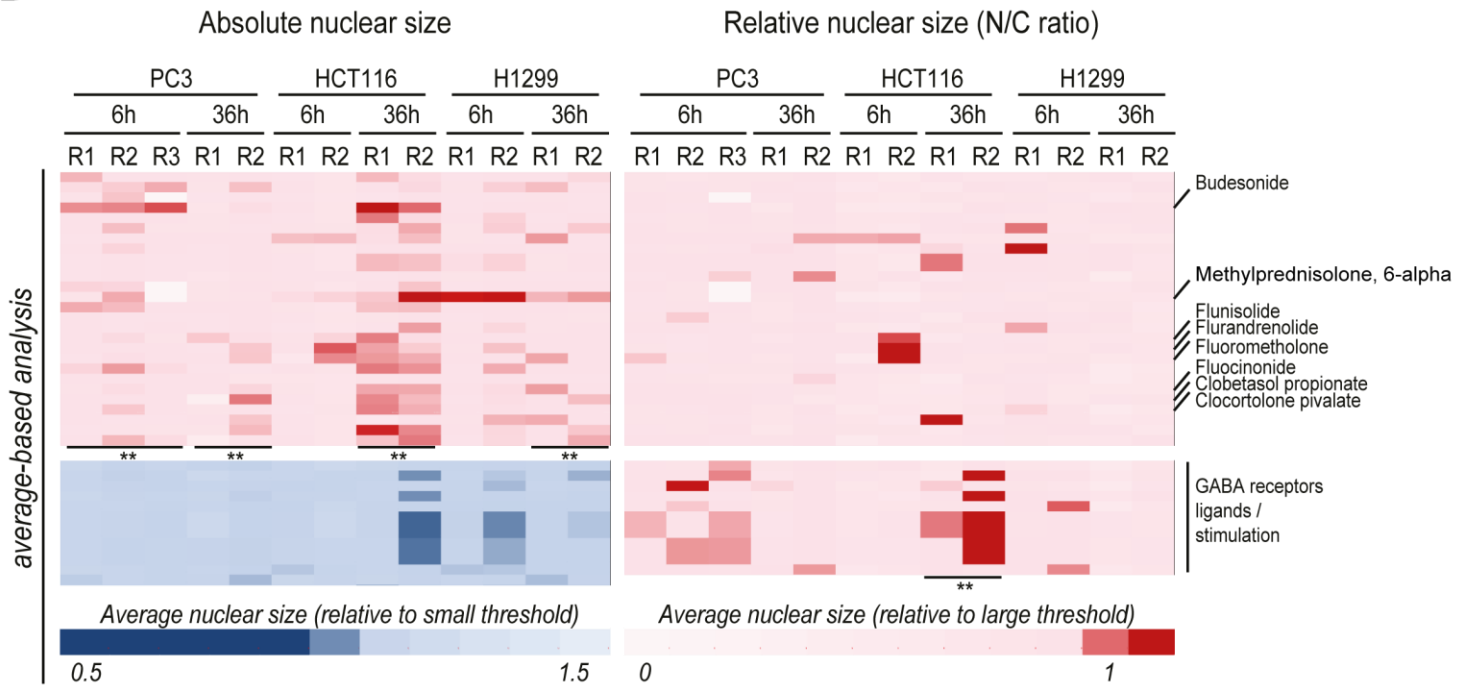
Class enrichment scores larger than 95% (resp. 99%) are indicated as \* (resp. \*\*) for compound classes of interest for specific phenotypes (i.e. cell line/time point/direction of nuclear size change). A. Heat maps showing nuclear size (top maps) and the N/C ratio (bottom maps) across tumour type/replicates (horizontal) treated with DNA intercalating agents (vertical), as determined by average-based analysis (left) and outliers-based analysis (right). Both averages, and the fractions of outlier cells for nuclear size and N/C ratio metrics were normalized to the detection thresholds for large/small nucleus or N/C ratio (see Methods), and colour-coded as indicated. Darker colours correspond to stronger phenotypes. Data for the fraction of outlier cells with abnormally small N/C ratio couldn't be determined due to renormalization issues (\*\*\*, see Methods). B. Heat maps showing absolute nuclear size across tumour type/replicates (horizontal) treated with microtubule poisons (vertical), as determined by outliers-based analysis (right) and average-based analysis (left). Compounds are indicated as numbers: 1-lumicolchicine  $\gamma$ , 2-tiabendazole, 3-fenbendazole, 4-colchicine; 5-nocodazole, 6-paclitaxel, 7-albendazole, 8-podophyllotoxin, 9-trimethylcolchicinic acid. Data normalization and colour-coding were performed similarly to panel (A). C. Heat maps showing absolute nuclear size (left) and relative nuclear size (N/C ratio, right) across PC3 replicates (horizontal) treated with microtubule poisons (vertical), as determined by outliers-based analysis. Compounds are numbered as on panel (B). Fractions of outlier cells data was normalized and colour-coded as indicated on panel (B). D. Heat maps showing the mean nuclear size (left) and the mean N/C ratio (right) across tumour type/replicates (horizontal) treated with all Prestwick compounds documented as antineoplastic. Nuclear size and N/C ratio have been normalized to both the detection thresholds for large (yielding a red heat map) and for small nucleus (yielding a blue heat map), both of which have been colour-coded as indicated. Then, both red and blue heat maps have been superimposed to yield the multi-colour heat map shown. Almost all antineoplastic agents affect the absolute nuclear size and/or the N/C ratio

in at least one condition as reflected by large class enrichment scores computed across all conditions.

A



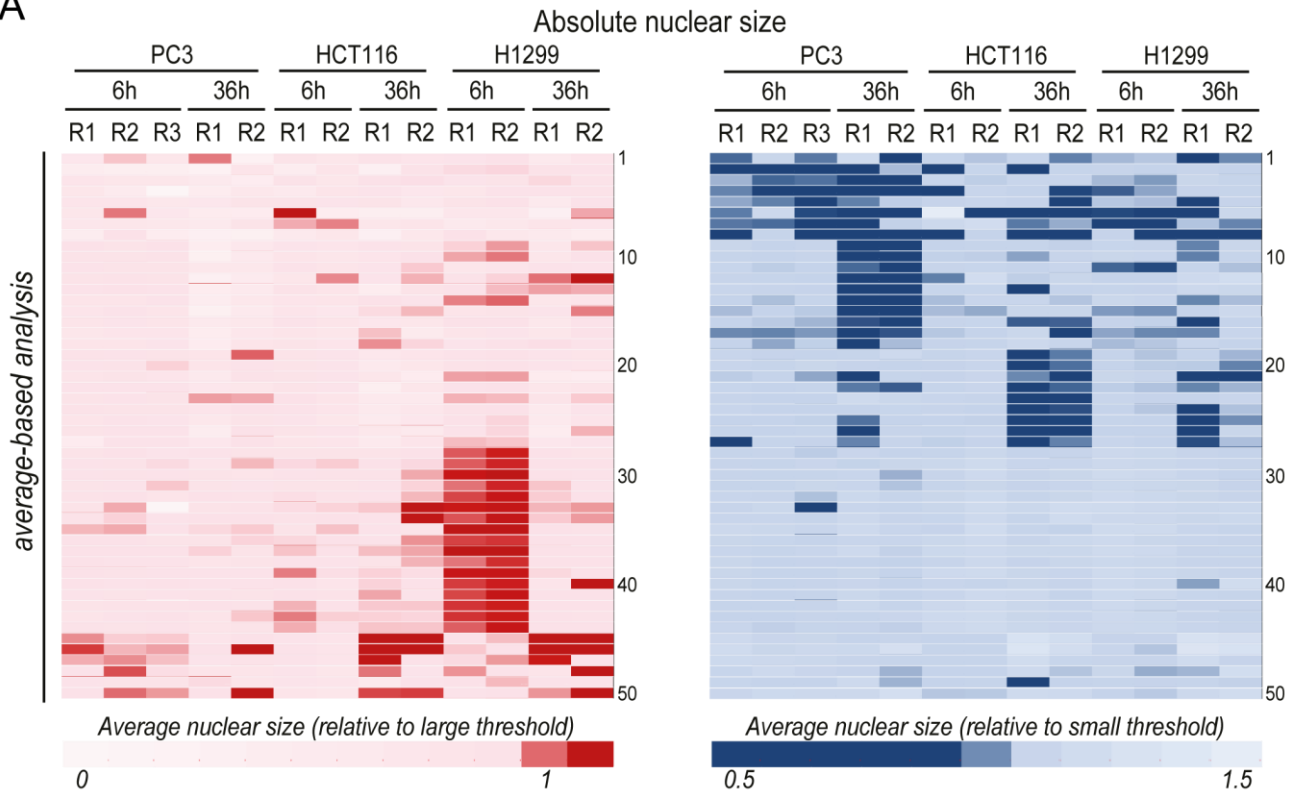
B



**Supplementary Figure S4. On the importance of knowing which of absolute or relative nuclear size actively contributes to metastasis.**

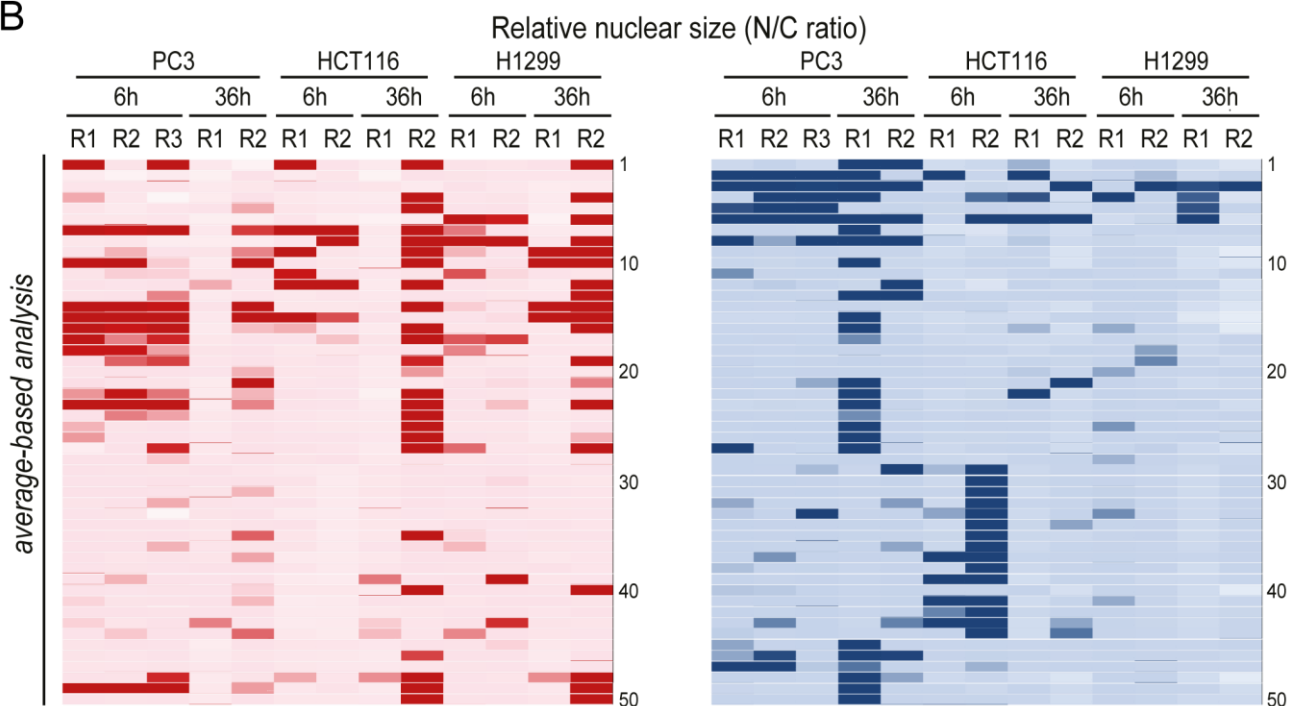
Class enrichment scores larger than 95% (resp. 99%) are indicated as \* (resp. \*\*) for compound classes of interest for specific phenotypes. A. Heat maps showing the mean nuclear size (left) and the mean N/C ratio (right) across tumour type/replicates (horizontal) treated with beta-adrenergic receptor agonists (top heat maps) or beta-adrenergic receptor antagonists (bottom heat map). Both heat maps show particular regions from Fig. 3, magnified for better visualization. Nuclear size and N/C ratio were normalized to the detection thresholds for large nucleus (red heat maps, see Methods), or for small nucleus (blue heat maps), and colour-coded as indicated. B. Heat maps showing the mean nuclear size (left) and the mean N/C ratio (right) across tumour type/replicates (horizontal) treated with glucocorticoids (top heat maps) or GABA receptor ligands/stimulators (bottom heat map). Nuclear size and N/C ratio were normalized to the detection thresholds for large nucleus or N/C (red heat maps, see Methods), or for small nucleus or N/C (blue heat maps), and colour-coded as indicated. Some compounds of particular interest are indicated on the side.

A



1	Disulfiram	14	Emetine di-HCl	27	Azacytidine 5	40	Proscillaridin A
2	Tomatine	15	Piperlongumine	28	Hydroflumethiazide	41	Etilefrin HCl
3	Astemizole	16	Lycorine HCl	29	Metaraminol bitartrate	42	Letrozole
4	Perhexiline maleate	17	Sertraline	30	Flufenamic acid	43	(+,-)-Synephrine
5	Ebselen	18	Paroxetin HCl	31	Trimethoprim	44	Verteporfin
6	Alexidine di-HCl	19	Danazol	32	Fenspiride HCl	45	Monobenzone
7	Cantharidin	20	Griseofulvin	33	Methylprednisolone 6- $\alpha$	46	Trifluridine
8	Oxyphenbutazone	21	Puromycin di-HCl	34	Debrisoquin sulfate	47	Antimycin A
9	Anisomycin	22	Resveratrol	35	Harmol HCl mono-H <sub>2</sub> O	48	Mitoxantrone di-HCl
10	Roxatidine acetate	23	Cilostazol	36	Metoxy-6-harmalan	49	Parbendazole
11	Metixene HCl	24	Eburnamonine	37	Levonordefrin	50	Camptothecine (S,+)
12	Parthenolide	25	Monensin Na salt	38	N-acetyl-L-leucine		
13	Prenylamine lactate	26	Dienestrol	39	(+)-Isoproterenol bitartrate		

B



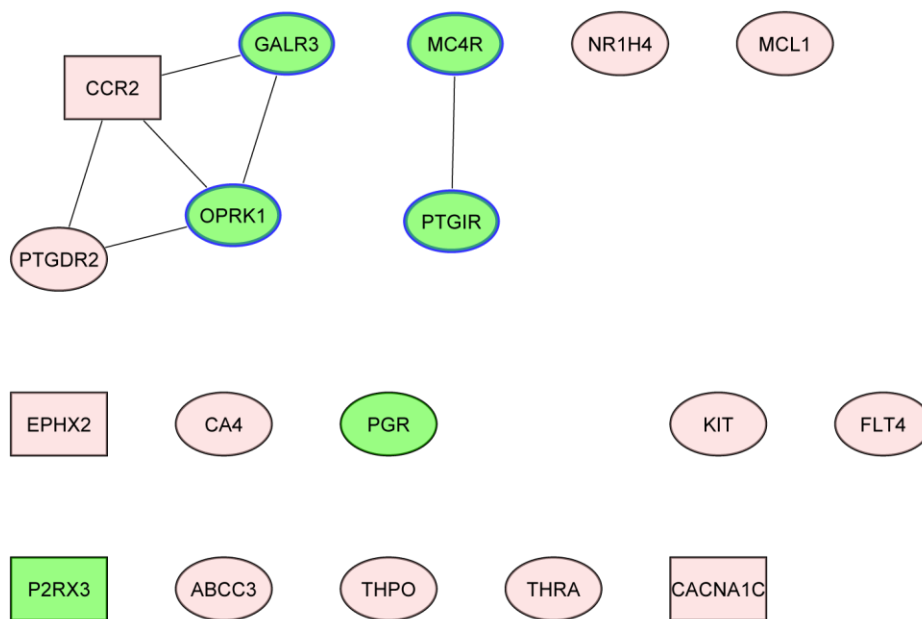
Tollis et al.  
Figure S5

**Supplementary Figure S5. Individual compounds spanning many pharmacological classes can correct cancer-associated nuclear size changes.**

A. Heat maps showing the mean nuclear size (A) and the mean N/C ratio (B) across tumour type/replicates (horizontal) treated with the Prestwick compounds (individual rows) that showed the strongest effects in one or several conditions (as listed in Table 1). For clarity, compounds are labeled with numbers on heat maps and listed in the Table shown on panel (A). Cell population-averaged nuclear size and N/C ratio have been normalized to both the detection thresholds for large (yielding a red heat map) and for small nucleus (yielding a blue heat map), and colour-coded as indicated.

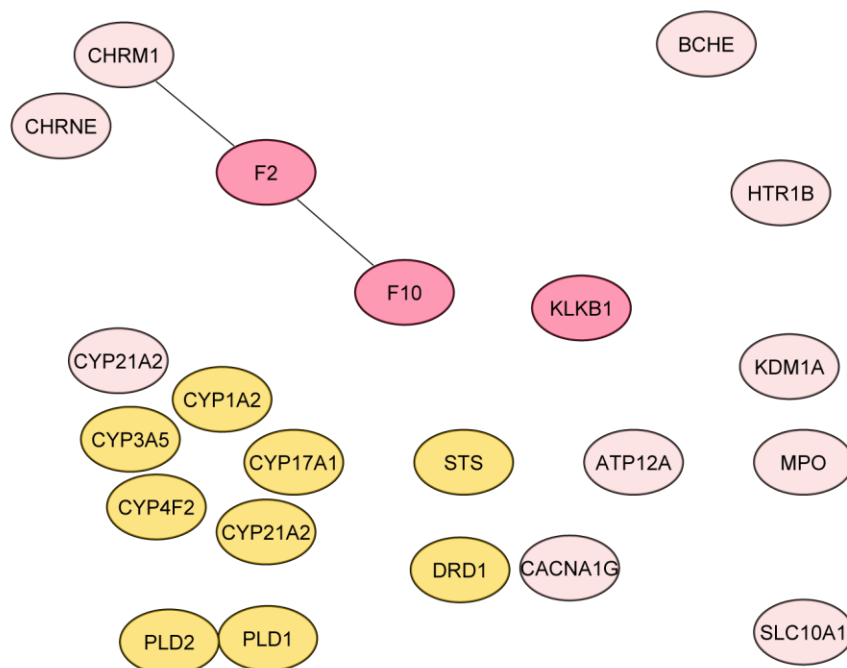
A

H1299-specific NSR target network



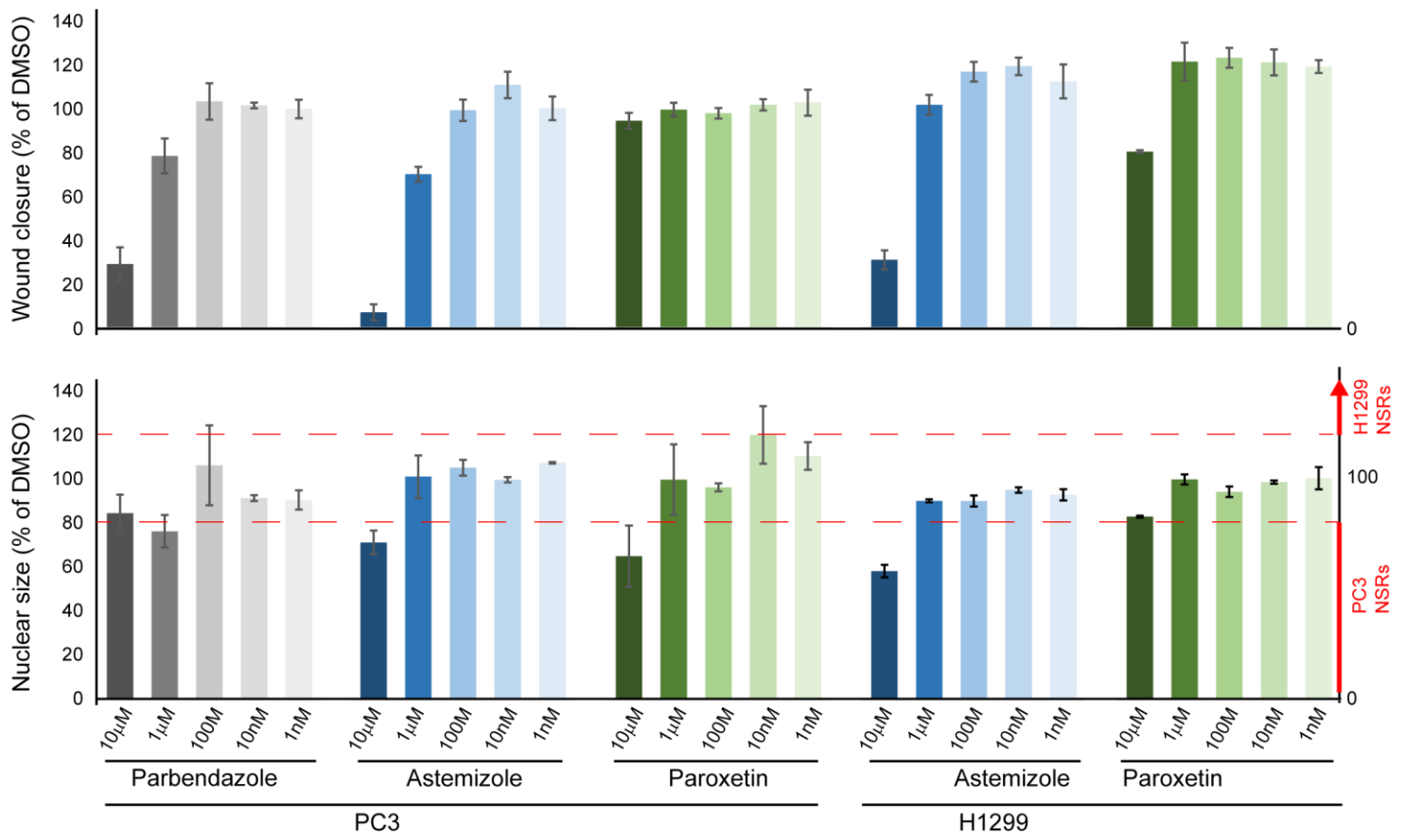
B

HCT116-specific NSR target network

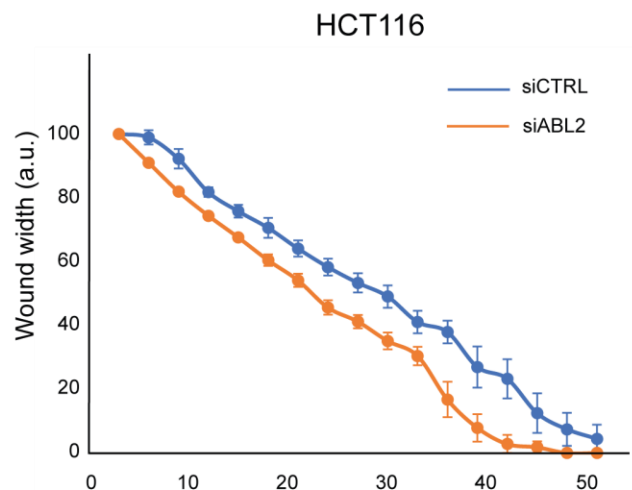
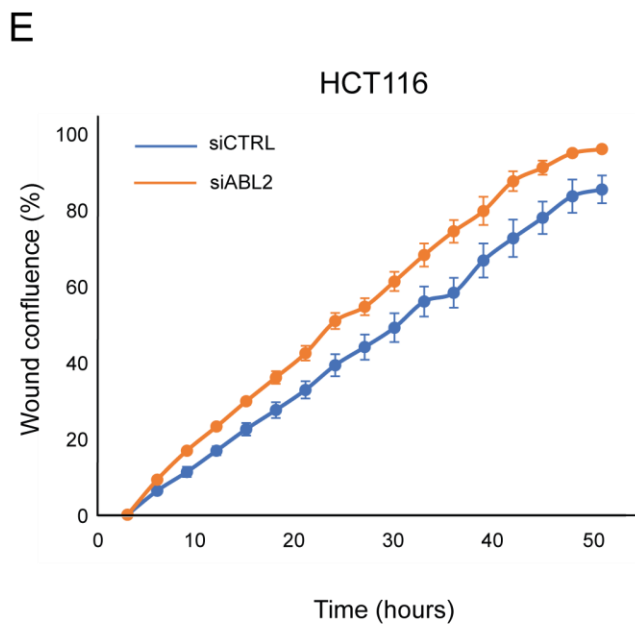
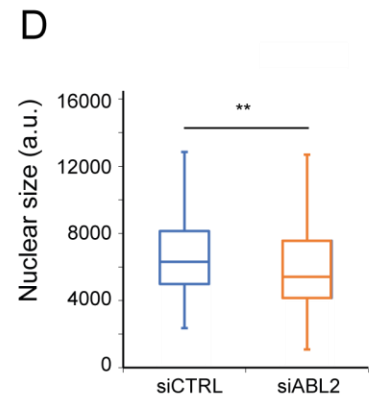
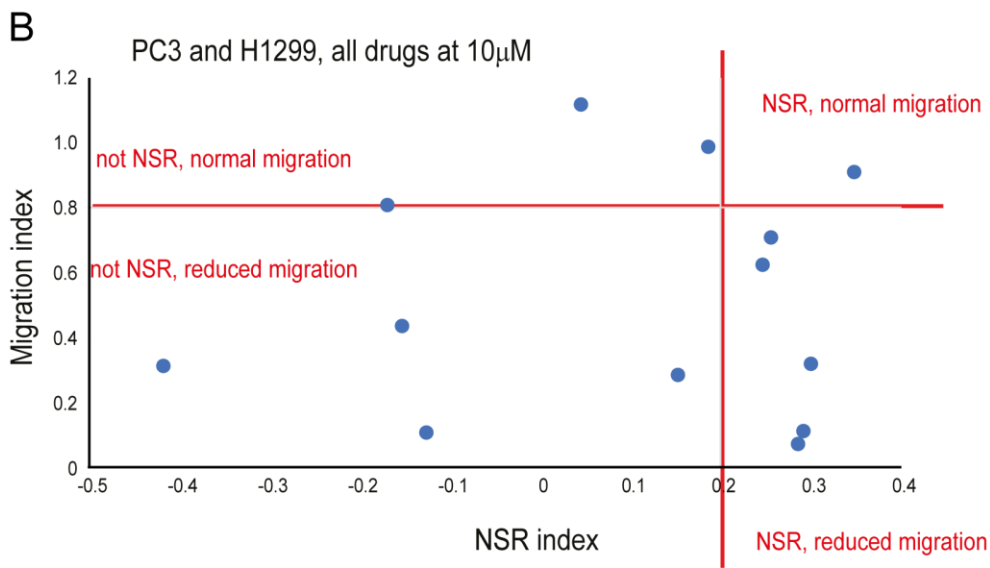
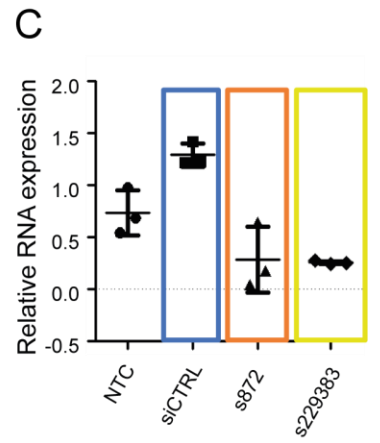
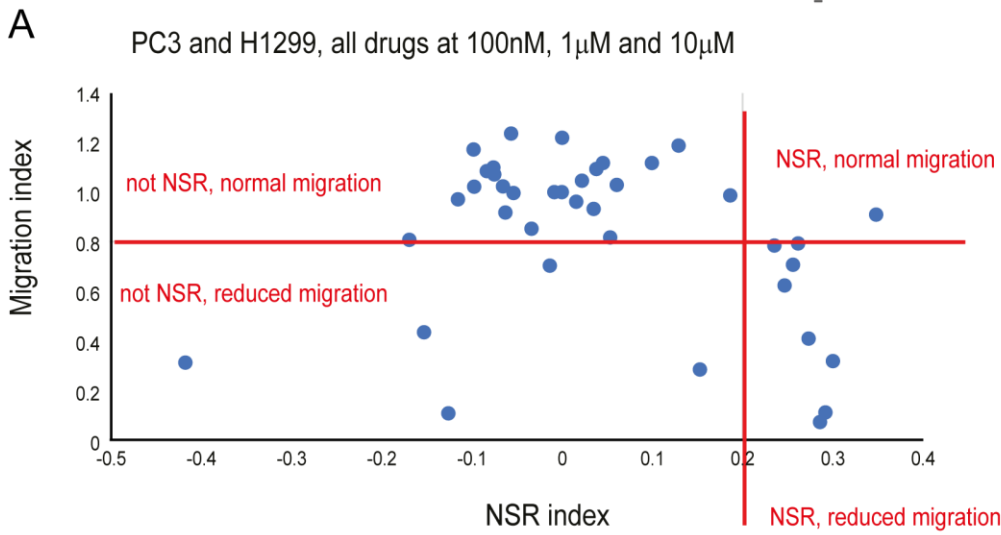


**Supplementary Figure S6. Cell line-specific NSRs target specific protein networks, additional data.** **a** Network targeted by H1299-specific NSRs. Only compounds that were not NSR in any condition in any of the two other cell lines were included. Default node colour is pink, default node shape is elliptic. Green nodes represent the cell-cell communication and signaling GO terms (7154; 7267); nodes circled in blue represent regulation of cAMP metabolic process (e.g. 30817; 30814) and of adenylate cyclase activity (e.g. 7194; 45761; 31279), and G-protein signaling, coupled to cyclic nucleotide second messenger (7187); Square nodes represent cellular ion homeostasis GO terms (6873; 6874). **b** Network targeted by HCT116-specific NSRs. Only compounds that were not NSR in any condition in any of the two other cell lines were included. Default node colour is light pink. Yellow nodes represent proteins belonging to the lipid metabolism/catabolism GO terms (6629; 16042), and dark red nodes the hemostasis GO term (7599).

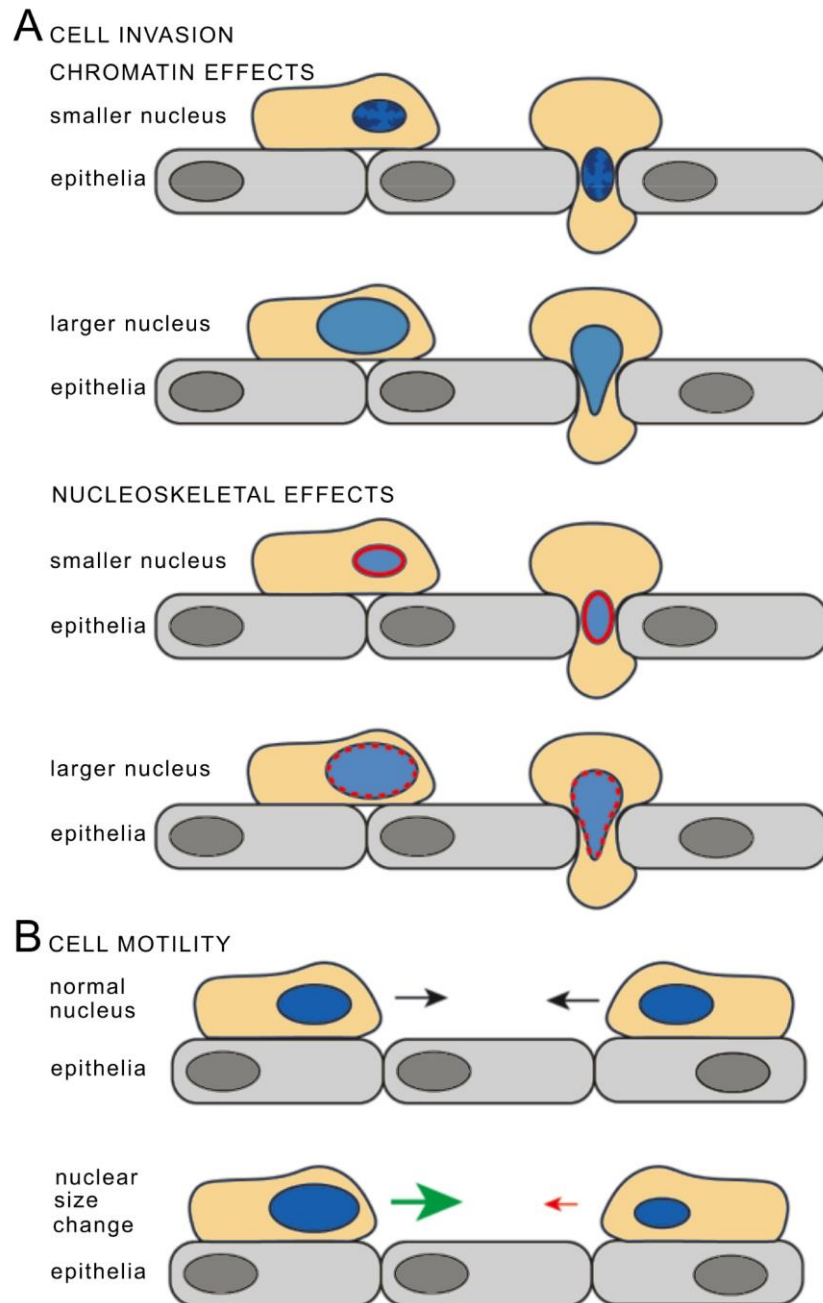


**A**

**Supplementary Figure S7. NSR compounds affecting nuclear size also affect cell migration, additional data. a** Wound healing assay. Top row: wound confluence, in % of the wound confluence of DMSO-treated control cells, for PC3 and H1299 cells treated with varying concentrations of Parabendazole, Astemizole and Paroxetine (from left to right) as indicated below the bottom row. Bottom row: average nuclear size, in % of the average nuclear size of DMSO-treated control cells, for PC3 and H1299 cells in the indicated conditions. Dashed red lines represent cutoff values for strong NSR phenotypes (see Supplementary Fig. S8a) for PC3 (20% reduction of nuclear size vs DMSO) and H1299 (20% increase of nuclear size vs DMSO).



**Supplementary Figure S8. Nuclear size rectification is a good predictor of cell migration impairment.** **a** Scatter plot showing the migration index (vertical) as a function of the NSR index (horizontal, see Methods) across PC3 and H1299 cell lines and all compound treatments at concentrations larger or equal to 100nM. 1 dot = 1 condition (cell line/compound /concentration). The vertical red line distinguishes the strong NSR phenotypes (NSR index>0.2), and the horizontal red line the migration phenotypes (migration index < 0.8 = reduced migration). The number of dots within each region delimited by the red lines was used to estimate the probability that a compound that is NSR at a given concentration, reduces migration at this concentration (see Methods). **c** Quantification of ABL2 expression at the mRNA level in presence of the indicated siRNAs in PC3 cells. **d** Whisker and Box plots showing the distribution of absolute nuclear size in PC3 cells treated with control siRNA (blue, N=132) and siABL2 (orange, N=354) as indicated, as determined by fluorescence microscopy (see Methods). The distribution of nuclear sizes in cells treated with siCTRL and siABL2 were compared using a Wilcoxon Rank test (\*\*: p=0.0013). **e** Wound healing assay in presence of siRNA-mediated ABL2 knock-out. Left and right plots show respectively the wound confluence and wound width normalized to the width at the first time-point, as a function of time for HCT116 cells, treated with 20 nM siCTRL (blue) and 20 nM siABL2 (orange). Data points show confluence and width values averaged over 8 replicates, and error bars represent the standard error on the mean.



**Supplementary Figure S9.** Model for how nuclear size changes may affect cancer cell invasiveness. **a** Chromatin effects on nuclear size and stiffness (top). For cell invasion through an epithelial layer, condensation of chromatin in a smaller nucleus could allow facile transit through a tight junction while looser chromatin in a larger nucleus could make the nucleus more malleable and also facilitate transit through a tight junction. Nucleoskeletal effects on nuclear size and stiffness (bottom). Reduced lamin A production might result in a smaller nucleus that could squeeze through tight junctions. Conversely scaling defects that cause a larger nucleus with lower lamin density would be more malleable to facilitate tight junction transit. **b** Cell motility may also be affected by nuclear size. Altered connections between the nucleoskeleton and cytoplasmic filaments in cells with larger or smaller nuclear size may influence cell mobility.

## Supplementary Tables legends:

**Supplementary Table 1.** Summary table showing the fraction of hits replicated once, twice or three times, using the two metrics and two analysis strategies introduced in the main text, and that yielded a p-value lower than 0.05 upon a compound vs DMSO Wilcoxon rank-test.

**Supplementary Table 2.** Effects across cell lines and duration of treatment of compounds identified as affecting the average absolute nuclear size in at least one condition.

**Supplementary Table 3.** Effects across cell lines and duration of treatment of compounds identified as affecting the average N/C ratio in at least one condition.

**Supplementary Table 4.** Effects across cell lines and duration of treatment of compounds identified as affecting the fractions of outlier cells with abnormally large or small nucleus in at least one condition.

**Supplementary Table 5.** Effects across cell lines and duration of treatment of compounds identified as affecting the fractions of outlier cells with abnormally large or small N/C ratio in at least one condition

**Supplementary Table 6.** Targets of NSR compounds. Sheet 1 lists all NSR and NSW compound targets from all cell lines and any analysis method. Sheet 2 lists specific nuclear size increasers and decreasers. Sheet 3 lists unique rectifier compound targets. Sheet 4 lists All PC3 NSR and NSW compound targets while sheet 5 lists those for compounds identified using any of the 4 measures. Sheets 6 and 7 respectively list All and Any for the HCT116 cell line and sheets 8 and 9 for H1299s. Sheet 10 lists the ChEMBL target hit count. Sheet 11 lists the number of compounds in the screen that hit a particular target. Sheet 12 lists the known targets of each compound.

**Supplementary Table 7.** Compounds tested in detail with chemical structures.

**Supplementary Table 1 :**

<b>Metric</b>	<b>Analysis strategy</b>	<b>% of 1-rep hits with p&lt;0.05</b>	<b>% of 2-rep hits with p&lt;0.05</b>	<b>% of 3-rep hits with p&lt;0.05</b>
Nuclear size	Average	80,6	66,7	100
Nuclear size	Outliers	16,3	87,5	100
N/C ratio	Average	40	93,3	100
N/C ratio	Outliers	38,6	88,9	100



Supplementary Table 2

Compound	Chemical name	Therapeutic group	Mechanism/class	Hit PC3 6h	Hit PC3 36h	Hit HCT116 6h	Hit HCT116 36h	Hit H1299 6h	Hit H1299 36h
Plate09A09	Betonidine	-	-			-			
Plate09F02	Fillalbin	-	-					-	
Plate07A02	Serotonin hydrochloride	Neurotransmitter	5HT agonist			-			
Plate09C09	Skimmianine	Sedative	5HT ligand			-			
Plate07D02	Fluoxetine hydrochloride	Antidepressant	5HT uptake inhibitor		-				
Plate09F03	Citalopram Hydrobromide	Antidepressant	5HT uptake inhibitor	-				-	
Plate11F02	Paroxetine Hydrochloride	Antidepressant	5HT uptake inhibitor		-				
Plate13F05	Sertraline	Antidepressant	5HT uptake inhibitor		-		-		
Plate06B03	Anisomycin	Antiprotozoal	Acetylcholine esterase inhibitor		-				
Plate14E03	(-)-Eseroline fumarate salt	Potent analgesic	Acetylcholine esterase inhibitor		-				
Plate10E09	Vidarabine	Antiviral	Adenosine antimetabolite	+	+		-		+
Plate01D05	Triamterene	Diuretic	Aldosterone antagonist (non competitive)		+				
Plate09D09	Ricinine		Alkaloid			-			
Plate08E05	Piperlongumine	Antifungal	Alkaloid		-				
Plate08E08	Eburnamonine (-)	Cerebral vasodilator	Alkaloid				-		-
Plate14E09	(+,-)-Synephrine	Adrenergic	Alpha adrenergic agonist					+	
Plate03D08	Metaraminol bitartrate	Vasoconstrictor	alpha Adrenergic agonist					+	
Plate13F08	Etilefrine hydrochloride	Antihypertensive	Alpha Adrenergic agonist (alpha1)					+	
Plate13H09	Methyldopate hydrochloride	Antihypertensor	Alpha Adrenergic agonist (alpha2)		-				
Plate10B10	Levonordefrin	Vasoconstrictor	Alpha Adrenergic agonist (alpha2)					+	
Plate10D02	Terazosin hydrochloride	Antihypertensor	Alpha adrenergic antagonist		-				
Plate09F09	Tetrahydrozoline hydrochloride	Vasoconstrictor	Alpha adrenergic ligand			-		-	
Plate08H03	Dipivefrin hydrochloride	Adrenergic (ophthalmic)	alpha beta Agrenergic agonist				+	+	
Plate10G08	Merbromin	Antibacterial	Antibacterial			+			
Plate12H06	Florfenicol	Antibacterial	Antibacterial					-	
Plate13A11	Roxarsone	Antibacterial	Antibacterial	-					
Plate09A03	Epicatchin(-)	Antidiarrhoeic	Antidiarrhoeic	-					
Plate14G11	Parbendazole	Anthelmintic (VET)	Anthelmintic				-		
Plate13H11	Pyruvium pamoate	Anthelmintic (Nematodes, enterobiasis)	Anthelmintic	-	-				
Plate10A02	Althiazide	Antihypertensor	Antihypertensor		-				
Plate13H02	Halofantrine hydrochloride	Antimalarial	Antimalarial		-				
Plate07A04	Azathymine, 6	Anticancer	Antimetabolite			-			
Plate11G07	Azacytidine-5	Antineoplastic	Antimetabolite	-			-		-
Plate06H11	Puromycin dihydrochloride	Antiprotozoal	Antimetabolite		-		-		-
Plate10E06	Ethoxyquin	Antifungal	Antioxydant		-				
Plate14A09	Piperacetazine	Antipsychotic	Antipsychotic				-		
Plate14B05	Levopropoxyphene napsylate	Antitussive	Antitussive				-		
Plate09G11	Strophanthidin	Cardiotonic	ATPase inhibitor					+	+
Plate08G02	Methoxy-6-harmalan	Psoriasis treatment	Benzodiazepine receptor ligand					+	
Plate03D09	Salbutamol	Bronchodilatator	Beta adrenergic agonist			+		+	
Plate04E03	Fenoterol hydrobromide	Bronchodilatator	Beta adrenergic agonist	-			+	+	
Plate05C06	Clenbuterol hydrochloride	Bronchodilatator	Beta adrenergic agonist					+	
Plate07C06	Metaproterenol sulfate, orciprenaline sulfate	Bronchodilatator	Beta adrenergic agonist				+		
Plate10C10	Isoetharine mesylate salt	Bronchodilator	Beta adrenergic agonist					+	

Plate14F08	(-)-Isoproterenol hydrochloride	Bronchodilator	Beta adrenergic agonist						+	
Plate05D03	Dobutamine hydrochloride	Bronchodilator	Beta adrenergic agonist (beta1)						+	
Plate05H02	Terbutaline hemisulfate	Bronchodilator	Beta adrenergic agonist (beta2)			-			+	
Plate12G06	Salmeterol	Bronchodilator	Beta adrenergic agonist (beta2)				+		+	
Plate05C10	Ritodrine hydrochloride	Tocolytic	Beta adrenergic agonist (beta2)						+	
Plate12G10	(+,-)-Octopamine hydrochloride	Adrenergic	Beta adrenergic agonist (beta3)						+	
Plate05G03	Betaxolol hydrochloride	Antihypertensor	Beta adrenergic antagonist						-	
Plate14A04	Penbutolol sulfate	Antihypertensor	Beta adrenergic antagonist			-				
Plate12H03	Propranolol hydrochloride	Antianginal	Beta adrenergic blocker						-	
Plate07F07	(S)-(-)-Atenolol	Antihypertensor	beta adrenergic blocker						+	
Plate14B08	Oxprenolol hydrochloride	Antihypertensor	Beta adrenergic blocker			+				
Plate12H04	(R)-(+)-Atenolol	Antihypertensor	Beta adrenergic blocker (beta1)						-	
Plate03F04	Fenspiride hydrochloride	Antiinflammatory	Bradykinin antagonist						+	
Plate12D02	(+)-Isoproterenol (+)-bitartrate salt	Bronchodilator	Bronchodilator						+	
Plate05E09	Bepidil hydrochloride	Antianginal	Ca2+ channel blocker			-				
Plate09D03	(d,l)-Tetrahydroberberine	Sedative	Ca2+ channel blocker	-						
Plate04E07	Perhexiline maleate	Vasodilatator	Ca2+ channel blocker	-	-	-	-	-	-	
Plate06H09	Felodipine	Antihypertensor	Ca2+ channel blocker (L-Type)			-				
Plate07H11	Prenylamine lactate	Vasodilatator	Ca2+ channel stimulation			-		-		
Plate13C07	Proscillaridin A	Cardiotonic	Cardiac glycoside						+	+
Plate05F03	Debrisoquin sulfate	Antihypertensor	Catecholamine depletor					+	+	
Plate07G02	Ciclopirox ethanolamine	Antifungal	Cell membrane proteins synthesis inhibitor					+		+
Plate14H09	Cefepime hydrochloride	Antibacterial	Cell wall destruction agent						+	
Plate06G11	Ceforanide	Antibacterial	Cell wall synthesis inhibitor	-						
Plate14D09	Benzylpenicillin sodium	Antibacterial	Cell wall synthesis inhibitor						+	
Plate10A06	Deferoxamine mesylate		chelating agent					+		+
Plate03E03	Tiratricol, 3,3',5-triiodothyroacetic acid	Hypocholesterolemic drug	Cholesterol downregulation					+		+
Plate12H09	Urosiol	Anticholelithogenic	Cholesterol regulation						-	
Plate07B02	Metixene hydrochloride	Antiparkinsonian	cholinergic inhibition			-			-	
Plate09G02	Trihexyphenidyl-D,L Hydrochloride	Antiparkinsonian	cholinergic inhibition						-	
Plate02C08	Tomatine	Antifungal	Cholinergic inhibition	-	-	-	-			
Plate10C02	Nadide	-	CoA nicotinamide adenine dinucleotide			-				
Plate07D07	Lovastatin	Antihypercholesterolemic	CoA reductase inhibitor (HMG CoA)			-				
Plate13A10	3-Acetamidocoumarin	Antiinflammatory	coumarin	-						
Plate03E04	Flufenamic acid	Analgesic	cyclooxygenase inhibition						+	
Plate03E06	Tolfenamic acid	Antiinflammatory	cyclooxygenase inhibition						-	
Plate07C09	Resveratrol	Antiinflammatory	cyclooxygenase inhibition			-		-		
Plate10A03	Isopyrin hydrochloride	Antiinflammatory	cyclooxygenase inhibition							+
Plate10B11	Ebselen	Antiinflammatory	cyclooxygenase inhibition	-				-		-
Plate10H02	(R) -Naproxen sodium salt	Antiinflammatory	cyclooxygenase inhibition			-				+
Plate11B07	Suprofen	Antiinflammatory	cyclooxygenase inhibition	-						
Plate11D07	Indoprofen	Antiinflammatory	cyclooxygenase inhibition	-						
Plate11F07	Tolmetin sodium salt dihydrate	Antiinflammatory	cyclooxygenase inhibition	-						

Plate13E04	Azapropazone	Anti-inflammatory	cyclooxygenase inhibition		-				
Plate14A10	Oxyphenbutazone	Anti-inflammatory	cyclooxygenase inhibition	-	-	-	-	-	-
Plate09G06	Methyl benzethonium chloride	Antibacterial	Detergent				-		
Plate09G09	Benzethonium chloride	Antibacterial	Detergent			-			
Plate10F08	Alexidine dihydrochloride	Antibacterial	Detergent	-	-	+/-	-	-	-
Plate10H03	Propidium iodide	Antibacterial	Detergent						+
Plate02G09	Canrenoic acid potassium salt	Antihypercholesterolemic	Detergent						-
Plate02G04	Chlorhexidine	Bacteriostatic	Detergent						+
Plate12E06	Thonzonium bromide		Detergent		-		-		
Plate14F05	Sulfadoxine	Antibacterial	dihydropteroate synthase inhibitor				-		
Plate07H06	Nifuroxazide	Antibacterial	DNA damage (bacterial)						+
Plate01D11	Nicosamide	Anthelmintic	DNA damage (Helminthic)		-				
Plate06D09	Doxorubicin hydrochloride	Antibacterial	DNA intercalating agent		+		+		+
Plate08F05	Ellipticine	Anticancer	DNA Intercalating agent	+	+		+	+	+
Plate07A08	Daunorubicin hydrochloride	Antineoplastic	DNA intercalating agent		+/-				
Plate14B07	Trifluridine	Antiviral (ophthalmic)	DNA replication inhibitor (viral)	+	+		+		+
Plate08G09	Salsolinol hydrobromide	-	Dopamine analog					+	
Plate06F02	Alizapride HCl	Antiemetic	Dopamine antagonist		+/-				+
Plate08E02	Scoulerine	Antiemetic	Dopamine antagonist		+		-		
Plate09G05	Bromopride	Antiemetic	Dopamine antagonist					-	
Plate07C10	Bromperidol	Antipsychotic	Dopamine antagonist				-		
Plate09F04	Promazine hydrochloride	Antipsychotic	Dopamine antagonist					-	
Plate04G09	Pimozide	Antipsychotic	Dopamine antagonist ?	-			-		
Plate02B08	Disulfiram	Alcohol deterrent	Dopamine beta hydroxylase inhibitor	-	-				-
Plate05G07	GBR 12909 dihydrochloride	Antidepressant	Dopamine uptake inhibitor	+			-		
Plate03G07	Griseofulvin	Antifungal	Enzymatic inductor				-		
Plate11A11	Sulconazole nitrate	Antifungal	Ergosterol synthesis inhibition	-					
Plate11G11	Luteolin	Expectorant	Flavonoid		+		+		
Plate10B09	Folinic acid calcium salt	Antianemic	Folic acid antagonist				-		
Plate03E09	Trimethoprim	Antibacterial	Folic acid antagonist					+	
Plate01D08	Pyrimethamine	Antiprotozoal	Folic acid antagonist		+		+		+
Plate09G03	Succinylsulfathiazole	Antibacterial	Folic acid synthesis inhibition	-				-	
Plate09H02	Sulfabenzamide	Antibacterial	Folic acid synthesis inhibition			+			
Plate10B02	Sulfaquinoxaline sodium salt	Antibacterial	Folic acid synthesis inhibition		-				
Plate10A09	Sulfadimethoxine	Antibacterial	Folic acid synthesis inhibitor				-		
Plate08A10	Dihydroergotoxine mesylate	Anticonvulsant	GABA A receptor Cl-channel high affinity		-				
Plate07F10	Thiocolchicoside	Muscle relaxant	GABA agonist ?				+		
Plate09C03	Gelsemine	Tumour inhibitor	GABA antagonist	-					
Plate09B03	Picrotoxinin	Analeptic	GABA channel blocker	-					
Plate13E03	Alfaxalone	In combination with alfadolone acetate as anesthetic (intravenous)	GABA receptor stimulation				-		
Plate13E02	Alfadolone acetate	In combination with alfaxalone as anesthetic (intravenous)	GABA receptor stimulation				-		
Plate07D09	Budesonide	Antiinflammatory	Glucocorticoid	+			+		
Plate04D10	Methylprednisolone, 6-alpha	Glucocorticoid	Glucocorticoid	-			+	+	
Plate09A06	Flurandrenolide	Glucocorticoid	Glucocorticoid			+			
Plate09H09	Fluorometholone	Glucocorticoid	Glucocorticoid			-			

Plate10G02	Clobetasol propionate	Glucocorticoid	Glucocorticoid		-				
Plate14A05	Prednicarbate	Glucocorticoid (topical)	Glucocorticoid				-		
Plate08B03	Mometasone furoate	Antiinflammatory	glucocorticoid receptor agonist				+		
Plate10F02	Alclometasone dipropionate	Anti-inflammatory	glucocorticoid receptor agonist		-				
Plate03F08	Mebendazole	Parasite suppressor	Glucose transport inhibitor ?		+				
Plate02E07	Mefloquine hydrochloride	Antimalarial	Heme polymerase inhibitor		-		-		
Plate06H07	Primaquine diphosphate	Antimalarial	Heme polymerase inhibitor		-		+		+
Plate10H08	Methotrimeprazine maleat salt	Analgesic	Histamine antagonist			+			
Plate10H04	Cloperastine hydrochloride	Antitussive	Histamine antagonist						-
Plate07C11	Cyclizine hydrochloride	Antiemetic	Histamine antagonist (H1)				-		
Plate02F07	Astemizole	Antihistaminic	Histamine antagonist (H1)	-	-				
Plate07C04	Cetirizine dihydrochloride	Antihistaminic	Histamine antagonist (H1)				-		
Plate13F04	Deptropine citrate	Antihistaminic	Histamine antagonist (H1)		-				
Plate06C09	Roxatidine Acetate HCl	Antiulcerative	Histamine antagonist (H2)		-				
Plate14D05	Cyproterone acetate	Antiandrogen	hormone antiandrogen				-		
Plate09E09	Estropipate	Estrogen	Hormone estrogen			-			
Plate10D07	Diethylstilbestrol	Estrogen	Hormone estrogen		+		-		
Plate11E07	Ethinylestradiol 3-methyl ether	Estrogen	Hormone estrogen	-					
Plate05H08	Clomiphene citrate (Z,E)	Antineoplastic	hormone Estrogen agonist		-				
Plate02C06	Danazol	Antigonadotropin	hormone Estrogen antagonist		+		-		
Plate12H07	Megestrol acetate	Progestogen	Hormone progestogen					-	
Plate07H07	Mycophenolic acid	Antineoplastic	Inosine monophosphate dehydrogenase inhibitor		-				+
Plate02E03	Metanephrine hydrochloride DL		Isoprenaline uptake inhibitor extraneuronal			+		+	
Plate07H05	Tolazamide	Antidiabetic	K+ channel blocker (ATP-dependent channels)					+	
Plate03C11	Tolbutamide	Hypoglycemic	K+ channel blocker (ATP-dependent channels)	+			+		+
Plate08F03	Harmol hydrochloride monohydrate	Anxiolytic	Liver conjugation probe					+	
Plate11H07	Arcaine sulfate		Lowers blood sugar	-					
Plate12A04	Digoxigenin	Diagnosis	Mainly used as a non-isotopic label for DNA					+	
Plate03A11	Phenelzine sulfate	Antidepressant	MAO inhibitor	-					
Plate10H06	Isocarboxazid	Antidepressant	MAO inhibitor				-		
Plate08F04	Harmine hydrochloride	Anthelmintic	MAO inhibitor		+				
Plate04H09	Quinacrine dihydrochloride dihydrate	Antimalarial	MAO inhibitor	-			-		+
Plate07G11	Parthenolide	Antiinflammatory	MAPK inhibitor		-				+
Plate06B05	Apigenin	Antiproliferative	MAPK inhibitor		+			+	
Plate12D03	Monobenzone	Depigmentor	melanin inhibition				+		+
Plate09A07	Helveticoside	Cardiotonic	membrane ATP inhibitor					+	
Plate10C09	Monensin sodium salt	Antibacterial	Membrane ionophores producer		-		-		-
Plate03E11	Fenbendazole	Anthelmintic	microtubule polymerisation inhibitor		+				-
Plate05E04	Colchicine	Antiinflammatory	microtubule polymerisation inhibitor				-		-
Plate02B11	Nocodazole	Antineoplastic	microtubule polymerisation inhibitor		+		-		
Plate02H06	Paclitaxel	Antineoplastic	microtubule polymerisation inhibitor				-		-

Plate04A08	Albendazole		microtubule polymerisation inhibitor	-	+		+		+
Plate10G03	Podophyllotoxin	Antiviral	microtubule polymerisation inhibitor				-		
Plate12H08	Deoxycorticosterone	Mineralocorticoid	Mineralocorticoid					-	
Plate03G03	Antimycin A	Antifungal	Mitochondrial electron transport inhibitor				+		+
Plate14C05	Mepylcaine hydrochloride	Local anesthetic	Momoamine transport inhibition				-		
Plate09D07	Beta-Escin	Peripheral vascular disorders	Momoamine transport inhibition		-				
Plate14B06	Piperidolate hydrochloride	Antispasmodic	Muscarinic blocking agent		+				
Plate09H03	Benzocaine	Anesthetic	Na+ channel blocker	-		+			
Plate10E02	Butamben	Anesthetic	Na+ channel blocker		-				
Plate03D10	Prilocaine hydrochloride	Local anesthetic	Na+ channel blocker		+				+
Plate10G09	Hexylcaine hydrochloride	Local anesthetic	Na+ channel blocker				-		
Plate09H07	Pramoxine hydrochloride	Local anesthetic	Na+ channel inhibitor (voltage-dependent)			+			
Plate12H10	Proparacaine hydrochloride	Topical anesthetic (ophthalmic)	Na+ channel inhibitor (voltage-dependent)					-	
Plate01B04	Hydroflumethiazide	Antihypertensor	Na+ Cl- transport inhibitor					+	
Plate03F11	Indapamide	Antihypertensor	Na+ Cl- uptake inhibitor		+				
Plate06D07	Digitoxigenin	Cardiotonic	Na+ K+ ATPase inhibitor				-	+	+
Plate06D08	Digoxin	Cardiotonic	Na+ K+ ATPase inhibitor				+	+	+
Plate06H02	Strophantine octahydrate	Cardiotonic	Na+ K+ ATPase inhibitor					+	+
Plate09B07	Lanatoside C	Cardiotonic	Na+ K+ ATPase inhibitor					+	+
Plate03F03	Pyrantel tartrate	Anthelmintic	Neuromuscular depolarizing agent		+				
Plate09E03	beta- Belladonnine dichloroethylate	Muscle relaxant	Nicotinic receptor ligand	-					
Plate11A07	Trimipramine maleate salt	Antidepressant	Noradrenaline uptake inhibitor	-					
Plate09G04	Famprofazone	Analgesic	NSAI					-	
Plate14G05	Clonixin Lysinate	Analgesic	NSAI				-		
Plate09B09	Suxibuzone	Antiinflammatory	NSAI			-			
Plate11C07	Oxalamine citrate salt	Antiinflammatory	NSAI	-					
Plate09F10	Hexestrol	Estrogen antineoplastic	Nuclear receptor ligand					-	
Plate10H09	Dienestrol	Non-steroidal estrogen	Nuclear receptor ligand		-		-		-
Plate13G06	Letrozole	Antineoplastic	P450 inhibitor					+	
Plate10F09	Proadifen hydrochloride	Local anesthetic	P450 inhibitor (mono-oxygenases)	-	-		-		
Plate05G10	Ketoconazole	Antifungal	P450 inhibitor (P450c17)				-	-	
Plate08C08	Cilostazol	Antithrombotic	Phosphodiesterase inhibitor				-		
Plate14H05	Saquinavir mesylate	Antiviral (HIV)	Protease inhibitor				-		
Plate02G07	Tamoxifen citrate	Anticancer	Protein kinase C inhibitor						+
Plate08A11	Emetine dihydrochloride	Antiamoebic	Protein synthesis inhibitor		-			+	
Plate10G11	Cycloheximide	Antibacterial	Protein synthesis inhibitor		-				
Plate09E07	Lycorine hydrochloride	Antitumoral	Protein translation inhibitor		-		-		-
Plate13E09	Gabexate mesilate	Severe acute pancreatitis	Proteinase inhibitor				-		
Plate05H05	Kanamycin A sulfate	Antibacterial	Ribosomal protein synthesis inhibitor			+			
Plate10D09	Ribostamycin sulfate salt	Antibacterial	Ribosomal protein synthesis inhibitor				-		
Plate12H02	Crotamiton	Scabicide	Scabicide					-	
Plate13F10	Tribenoside	Sclerosing agent	Sclerosing agent	-	-		-		
Plate12A06	Cantharidin	Rubefiant	Serine protease releaser	-	-		-	-	
Plate05G08	Carbetapentane citrate	Antitussive	Sigma1 receptor ligand				-	-	
Plate10G10	Drofenine hydrochloride	Spasmolytic	Spasmolytic				-		
Plate02E08	Isoconazole	Antibacterial	Sterol 14-demethylase inhibitor		-				

Plate03D11	Camptothecine (S,+)	Antitumor agent	Topoisomerase I inhibitor		+		+		+
Plate14F09	Kaempferol	Anti-inflammatory	Topoisomerase I inhibitor		+				
Plate05G06	Mitoxantrone dihydrochloride	Antineoplastic	topoisomerase II inhibitor	+					+
Plate05H07	Etoposide	Antineoplastic	Topoisomerase II inhibitor	+	+		+		
Plate09F11	Cefmetazole sodium salt	Antibacterial	transpeptidase inhibitor (bacterial)					-	
Plate14G06	Verteporfin	Treatment of age-related macular degeneration	Treatment of age-related macular degeneration					+	
Plate11H10	Capsaicin	Topical analgesic	Vanilloid receptor ligand		+				
Plate06C02	Suloctidil	Vasodilatator	Vasodilatator		-				
Plate12B07	N-Acetyl-L-leucine	Vertigo	Vertigo					+	
Plate08H05	Riboflavine	Vitamin	Vitamin					+	
Plate06F10	Menadione	Vitamin K3	Vitamin precursor		+/-				
Plate09F08	3-alpha-Hydroxy-5-beta-androstan-17-one							-	
Plate14D11	Methiazole						-		
Plate14E05	Leucomisine						-		

Supplementary Table 3

Compound	Chemical name	Therapeutic group	Mechanism/class	Hit PC3 6h	Hit PC3 36h	Hit HCT116 6h	Hit HCT116 36h	Hit H1299 6h	Hit H1299 36h
Plate08C11	Yohimbic acid monohydrate	-	-	+					
Plate09A09	Betonicine	-	-			-			
Plate09F02	Fillalbin	-	-			+	+	+	
Plate07D11	Sulfasalazine	Treatment of ulcerative colitis	15-hydroxydehydrogenase inhibitor	-					
Plate09H08	Finasteride	Antialopecia agent	5A-reductase inhibitor			+			
Plate05F06	Methiothepin maleate	-	5HT antagonist		-				
Plate04F08	Benzydamine hydrochloride	Analgesic	5HT antagonist		-				
Plate13D03	Pizotifen malate	Antimigraine	5HT antagonist				+	+	
Plate02C04	Cyproheptadine hydrochloride	Antipruritic	5HT antagonist		-				
Plate06C11	Cisapride	Peristaltic stimulant	5HT antagonist	+			-		
Plate08A03	Dihydroergocristine mesylate	Vasodilatator	5HT antagonist		-				
Plate05E05	Metergoline	Antiprolactin	5HT antagonist (5HT1)			-			
Plate07F02	Pirenperone		5HT antagonist (5HT2)		-				
Plate14B09	Ondansetron Hydrochloride	Antiemetic	5HT antagonist (5HT3)	-			+		
Plate09C09	Skimianine	Sedative	5HT ligand			-			
Plate01H03	Imipramine hydrochloride	Antidepressant	5HT transport inhibitor				-		-
Plate02B03	Zimelidine dihydrochloride monohydrate	Antidepressant	5HT uptake inhibitor			+			
Plate07A09	Dosulepin hydrochloride	Antidepressant	5HT uptake inhibitor		-				-
Plate07D02	Fluoxetine hydrochloride	Antidepressant	5HT uptake inhibitor				-		
Plate09F03	Citalopram Hydrobromide	Antidepressant	5HT uptake inhibitor	-				+	
Plate11F02	Paroxetine Hydrochloride	Antidepressant	5HT uptake inhibitor	+					
Plate13F05	Sertraline	Antidepressant	5HT uptake inhibitor	+	-		+	+	
Plate06B03	Anisomycin	Antiprotozoal	Acetylcholine esterase inhibitor			+	+		+
Plate14E03	(-)-Eseroline fumarate salt	Potent analgesic	Acetylcholine esterase inhibitor						-
Plate10E04	Meclofenoxate hydrochloride	Cerebral stimulant	Acetylcholine precursor					-	
Plate10E09	Vidarabine	Antiviral	Adenosine antimetabolite	-	-		+		
Plate11H05	Theobromine	Bronchodilator	Adenosine receptor antagonist		-				
Plate03H07	Dilazep dihydrochloride	Vasodilatator	Adenosine uptake inhibitor				-		
Plate11B04	Bucladesine sodium salt	Cardiotonic	Adenylate cyclase modulator		-		+		
Plate01E08	Ticlopidine hydrochloride	Platelet antiaggregant	ADP antagonist		+				-
Plate04C04	Doxepin hydrochloride	Anticonvulsant	Adrenaline uptake inhibitor		-				
Plate09C11	Tetrandrine	Analgesic	Alkaloid	+	-		-	-	
Plate09D09	Ricinine		Alkaloid			-			
Plate08E05	Piperlongumine	Antifungal	Alkaloid	+	+/-	+			+
Plate08E07	(-)-Cinchonidine	Antimalarial	Alkaloid	+					
Plate08E08	Eburnamonine (-)	Cerebral vasodilatator	Alkaloid				+		
Plate08F02	Harmalol hydrochloride dihydrate	Vasorelaxant	Alkaloid			-			
Plate03D02	Midodrine hydrochloride	Hypotensor	Alpha adrenergic		-				
Plate14E09	(+,-)-Synephrine	Adrenergic	Alpha adrenergic agonist	-	-	-		+	
Plate03F05	Gemfibrozil	Antihyperlipoproteinemic	Alpha adrenergic agonist		-				
Plate07F06	Methoxamine hydrochloride	Antihypotensive	alpha Adrenergic agonist	-				-	
Plate05A05	Phenylpropanolamine hydrochloride	Decongestant	alpha Adrenergic agonist		-				
Plate03D08	Metaraminol bitartrate	Vasoconstrictor	alpha Adrenergic agonist		-	-			

Plate13F08	Etilefrine hydrochloride	Antihypotensive	Alpha Adrenergic agonist (alpha1)			-		
Plate13H09	Methyldopate hydrochloride	Antihypertensor	Alpha Adrenergic agonist (alpha2)	+			+	
Plate10B10	Levonordefrin	Vasoconstrictor	Alpha Adrenergic agonist (alpha2)			-		
Plate01E03	Moxisylyte hydrochloride	Vasodilatator	Alpha adrenergic antagonist				-	
Plate01F11	Tolazoline hydrochloride	Vasodilatator	Alpha adrenergic antagonist		+/-			
Plate02G02	Verapamyl hydrochloride	Antihypertensive	Alpha adrenergic antagonist (alpha1)			+		
Plate01H05	Amityptiline hydrochloride	Antidiabetic	Alpha Adrenergic antagonist (alpha1)			+	-	-
Plate05A03	Alfuzosin hydrochloride	Antihypertensor	Alpha Adrenergic antagonist (alpha1)		-			
Plate08B08	Rauwolscine hydrochloride	Antidepressant	Alpha adrenergic antagonist (alpha2)				+	
Plate09F09	Tetrahydrozoline hydrochloride	Vasoconstrictor	Alpha adrenergic ligand			-		
Plate08H03	Dipivefrin hydrochloride	Adrenergic (ophthalmic)	alpha beta Agrenergic agonist	+		-		
Plate10D03	Phenazopyridine hydrochloride	Analgesic	Analgesic			-		
Plate11B02	Bergenin monohydrate	Antiarrhythmic	Antiarrhythmic			-		
Plate11B03	Cromolyn disodium salt	Antiasthmatic	Antiasthmatic			-		-
Plate07E03	Thiostrepton	Antibacterial	Antibacterial			-		
Plate12H06	Florfenicol	Antibacterial	Antibacterial			+		+
Plate13D11	Lymecycline	Antibiotic	Antibacterial				+	+
Plate13A11	Roxarsone	Antibacterial	Antibacterial		-		+	+
Plate08D10	Seneciophylline	Antitumor activity	Anticancer		+			
Plate10H07	Lithocholic acid	Cholagogue	Anticholelithogenic					+
Plate09A03	Epicatechin(-)	Antidiarrhoeic	Antidiarrhoeic	+/-		+		
Plate13A04	Enilconazole	Antifungal	Antifungal		-		+	
Plate14G11	Parbendazole	Anthelmintic (VET)	Anthelmintic	+	-		+	+
Plate13H11	Pyrvinium pamoate	Anthelmintic (Nematodes, enterobiasis)	Anthelmintic	+/-				+
Plate14D07	Ciprofibrate	Antihyperlipoproteine-mic	Antihyperlipoproteine-mic			+		
Plate01H02	Todralazine hydrochloride	Antihypertensor	Antihypertensor	+				
Plate10A02	Althiazide	Antihypertensor	Antihypertensor			-	+	
Plate13H02	Halofantrine hydrochloride	Antimalarial	Antimalarial	+		+		
Plate05C08	Thioguanosine	Anticancer	Antimetabolite					+
Plate11G07	Azacytidine-5	Antineoplastic	Antimetabolite	+/-	-		+	+
Plate06H11	Puromycin dihydrochloride	Antiprotozoal	Antimetabolite		+/-		-	
Plate02B05	Azathioprine	Immunosuppressant	Antimetabolite					-
Plate07A11	Iobenguane sulfate	Antineoplastic if radiolabeled	Antineoplastic				+	
Plate10E06	Ethoxyquin	Antifungal	Antioxydant			-		-
Plate06A05	Tocopherol (R,S)	Anti-oxidant	Antioxydant			-		
Plate06B04	Carbarsone	Antiamebic	Antiprotozoal					+
Plate12C07	Fluspirilen	Antipsychotic	Antipsychotic		-			
Plate14A09	Piperacetazine	Antipsychotic	Antipsychotic		-			
Plate14B05	Levopropoxyphene napsylate	Antitussive	Antitussive				+	
Plate07D04	Norcyclobenzaprine	Antilucerative	Antilucerative			+	-	
Plate06H10	Methoxy-8-psoralen	Psoriasis treatment	Apoptosis inducer with UV					+
Plate09G11	Strophanthidin	Cardiotonic	ATPase inhibitor				+	+
Plate07B08	Vancomycin hydrochloride	Antibacterial	Bacterial mucopeptide biosynthesis inhibitor		+			
Plate08G02	Methoxy-6-harmalan	Psoriasis treatment	Benzodiazepine receptor ligand			-		
Plate03D09	Salbutamol	Bronchodilatator	Beta adrenergic agonist			-		
Plate04E03	Fenoterol hydrobromide	Bronchodilatator	Beta adrenergic agonist			-		-
Plate05C06	Clenbuterol hydrochloride	Bronchodilatator	Beta adrenergic agonist			-		



Plate07C06	Metaproterenol sulfate, orciprenaline sulfate	Bronchodilatator	Beta adrenergic agonist			-		-	
Plate10C10	Isoetharine mesylate salt	Bronchodilatator	Beta adrenergic agonist			-			
Plate14F08	(-)-Isoproterenol hydrochloride	Bronchodilatator	Beta adrenergic agonist		-	-			+
Plate01G09	Isosuprine hydrochloride	Vasodilatator	Beta adrenergic agonist		+	-			
Plate05D03	Dobutamine hydrochloride	Bronchodilatator	Beta adrenergic agonist (beta1)			-			
Plate05H02	Terbutaline hemisulfate	Bronchodilatator	Beta adrenergic agonist (beta2)		-				
Plate12G06	Salmeterol	Bronchodilatator	Beta adrenergic agonist (beta2)			-	+/-		
Plate05C10	Ritodrine hydrochloride	Tocolytic	Beta adrenergic agonist (beta2)			-			
Plate12G10	(+,-)-Octopamine hydrochloride	Adrenergic	Beta adrenergic agonist (beta3)			-			
Plate02A11	Pindolol	Antiarrhythmic	Beta adrenergic antagonist		+			-	
Plate07B10	Propafenone hydrochloride	Antiarrhythmic	Beta adrenergic antagonist		-			-	
Plate10B04	Metoprolol-(+,-) (+)-tartrate salt	Antihypertensor	Beta adrenergic antagonist					-	
Plate14A04	Penbutolol sulfate	Antihypertensor	Beta adrenergic antagonist			-			
Plate01G10	Acebutolol hydrochloride	Antianginal	Beta adrenergic antagonist (beta1)			-			
Plate04A11	Alprenolol hydrochloride	Antihypertensor	Beta adrenergic antagonist (beta1)			-			
Plate04D08	Labetalol hydrochloride	Antihypertensor	Beta adrenergic antagonist (beta1)			-		-	
Plate03A10	Hydralazine hydrochloride	Antihypertensor	Beta adrenergic antagonist (could be, not shown)						+
Plate12H03	Propranolol hydrochloride	Antianginal	Beta adrenergic blocker		-			+	
Plate07F07	(S)-(-)-Atenolol	Antihypertensor	beta adrenergic blocker		+				
Plate14B08	Oxprenolol hydrochloride	Antihypertensor	Beta adrenergic blocker		-	-			
Plate14D06	(R)-Propranolol hydrochloride	Antihypertensor	Beta adrenergic blocker				+		
Plate12H04	(R)-(+)-Atenolol	Antihypertensor	Beta adrenergic blocker (beta1)					+	
Plate05C04	Desipramine hydrochloride	Antidepressant	Beta Adrenergic transport inhibitor					-	
Plate07G10	Trimetazidine dihydrochloride	Antianoxic	Beta-oxidation inhibition		+				
Plate13A02	Denatonium benzoate		Bittering agent to prevent poisoning						+
Plate03F04	Fenspiride hydrochloride	Antiinflammatory	Bradykinin antagonist			-			
Plate12D02	(+)-Isoproterenol (+) bitartrate salt	Bronchodilatator	Bronchodilatator			-		+	
Plate02G05	Loperamide hydrochloride	Antidiarrhoeic	Ca2+ channel antagonist					-	
Plate01H09	Thioridazine hydrochloride	Neuroleptic	Ca2+ channel antagonist					-	
Plate05D07	Adenosine 5'-monophosphate monohydrate	Nutrient	Ca2+ channel blocker					-	
Plate09D03	(d,l)-Tetrahydroberberin	Sedative	Ca2+ channel blocker		-				
Plate04E07	Perhexiline maleate	Vasodilatator	Ca2+ channel blocker		-	-	+/-	-	+/-
Plate08D06	Calycanthine		Ca2+ channel blocker						-
Plate03A06	Ethosuximide	Anticonvulsant	Ca2+ channel inhibitor voltage dependant						+
Plate07D06	Trimethadione	Anticonvulsant	Ca2+ channel inhibitor voltage dependant ?					-	
Plate07H11	Prenylamine lactate	Vasodilatator	Ca2+ channel stimulation		-				+
Plate01G04	Nifedipine	Antihypertensor	Ca2+ channels blocker (L type)			+			
Plate11G04	Etidronic acid, disodium salt	Calcium regulator	Calcium regulator					-	
Plate01A05	Metformin hydrochloride	Antidiabetic	cAMP/PKA		+				
Plate05E06	Brinzolamide	Antiglaucoma drug	Carbonic anhydrase inhibitor		-				
Plate14H07	Dorzolamide hydrochloride	Antiglaucoma drug	Carbonic anhydrase inhibitor		-				

Plate01A04	Acetazolamide	Diuretic	Carbonic anhydrase inhibitor	+		+			+
Plate11A03	Methazolamide	Diuretic	Carbonic anhydrase inhibitor	-					
Plate13C07	Proscillaridin A	Cardiotonic	Cardiac glycoside				+		+
Plate14E08	2-Chloropyrazine	Cardiotonic	Cardiotonic			-	+		
Plate08A05	Syrosingopine	-	Catecholamine depletor	-					
Plate05F03	Debrisoquin sulfate	Antihypertensor	Catecholamine depletor			-			
Plate11H06	Reserpine	Neuroleptic	Catecholamine pump inhibitor	+	-				
Plate07G02	Ciclopirox ethanolamine	Antifungal	Cell membrane proteins synthesis inhibitor						+
Plate07A10	Ceftazidime pentahydrate	Antibacterial	Cell wall destruction agent				+		
Plate07E07	Ethionamide	Antibacterial	Cell wall destruction agent		+				
Plate13E10	Pivampicillin	Antibacterial	Cell wall destruction agent				+	+	
Plate13F02	Flucloxacillin sodium	Antibacterial	Cell wall destruction agent				+		
Plate13G09	Benzathine benzylpenicillin	Antibacterial	Cell wall destruction agent					+	
Plate14H09	Cefepime hydrochloride	Antibacterial	Cell wall destruction agent			-			
Plate06G11	Ceforanide	Antibacterial	Cell wall synthesis inhibitor (bacterial)	+	-				
Plate06H04	Cefotetan	Antibacterial	Cell wall synthesis inhibitor (bacterial)		-		-		+
Plate14E07	D-cycloserine	Antibacterial	Cell wall synthesis inhibitor (bacterial)		-	-			
Plate14E10	(S)-(-)-Cycloserine	Antibacterial	Cell wall synthesis inhibitor (bacterial)			-			
Plate14G07	Meropenem	Antibacterial	Cell wall synthesis inhibitor (bacterial)				+		
Plate07C05	Etifenin	Diagnostic agent	Chelating agent				-		
Plate12G02	Pentetic acid		Chelating agent (iron)					+	
Plate12A07	Clioquinol	Anti-infective	Chelating agent, chymotrypsin-like proteasome activity inhibitor		-				+
Plate02E04	Dehydrocholic acid	Choleretic	Choleretic		-				
Plate05G05	Probucol	Antihyperlipoproteinemic	Cholesterol downregulation				+		
Plate06A03	Arecoline hydrobromide	Anthelmintic	Cholinergic	+	-	+			
Plate06E10	Pilocarpine nitrate	Antiglaucoma drug	Cholinergic		+			+	
Plate03H04	Hyoscyamine (L)	Antispasmodic	Cholinergic	+					
Plate09A08	Myosmine	Cholinergic	Cholinergic			+			
Plate02A04	Edrophonium chloride	Myasthenia Gravis test	Cholinergic						+
Plate01F03	Carbamazepine	Anticonvulsivant	Cholinergic antagonist		-				
Plate09E11	Napelline	Antiarrhythmic	cholinergic inhibition	+					
Plate04F05	Pimethixene maleate	Antihistaminic	cholinergic inhibition				-		
Plate07B02	Metixene hydrochloride	Antiparkinsonian	cholinergic inhibition			+		+	
Plate10H10	Pridinol methanesulfonate salt	Antiparkinsonian	cholinergic inhibition				+/-		
Plate01E09	Dicyclomine hydrochloride	Antispasmodic	cholinergic inhibition		+				
Plate14A03	Tridihexethyl chloride	Antispasmodic	cholinergic inhibition				+		
Plate04E08	Oxybutynin chloride	Spasmolytic	cholinergic inhibition					-	
Plate10H05	Eucatropine hydrochloride		cholinergic inhibition			+	+	-	+
Plate02A03	Cotinine (-)	Antidepressant	cholinergic inhibition (and nicotinic inhibition)						+
Plate05H04	Hemicholinium bromide	Anticholinergic	Cholinergic inhibition (partial, Acetylcholine stores depletor)		+				
Plate02C08	Tomatine	Antifungal	Cholinergic inhibition (pH-dependent competitive inhibition of the enzyme acetylcholinesterase)	-	-	-	-		
Plate01F02	Trichlorfon	Anthelmintic	cholinergic inhibition Cholinesterase inhibitor	+	-			-	

Plate05A10	Tacrine hydrochloride hydrate	Cognition enhancer	Cholinesterase inhibitor				-		
Plate12A03	Bemegride	CNS stimulant	CNS stimulant	+					
Plate10C02	Nadide	-	CoA nicotinamide adenine dinucleotide					-	
Plate11G06	Simvastatin	Anthyperlipidemic	CoA reductase inhibitor (HMG CoA)					-	
Plate01C03	Panthenol (D)	Vitamin	CoA synthesis precursor					-	
Plate06H03	Pantothenic acid calcium salt monohydrate	Nutritional factor	CoA synthesis role			-			
Plate04H05	Enalapril maleate	Antihypertensor	Converting enzyme inhibitor				+		
Plate14G08	Ramipril	Antihypertensor	Converting enzyme inhibitor			+			
Plate13A10	3-Acetamidocoumarin	Antiinflammatory	coumarin	-				+	
Plate13A03	Scopoletin	Antispasmodic	Coumarin					+	
Plate12B02	3-Acetylcoumarin		coumarin					+	
Plate08A02	Tubocurarine chloride pentahydrate (+)	Muscle relaxant	Curarising	+					
Plate01C10	Antipyrine	Analgesic	cyclooxygenase inhibition			+			
Plate03E04	Flufenamic acid	Analgesic	cyclooxygenase inhibition				-		
Plate09H04	Dipyrone	Analgesic	cyclooxygenase inhibition				+		-
Plate11B06	Fosfosal	Analgesic	cyclooxygenase inhibition			-			
Plate01E06	Naproxen	Antiinflammatory	cyclooxygenase inhibition			+			
Plate01F05	Mefenamic acid	Antiinflammatory	cyclooxygenase inhibition			-			
Plate01H04	Sulindac	Antiinflammatory	cyclooxygenase inhibition	+					
Plate02B09	Acetylsalicylsalicylic acid	Antiinflammatory	cyclooxygenase inhibition						-
Plate03E06	Tolfenamic acid	Antiinflammatory	cyclooxygenase inhibition						+
Plate03E07	Meclofenamic acid sodium salt monohydrate	Antiinflammatory	cyclooxygenase inhibition	-					
Plate03F09	Fenbufen	Antiinflammatory	cyclooxygenase inhibition			-			
Plate03F10	Ketoprofen	Antiinflammatory	cyclooxygenase inhibition			-			
Plate07C09	Resveratrol	Antiinflammatory	cyclooxygenase inhibition	+		-		+/	
Plate07E08	Tenoxicam	Antiinflammatory	cyclooxygenase inhibition			+			
Plate10A03	Isopyrin hydrochloride	Antiinflammatory	cyclooxygenase inhibition			-		+	
Plate10B11	Ebselen	Antiinflammatory	cyclooxygenase inhibition	-				+	
Plate10H02	(R) -Naproxen sodium salt	Antiinflammatory	cyclooxygenase inhibition				+		-
Plate11B07	Suprofen	Antiinflammatory	cyclooxygenase inhibition			-			
Plate11D07	Indoprofen	Antiinflammatory	cyclooxygenase inhibition	-					
Plate11F07	Tolmetin sodium salt dihydrate	Antiinflammatory	cyclooxygenase inhibition	-					+
Plate10A11	Balsalazide Sodium	Anti-inflammatory	cyclooxygenase inhibition			-			
Plate13E04	Azapropazone	Anti-inflammatory	cyclooxygenase inhibition	+		-		+	
Plate14A10	Oxyphenbutazone	Anti-inflammatory	cyclooxygenase inhibition	-		-		+	+
Plate14B11	Oxaprozin	Anti-inflammatory	cyclooxygenase inhibition					+	+
Plate01C11	Antipyrine, 4-hydroxy	Antipyrine metabolite	cyclooxygenase inhibition			+			
Plate09G06	Methyl benzethonium chloride	Antibacterial	Detergent	-			+	-	-
Plate09G09	Benzethonium chloride	Antibacterial	Detergent	-			-	+/	
Plate10F08	Alexidine dihydrochloride	Antibacterial	Detergent	-		-		-	+
Plate10H03	Propidium iodide	Antibacterial	Detergent	+				+	
Plate04E06	Chenodiol	Anticholelithogenic	Detergent				-		-
Plate02G04	Chlorhexidine	Bacteriostatic	Detergent			-			+

Plate12E06	Thonzonium bromide		Detergent	+			+		
Plate13D10	Proguanil hydrochloride	Antimalarial	dihydrofolate reductase inhibitor					+	
Plate14F05	Sulfadoxine	Antibacterial	dihydropteroate synthase inhibitor		+/-		+		
Plate09A05	N-Acetyl-DL-homocysteine Thiolactone	Expectorant	Disulfure bridge breaker	-					
Plate02A10	Ursolic acid	Diuretic	Diuretic			-			
Plate02A02	Metronidazole	Antibacterial	DNA damage (bacterial)			-	+		+
Plate07B03	Nitrofurural	Antibacterial	DNA damage (bacterial)	+		-			
Plate07H06	Nifuroxazide	Antibacterial	DNA damage (bacterial)						+
Plate10E05	Furaltadone hydrochloride	Antibacterial	DNA damage (bacterial)					-	
Plate03A09	Nitrofurantoin	Urinary antiseptic	DNA damage (bacterial)						+
Plate06G10	Niridazole	Anthelmintic	DNA damage ('Helminthic')			+			
Plate10E07	Tinidazole	Antiprotozoal	DNA damage (protozoal)					-	
Plate05D06	Hycanthone	Anthelmintic	DNA intercalating agent			-			
Plate06D09	Doxorubicin hydrochloride	Antibacterial	DNA intercalating agent			-			+
Plate08F05	Ellipticine	Anticancer	DNA Intercalating agent			-	-		
Plate07A08	Daunorubicin hydrochloride	Antineoplastic	DNA intercalating agent				+		+
Plate11D04	Ifosfamide	Antineoplastic	DNA replication inhibitor					-	
Plate14D10	Chlorambucil	Antineoplastic	DNA replication inhibitor				-	+	
Plate05F07	Clofazimine	Antileprosy	DNA replication inhibitor (mycobacterial DNA)					-	
Plate14B07	Trifluridine	Antiviral (ophthalmic)	DNA replication inhibitor (viral)	-	-		+		
Plate10B03	Streptozotocin	Antineoplastic	DNA synthesis inhibitor					-	+
Plate10A08	Ergocryptine-alpha	Vasoconstrictor	Dopamine activator			+			
Plate04F06	Pergolide mesylate	Antiparkinsonian	Dopamine agonist					-	
Plate13B11	Piribedil hydrochloride	Vasodilator (peripheral)	Dopamine agonist				+		
Plate02C02	R(-) Apomorphine hydrochloride hemihydrate	Emetic	Dopamine agonist (D1)		+	+			
Plate14F04	(-)-Quinpirole hydrochloride	Anti-Parkinsonian	dopamine agonist (D2)				+		
Plate08G09	Salsolinol hydrobromide	-	Dopamine analog				-		
Plate01G05	Chlorpromazine hydrochloride	Antiemetic	Dopamine antagonist	+					
Plate06F02	Alizapride HCl	Antiemetic	Dopamine antagonist				+		
Plate08E02	Scoulerine	Antiemetic	Dopamine antagonist	+	-		+		+
Plate09G05	Bromopride	Antiemetic	Dopamine antagonist				+		
Plate04H11	Fluphenazine dihydrochloride	Antipsychotic	Dopamine antagonist						-
Plate07C10	Bromperidol	Antipsychotic	Dopamine antagonist		+				
Plate07E10	Mesoridazine besylate	Antipsychotic	Dopamine antagonist		+				
Plate09F04	Promazine hydrochloride	Antipsychotic	Dopamine antagonist				-	+	-
Plate04H04	Trifluoperazine dihydrochloride	Psycholeptic	Dopamine antagonist				-	-	
Plate01F04	Triflupromazine hydrochloride	Antipsychotic	Dopamine antagonist ?		-		-		
Plate01H11	Trimethobenzamide hydrochloride	Antiemetic	Dopamine antagonist (D2)					-	-
Plate01F07	Sulpiride	Antipsychotic	Dopamine antagonist (D2)			+/-			
Plate05C09	Chlorprothixene hydrochloride	Neuroleptic	Dopamine antagonist (D2)				-	-	
Plate07H10	DO 897/99	-	Dopamine antagonist (D3)			-			
Plate04G09	Pimozide	Antipsychotic	Dopamine antagonist ?				-		
Plate02B08	Disulfiram	Alcohol deterrent	Dopamine beta hydroxylase inhibitor	+	-	+	+		+
Plate02C03	Amoxapine	Antidepressant	Dopamine uptake inhibitor			-	-		
Plate05G07	GBR 12909 dihydrochloride	Antidepressant	Dopamine uptake inhibitor				+		

Plate09E10	Ungerine nitrate	Sedative	Enhancer of analgesics					-	
Plate06H05	Piperine	Antidiarrhoeic	Enzyme inhibitor						+
Plate06A09	Butoconazole nitrate	Antifungal	Ergosterol inhibitor				-		+
Plate06A11	Amphotericin B	Antibacterial	Ergosterol ligand	-					
Plate01G11	Tolnaftate	Antifungal	Ergosterol synthesis inhibition		+				
Plate11A11	Sulconazole nitrate	Antifungal	Ergosterol synthesis inhibition	-					
Plate10F07	Guaifenesin	Expectorant	Expectorant					-	
Plate03E09	Trimethoprim	Antibacterial	Folic acid antagonist				-		
Plate01D06	Dapsone	Antiinflammatory	Folic acid antagonist		+				
Plate01D08	Pyrimethamine	Antiprotozoal	Folic acid antagonist		-				
Plate09G03	Succinylsulfathiazole	Antibacterial	Folic acid synthesis inhibition	-		+		+/-	
Plate09H02	Sulfabenzamide	Antibacterial	Folic acid synthesis inhibition			+			
Plate09H06	Sulfachloropyridazine	Antibacterial	Folic acid synthesis inhibition			+		-	
Plate10B02	Sulfaquinoxaline sodium salt	Antibacterial	Folic acid synthesis inhibition					-	
Plate10E10	Sulfameter	Antibacterial	Folic acid synthesis inhibition		+				
Plate10F06	Sulfamethazine sodium salt	Antibacterial	Folic acid synthesis inhibition					-	
Plate01B05	Sulfacetamide sodic hydrate	Antibacterial	Folic acid synthesis inhibitor					-	
Plate01C02	Sulfaphenazole	Antibacterial	Folic acid synthesis inhibitor					-	
Plate03A07	Mafenide hydrochloride	Antibacterial	Folic acid synthesis inhibitor			+			
Plate03B08	Sulfamethoxazole	Antibacterial	Folic acid synthesis inhibitor					+	
Plate10A09	Sulfadimethoxine	Antibacterial	Folic acid synthesis inhibitor	-	-				
Plate10A10	Sulfanilamide	Antibacterial	Folic acid synthesis inhibitor		-				
Plate01G02	Morantel tartrate	Anthelmintic	Fumarate reductase inhibitor	+					
Plate08A10	Dihydroergotoxine mesylate	Anticonvulsant	GABA A receptor C1-channel high affinity	+			-		+
Plate13B03	THIP Hydrochloride		GABA Agonist				+		
Plate06D11	Epiandrosterone	Anabolic steroid	GABA agonist (non competitive)	+					
Plate07F10	Thiocolchicoside	Muscle relaxant	GABA agonist ?	+	-				
Plate03A03	Pentylenetetrazole	CNS stimulant	GABA antagonist			+		+	
Plate11E02	Securinine	CNS stimulant	GABA antagonist						-
Plate09C03	Gelsemine	Tumour inhibitor	GABA antagonist	-					
Plate08C10	Bicuculline (+)	Convulsant	GABA antagonist (GABAa)				+		
Plate09B03	Picrotoxinin	Analeptic	GABA channel blocker	-		+			
Plate14A02	Etomidate	Hypnotic	GABA receptor (GABAa)				+		
Plate11G02	Gabapentin	Anticonvulsant	GABA receptor ligand	+					
Plate13B07	Tracazolate hydrochloride		GABA receptor ligand				+		
Plate12F02	Propofol	Anesthetic (intravenous)	GABA receptor stimulation					+	
Plate13E03	Alfaxalone	In combination with alfadolone acetate as anesthetic (intravenous)	GABA receptor stimulation				+		
Plate13E02	Alfadolone acetate	In combination with alfaxalone as anesthetic (intravenous)	GABA receptor stimulation				+		
Plate09B11	Avermectin B1	Anthelmintic	GABA receptors ligand					-	
Plate01D09	Hexamethonium dibromide dihydrate	Antihypertensor	Ganglion blocker		+				
Plate14H02	Mecamylamine hydrochloride	Antihypertensor	Ganglion blocker	-			+		
Plate05A04	Chlorpropamide	Antidiabetic	Glucagon secretogen	-					
Plate13D08	Fluticasone propionate	Antiallergic	glucocorticoid					-	
Plate13F11	Rimexolone	Anti-inflammatory (local)	Glucocorticoid					+	
Plate04D10	Methylprednisolone, 6-alpha	Glucocorticoid	Glucocorticoid				-		

Plate09A04	Flunisolide	Glucocorticoid	Glucocorticoid			+			
Plate09A06	Flurandrenolide	Glucocorticoid	Glucocorticoid			+			
Plate09H09	Fluorometholone	Glucocorticoid	Glucocorticoid			+/-		-	
Plate10B05	Flumethasone	Glucocorticoid	Glucocorticoid						-
Plate10C04	Medrysone	Glucocorticoid	Glucocorticoid	-					
Plate10F05	Fluocinonide	Glucocorticoid	Glucocorticoid					-	
Plate10G02	Clobetasol propionate	Glucocorticoid	Glucocorticoid		-		-	-	
Plate14A05	Prednicarbate	Glucocorticoid (topical)	Glucocorticoid				+/-		
Plate10F02	Alclometasone dipropionate	Anti-inflammatory	glucocorticoid receptor agonist			-			
Plate03F08	Mebendazole	Parasite suppressor	Glucose transport inhibitor ?	+	-		+		
Plate09C06	Evoxine	Sedative	Glycine receptor antagonist					-	
Plate07B04	Omeprazole	Antiulcerative	H+ pump inhibitor (ATPase H+ pump, non competitive)	+					
Plate04D11	Quinidine hydrochloride monohydrate	Antiarrhythmic	Heme polymerase inhibitor			-			
Plate02E07	Mefloquine hydrochloride	Antimalarial	Heme polymerase inhibitor	+	+/-		+	-	
Plate04G10	Amodiaquin dihydrochloride dihydrate	Antimalarial	Heme polymerase inhibitor				-		-
Plate06H07	Primaquine diphosphate	Antimalarial	Heme polymerase inhibitor		+/-	+	+	-	+
Plate07G09	Chloroquine diphosphate	Antipaludic	Heme polymerase inhibitor		+				
Plate01E04	Betazole hydrochloride	Gastric secretion stimulant	Histamine analog	+					
Plate10H08	Methotrimeprazine maleate salt	Analgesic	Histamine antagonist	+			+		-
Plate09G07	Chlorcyclizine hydrochloride	Antihistaminic	Histamine antagonist			+		-	
Plate11E03	Trimeprazine tartrate	Antipruritic	Histamine antagonist		-		-		
Plate10H04	Cloperastine hydrochloride	Antitussive	Histamine antagonist	+			+/-		
Plate07C11	Cyclizine hydrochloride	Antiemetic	Histamine antagonist (H1)		+				
Plate01C08	Doxylamine succinate	Antihistaminic	Histamine antagonist (H1)		+				
Plate01F10	Pheniramine maleate	Antihistaminic	Histamine antagonist (H1)		+/-				
Plate01G06	Diphenhydramine hydrochloride	Antihistaminic	Histamine antagonist (H1)		+				
Plate02F07	Astemizole	Antihistaminic	Histamine antagonist (H1)	-	-		-	-	-
Plate04C03	Triprolidine hydrochloride	Antihistaminic	Histamine antagonist (H1)		-				
Plate04C06	Dimenhydrinate	Antihistaminic	Histamine antagonist (H1)					-	
Plate04E04	Homochlorcyclizine dihydrochloride	Antihistaminic	Histamine antagonist (H1)				-		
Plate04G07	Clemastine fumarate	Antihistaminic	Histamine antagonist (H1)				-	-	
Plate06F06	Mebhydroline 1,5-naphthalenedisulfonate	Antihistaminic	Histamine antagonist (H1)	+					
Plate06H06	Brompheniramine maleate	Antihistaminic	Histamine antagonist (H1)						+
Plate07C04	Cetirizine dihydrochloride	Antihistaminic	Histamine antagonist (H1)				+		
Plate11A08	Chloropyramine hydrochloride	Antihistaminic	Histamine antagonist (H1)			+			
Plate12A09	Promethazine hydrochloride	Antihistaminic	Histamine antagonist (H1)	+				-	
Plate06C09	Roxatidine Acetate HCl	Antiulcerative	Histamine antagonist (H2)	+	+/-		+		+
Plate12E02	Nizatidine	Antiulcerative	Histamine antagonist (H2)				+		
Plate09B10	6-Furfurylaminopurine	Plant growth accelerator	Hormone (plants)					-	
Plate06B02	Androsterone	Antihypertensor	Hormone (steroid)			-		-	
Plate11F04	Liothyronine	Thyroidic drug	Hormone (Thyroid)					-	
Plate06A02	Testosterone propionate	Androgen	hormone Androgen			+			
Plate07G07	Pregnenolone	Androgen	Hormone androgen		+			-	
Plate03B11	Flutamide	Anticancer	hormone androgen receptor antagonist	-			-		

Plate14D05	Cyproterone acetate	Antiandrogen	hormone antiandrogen					+		
Plate13E07	Epitiostanol	Antineoplastic	hormone antiestrogen					+		
Plate09E09	Estropipate	Estrogen	Hormone estrogen			-				
Plate10D07	Diethylstilbestrol	Estrogen	Hormone estrogen					+	-	-
Plate11E07	Ethinylestradiol 3-methyl ether	Estrogen	Hormone estrogen	-						
Plate11E11	Equilin	Estrogen	Hormone estrogen	-						
Plate11G03	Raloxifene hydrochloride		hormone Estrogen agonist	+				-		-
Plate05H08	Clomiphene citrate (Z,E)	Antineoplastic	hormone Estrogen agonist		-					
Plate02C06	Danazol	Antigonadotropin	hormone Estrogen antagonist	+				+	-	+
Plate06H08	Progesterone	Progestogen	Hormone progestogen							+
Plate09D02	Dydrogesterone	Progestogen	Hormone progestogen	-						
Plate12H07	Megestrol acetate	Progestogen	Hormone progestogen		-					
Plate09D06	Hippeastrine hydrobromide	Hypotensor	Hypotensor						-	
Plate09E06	Nitrarine dihydrochloride	Hypotensor	Hypotensor						-	
Plate11E06	Amiprilose hydrochloride	Immunomodulator	Immunomodulator						-	
Plate03D03	Thalidomide	Immunosuppressant	Immunosuppressant		-					
Plate07H07	Mycophenolic acid	Antineoplastic	Inosine monophosphate dehydrogenase inhibitor	-	-			+		+
Plate02E03	Metanephrine hydrochloride DL		Isoprenaline uptake inhibitor extraneuronal		-	-				
Plate01B11	Minoxidil	Antihypertensor	K+ channel activator		+					
Plate02C07	Nicorandil	Antihypertensor	K+ channel agonist (ATP-dependent channels)						-	
Plate13A07	Sotalol hydrochloride	Antianginal	K+ channel antagonist	+				+		
Plate07H05	Tolazamide	Antidiabetic	K+ channel blocker (ATP-dependent channels)					-	+	+
Plate01F06	Acetohexamide	Antidiabetic (type II, noninsulin-dependent)	K+ channel blocker (ATP-dependent channels)		+/-					
Plate05G09	Dequalinium dichloride	Antibacterial	K+ channel blocker (Ca2+-dependent channels, apamin-sensitive small conductance)					+		
Plate04D06	Fenofibrate	Hypolipidemiant	Lipoprotein lipase activator						-	
Plate10G04	Clofibric acid	Antihyperlipoproteinemic	Lipoprotein lipase activator ?		-					
Plate04E05	Diethylcarbamazine citrate	Antihelminthic	Lipoxygenase inhibitor			-			-	
Plate07C08	Quercetine dihydrate	Antimalarial	Lipoxygenase inhibitor		+					
Plate08F03	Harmol hydrochloride monohydrate	Anxiolytic	Liver conjugation probe		+	-		+		
Plate11H07	Arcaïne sulfate		Lowers blood sugar	+/-						
Plate12A04	Digoxigenin	Diagnosis	Mainly used as a non-isotopic label for DNA					+/-		+
Plate03A11	Phenelzine sulfate	Antidepressant	MAO inhibitor	-						
Plate10H06	Isocarboxazid	Antidepressant	MAO inhibitor					+		+
Plate14F10	Nialamide	Antidepressant	MAO inhibitor			-				
Plate08F04	Harmine hydrochloride	Antihelminthic	MAO inhibitor					+		+
Plate04H09	Quinacrine dihydrochloride dihydrate	Antimalarial	MAO inhibitor		-			-		+
Plate13B04	Pirlindole mesylate	highly selective reversible inhibitor of monoamine oxidase type A	MAO inhibitor							-
Plate07H03	Selegiline hydrochloride	Antiparkinsonian	MAO inhibitor (Monoamine B)							+
Plate07G11	Parthenolide	Antiinflammatory	MAPK inhibitor		-	+		+		+
Plate11H04	Theophylline monohydrate	Bronchodilatator	Mastocyte degranulation inhibitor in vitro	+	-				-	

Plate12D03	Monobenzene	Depigmentor	melanin inhibition		-				
Plate09A07	Helveticoside	Cardiotonic	membrane ATP inhibitor			+	+		+
Plate10C09	Monensin sodium salt	Antibacterial	Membrane ionophores producer		-		+		
Plate07D08	Nystatine	Antifungal	Membrane ionophores producer		+				
Plate04B11	Praziquantel	Anthelmintic	Membrane permeability modulator			-			
Plate03E11	Fenbendazole	Anthelmintic	microtubule polymerisation inhibitor	+	-		+/-		+
Plate05E04	Colchicine	Antiinflammatory	microtubule polymerisation inhibitor	+	-		+	-	+
Plate02B11	Nocodazole	Antineoplastic	microtubule polymerisation inhibitor	+	-	+	+		+
Plate02H06	Paclitaxel	Antineoplastic	microtubule polymerisation inhibitor	+	+/-	+	+		+
Plate04A08	Albendazole		microtubule polymerization inhibition	+	-		+		+
Plate10G03	Podophyllotoxin	Antiviral	Microtubule polymerization inhibitor	+	-		+/-	-	+
Plate12H08	Deoxycorticosterone	Mineralocorticoid	Mineralocorticoid					+	
Plate03G03	Antimycin A	Antifungal	Mitochondrial electron transport inhibitor	-	-				
Plate14C05	Mepylcaine hydrochloride	Local anesthetic	Monoamine transport inhibition				+		
Plate11D08	Carbenoxolone disodium salt	Antiulcerative	Mucus stimulating synthesis					-	
Plate11E05	Procyclidine hydrochloride	Antiparkinsonian	Muscarinic antagonist					-	
Plate01G03	Homatropine hydrobromide (R,S)	Antispasmodic	Muscarinic antagonist	+				-	
Plate11C11	Ethaverine hydrochloride	Antispasmodic	Muscarinic antagonist ?	-					
Plate03H05	Chlorphensin carbamate	Muscle relaxant	Muscle relaxant				-		
Plate09H03	Benzocaine	Anesthetic	Na+ channel blocker	-		+		-	
Plate01B02	Meticrane	Antihypertensor	Na+ channel blocker	+					
Plate01E02	Procaine hydrochloride	Local anesthetic	Na+ channel blocker					-	
Plate01E10	Amyleine hydrochloride	Local Anesthetic	Na+ channel blocker		+	-			
Plate01E11	Lidocaine hydrochloride	Local anesthetic	Na+ channel blocker		+				
Plate01F08	Benoxinate hydrochloride	Local anesthetic	Na+ channel blocker		-				
Plate01F09	Oxethazaine	Local anesthetic	Na+ channel blocker		+/-				
Plate04G06	Bupivacaine hydrochloride	Local anesthetic	Na+ channel blocker					-	
Plate09H07	Pramoxine hydrochloride	Local anesthetic	Na+ channel inhibitor (voltage-dependent)			+			
Plate12H10	Proparacaine hydrochloride	Topical anesthetic (ophthalmic)	Na+ channel inhibitor (voltage-dependent)					+	
Plate10G05	Bendroflumethiazide	Antihypertensor	Na+ Cl- transport inhibitor		-				
Plate01A10	Hydrochlorothiazide	Diuretic	Na+ Cl- transport inhibitor	+					
Plate03F11	Indapamide	Antihypertensor	Na+ Cl- uptake inhibitor		-				
Plate05C02	Furosemide	Diuretic	Na+ Cl- uptake inhibitor		-	+			
Plate14A11	Quinethazone	Diuretic	Na+ Cl- uptake inhibitor			-			
Plate13C08	Sanguinarine	Antimicrobial drug	Na+ K+ ATPase inhibitor					-	
Plate06D07	Digitoxigenin	Cardiotonic	Na+ K+ ATPase inhibitor				+		+
Plate06D08	Digoxin	Cardiotonic	Na+ K+ ATPase inhibitor				+		+
Plate06H02	Strophantine octahydrate	Cardiotonic	Na+ K+ ATPase inhibitor		-		+		+
Plate09B07	Lanatoside C	Cardiotonic	Na+ K+ ATPase inhibitor				+		+
Plate13G08	Tocainide hydrochloride	Antiarrhythmic	Na+ K+ transport inhibition					-	
Plate13G11	Torsemide	Diuretic	Na+ uptake inhibitor				+	+	
Plate14A08	Piretanide	Diuretic	Na+ uptake inhibitor		-				



Plate01A06	Atracurium besylate	Curarizing agent	Neuromuscular blocking agent						
Plate03F03	Pyrantel tartrate	Anthelmintic	Neuromuscular depolarizing agent		-				
Plate13A09	Decamethonium bromide	Muscle relaxant (skeletal)	Neuromuscular depolarizing agent				+		
Plate08H04	Thiorphan	Antinociceptive	Neutral endopeptidase inhibitor	+					
Plate09D10	Delsoline		Nicotinic antagonist	+	+				
Plate09C10	Anabasine	Insecticide	Nicotinic receptor ligand	+				-	
Plate09E03	beta- Belladonnine dichloroethylate	Muscle relaxant	Nicotinic receptor ligand	-					
Plate09H05	Isosorbide dinitrate	Antianginal	Nitric oxide donor				+		
Plate05E07	Ambroxol hydrochloride	Expectorant	Nitric oxide inhibitor					-	
Plate07G08	Molsidomine	Vasodilator	Nitric oxide production ?		+				
Plate13B09	Memantine Hydrochloride	Antiparkinsonian	NMDA receptor antagonist				+		
Plate14F02	Spaglumic acid		NMDA receptor ligands					-	
Plate02C10	Dizocilpine maleate	-	NMDA receptor probe		-				
Plate07F08	Piracetam	Nootropic drug	Nootropic agent		+				
Plate01B06	Heptaminol hydrochloride	Antihypertensive	Noradrenaline increase		+				
Plate12C11	Nisoxetine hydrochloride		Noradrenaline inhibitor						-
Plate04C10	Clomipramine hydrochloride	Antidepressant	Noradrenaline uptake inhibitor					-	
Plate05C07	Maprotiline hydrochloride	Antidepressant	Noradrenaline uptake inhibitor		-		-		
Plate11A07	Trimipramine maleate salt	Antidepressant	Noradrenaline uptake inhibitor	-					
Plate04B05	Nortriptyline hydrochloride	Antidepressant	Norepinephrine uptake inhibitor				-	-	
Plate01D03	Epirizole	Analgesic	NSAI					-	
Plate09G04	Famprofazone	Analgesic	NSAI				+		+/-
Plate14G05	Clonixin Lysinate	Analgesic	NSAI	+			+		
Plate09F10	Hexestrol	Estrogen antineoplastic	Nuclear receptor ligand	+					
Plate10H09	Dienestrol	Non-steroidal estrogen	Nuclear receptor ligand		-		+		
Plate01B09	Idoxuridine	Antiviral	Nucleic acid synthesis inhibitors		+/-				-
Plate02D02	Naloxone hydrochloride	Opiate antidote	Opioid antagonist				+		
Plate05D10	Dextromethorphan hydrobromide monohydrate	Antitussive	Opioid ligand						-
Plate13E05	Meptazinol hydrochloride	Analgesic (narcotic)	opioid recepto activator				+		
Plate14G04	Quinic acid		opioid receptor modulator	+			+		
Plate13G06	Letrozole	Antineoplastic	P450 inhibitor				-		
Plate02E05	Hesperetin		P450 inhibitor		-				
Plate10F09	Proadifen hydrochloride	Local anesthetic	P450 inhibitor (mono-oxygenases)	-	-			-	-
Plate05G10	Ketoconazole	Antifungal	P450 inhibitor (P450c17)				+		
Plate04A03	Flavoxate hydrochloride	Antispasmodic	Phosphodiesterase inhibitor				+		
Plate08C08	Cilostazol	Antithrombotic	Phosphodiesterase inhibitor	+	-		+		+
Plate01D04	Diprophylline	Cardiac analeptic	Phosphodiesterase inhibitor	+					
Plate03B03	Etofylline	Cardiac analeptic	Phosphodiesterase inhibitor					+	
Plate04C09	Vinpocetine	Nootropic drug	Phosphodiesterase inhibitor				-		
Plate13F03	Trapidil	Vasodilator (coronary)	phosphodiesterase inhibitor				+		
Plate09A02	Sulmazole	Cardiotonic	Phosphodiesterase inhibitor (III)				+		
Plate10H11	Amrinone	Cardiotonic	Phosphodiesterase inhibitor (III)				+		
Plate13B08	Zardaverine		Phosphodiesterase inhibitor (III)	+				-	
Plate12H11	Aminocaproic acid	Hemostatic	Plasminogen inhibitor					+	
Plate12D10	Bacitracin	Antibacterial	Polypeptide toxin		+				
Plate01A03	Allantoin	Vulnerary	Precipitate proteins				+		

Plate01C05	Norethynodrel	Progestogen	Progesterone receptor agonist					-	
Plate04C02	Ethisterone	Progestogen	Progesterone receptor agonist		-				
Plate02E02	Bromocryptine mesylate	Antiparkinsonian	Prolactin inhibitor		-				
Plate13F09	Alprostadil	Vasodilator	Prostaglandine E1 receptor ligand					+	
Plate04B06	Niflumic acid	Analgesic	Prostaglandine synthesis inhibitor					-	
Plate06F11	Dinoprost trometamol	Smooth muscle activator	Prostaglandin agonist	-					
Plate14H05	Saquinavir mesylate	Antiviral (HIV)	Protease inhibitor		-		+		
Plate02G07	Tamoxifen citrate	Anticancer	Protein kinase C inhibitor						+
Plate08A11	Emetine dihydrochloride	Antiemetic	Protein synthesis inhibitor	+	+		+		+
Plate10G11	Cycloheximide	Antibacterial	Protein synthesis inhibitor	+	-		+		+
Plate13A05	Methacycline hydrochloride	Antibacterial	Protein synthesis inhibitor (bacteria)				+		
Plate09E07	Lycorine hydrochloride	Antitumoral	Protein translation inhibitor	+	-		+		+
Plate13E09	Gabexate mesilate	Severe acute pancreatitis	Proteinase inhibitor				+		
Plate03F06	Mefexamide hydrochloride	Psychoanaesthetic	Psychoanaesthetic		-				
Plate01A02	Azaguanine-8	Antineoplastic	Purine antimetabolite	+	+		+		+
Plate11H02	Iopamidol	Diagnostic aid (radiopaque medium)	Radiocontrast agent	+	-			-	
Plate12F10	Iodipamide	Diagnostic aid (radiopaque medium-cholecystographic)	Radiocontrast agent		+				
Plate12A05	Meglumine	Expectorant	Radiocontrast agent	+					
Plate11H03	Iopromide		Radiocontrast agent		-			-	
Plate03C10	Aminopurine, 6-benzyl		Respiratory kinase inhibitor (plants)		+				
Plate13H08	Zalcitabine	Antiviral (HIV)	Reverse transcriptase inhibitor					-	
Plate01D02	Chloramphenicol	Antibacterial	Ribosomal peptidyltransferase inhibitor	+				-	
Plate01C06	Thiamphenicol	Antibacterial	Ribosomal protein synthesis inhibitor		+			-	
Plate02H02	Erythromycin	Antibacterial	Ribosomal protein synthesis inhibitor			+			
Plate02H03	Oleandomycin phosphate	Antibacterial	Ribosomal protein synthesis inhibitor			+			-
Plate04H06	Minocycline hydrochloride	Antibacterial	Ribosomal protein synthesis inhibitor					-	
Plate05A02	Streptomycin sulfate	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate05H05	Kanamycin A sulfate	Antibacterial	Ribosomal protein synthesis inhibitor						+
Plate07C07	Sisomicin sulfate	Antibacterial	Ribosomal protein synthesis inhibitor		+				
Plate07H08	Dirithromycin	Antibacterial	Ribosomal protein synthesis inhibitor						+
Plate09A11	Butirosin disulfate salt	Antibacterial	Ribosomal protein synthesis inhibitor					-	
Plate10D04	Demeclocycline hydrochloride	Antibacterial	Ribosomal protein synthesis inhibitor					-	
Plate11F05	Roxithromycin	Antibacterial	Ribosomal protein synthesis inhibitor				+		
Plate07E06	Rifampicin	Antibacterial	RNA polymerase inhibitor				-	-	
Plate13D04	Ribavirin	Antiviral	RNA synthesis inhibitor (viral)				+		
Plate12H02	Crotamiton	Scabicide	Scabicide					+	
Plate13F10	Tribenoside	Sclerosing agent	Sclerosing agent				+		
Plate12A06	Cantharidin	Rubefiant	Serine protease releaser	+	+/-	+	+		
Plate02G11	Dihydroergotamine tartrate	Antimigraine	Serotonin antagonist			-			
Plate12E11	Protriptyline hydrochloride	Antidepressant	serotonin reuptake inhibitor				-		
Plate13D06	Fluvoxamine maleate	Antidepressant	serotonin reuptake inhibitor						-
Plate05G08	Carbetapentane citrate	Antitussive	Sigma1 receptor ligand				+	-	
Plate12G03	Bretylum tosylate	Antiadrenergic	SNS inhibition					+	
Plate10G10	Drofenine hydrochloride	Spasmolytic	Spasmolytic				+		
Plate02E08	Isoconazole	Antibacterial	Sterol 14-demethylase inhibitor						+

Plate07B06	Terconazole	Antifungal	Sterol 14-demethylase inhibitor					-	-
Plate01B03	Benzonatate	Antitussive	Stretch receptor sensitivity decrease	+					
Plate01A09	Amprolium hydrochloride	Coccidiostatic	Thiamine transport inhibitor		+				
Plate14E11	Homosalate		Tool for uv screen				+		
Plate09F06	Acacetin	Anti-oxidant	Topoisomerase I inhibitor					-	
Plate03D11	Camptothecine (S,+)	Antitumor agent	Topoisomerase I inhibitor		-		+		+
Plate14F09	Kaempferol	Anti-inflammatory	Topoisomerase I inhibitor		+/-	-			
Plate03D04	Oxolinic acid	Antibacterial	Topoisomerase II inhibitor		-				
Plate03E05	Flumequine	Antibacterial	Topoisomerase II inhibitor					+	
Plate05G06	Mitoxantrone dihydrochloride	Antineoplastic	topoisomerase II inhibitor	+	-		+		+
Plate05H07	Etoposide	Antineoplastic	Topoisomerase II inhibitor		+/-			-	
Plate07H04	Pentamidine isethionate	Antiparasitic	Topoisomerase inhibition						+
Plate14H11	Nadifloxacin	Antibacterial	Topoisomerase inhibitor (topoisomerase II)	-	+	-			
Plate03H06	Metampicillin sodium salt	Antibacterial	transpeptidase inhibitor (bacterial)	+					
Plate06E11	Dicloxacillin sodium salt	Antibacterial	transpeptidase inhibitor (bacterial)	-					
Plate07A06	Cefaclor	Antibacterial	transpeptidase inhibitor (bacterial)	-				-	
Plate07D10	Imipenem	Antibacterial	transpeptidase inhibitor (bacterial)		+				
Plate09H10	Cephalothin sodium salt	Antibacterial	transpeptidase inhibitor (bacterial)				+		
Plate09H11	Cefuroxime sodium salt	Antibacterial	transpeptidase inhibitor (bacterial)	+		+			
Plate10A04	Phenethicillin potassium salt	Antibacterial	Transpeptidase inhibitor (bacterial)		-				
Plate13E11	Talampicillin hydrochloride	Antibacterial	Transpeptidase inhibitor (bacterial)				+	+	
Plate14G06	Verteporfin	Treatment of age-related macular degeneration	Treatment of age-related macular degeneration		+	-	-		
Plate06E06	Cyclobenzaprine hydrochloride	Muscle relaxant	Tricyclic antidepressant						-
Plate01B08	Levodopa	Antiparkinsonian	Tyrosine aminotransferase inhibitor		+				
Plate11H10	Capsaicin	Topical analgesic	Vanilloid receptor ligand		-				
Plate12B07	N-Acetyl-L-leucine	Vertigo	Vertigo				-		
Plate06A08	Adamantamine fumarate	Antiviral	Viral assembly inhibition (and uncoating inhibition)	+					
Plate14F11	Vitamin K2	Dietary factor for controlling blood pressure	Vitamin	-					
Plate06C10	Cholecalciferol	Vitamin	Vitamin		+				
Plate06D04	Cyanocobalamin	Vitamin	Vitamin				-		
Plate08G04	Pyridoxine hydrochloride	Vitamin	Vitamin		-				
Plate13E08	Fursultiamine Hydrochloride	Vitamin (enzyme cofactor)	Vitamin					-	
Plate07E11	Trolox	Vitamin E analog	Vitamin	-					
Plate07F09	Phenindione	Anticoagulant	Vitamin K inhibition		+				
Plate09F08	3-alpha-Hydroxy-5-beta-androstan-17-one							+	
Plate13A08	6-Hydroxytryptopine			+			+	-	
Plate14D02	Imidurea						+	+	
Plate14D08	Tropine						+		
Plate14D11	Methiazole			+	+		+		
Plate14E05	Leucomisine						+		

Supplementary Table 4

Compound	Chemical name	Therapeutic group	Mechanism/class	Hit PC3 6h	Hit PC3 36h	Hit HCT116 6h	Hit HCT116 36h	Hit H1299 6h	Hit H1299 36h
Plate08C11	Yohimbic acid monohydrate	-	-	+	+				
Plate09A09	Betonidine	-	-			-			
Plate07A02	Serotonin hydrochloride	Neurotransmitter	5HT agonist			-			
Plate02B10	Mianserine hydrochloride	Antidepressant	5HT antagonist		-				
Plate06F05	Lysergol	Antipsychotic	5HT antagonist		+		+		
Plate06G02	Tropisetron HCl	Antiemetic	5HT antagonist (5HT3)			-			
Plate09C09	Skimmianine	Sedative	5HT ligand			-			
Plate01H03	Imipramine hydrochloride	Antidepressant	5HT transport inhibitor			+			
Plate02B03	Zimelidine dihydrochloride monohydrate	Antidepressant	5HT uptake inhibitor		-				
Plate07D02	Fluoxetine hydrochloride	Antidepressant	5HT uptake inhibitor		-				
Plate11F02	Paroxetine Hydrochloride	Antidepressant	5HT uptake inhibitor		-				
Plate13F05	Sertraline	Antidepressant	5HT uptake inhibitor		-		-		
Plate06B03	Anisomycin	Antiprotozoal	Acetylcholine esterase inhibitor		-				-
Plate14E03	(-)-Eseroline fumarate salt	Potent analgesic	Acetylcholine esterase inhibitor		-				
Plate10E09	Vidarabine	Antiviral	Adenosine antimetabolite	+	+				
Plate01D05	Triamterene	Diuretic	Aldosterone antagonist (non competitive)		+				
Plate09D09	Ricinine		Alkaloid			-			
Plate08E05	Piperlongumine	Antifungal	Alkaloid		-		+/-		-
Plate08E08	Eburnamonine (-)	Cerebral vasodilator	Alkaloid		+/-		-		-
Plate14E09	(+,-)-Synephrine	Adrenergic	Alpha adrenergic agonist					+	
Plate03D08	Metaraminol bitartrate	Vasoconstrictor	alpha Adrenergic agonist					+	
Plate02G08	Nicergoline	Vasodilator	Alpha adrenergic agonist	-					
Plate13F08	Etilefrine hydrochloride	Antihypertensive	Alpha Adrenergic agonist (alpha1)					+	
Plate13H09	Methyldopate hydrochloride	Antihypertensor	Alpha Adrenergic agonist (alpha2)		-				
Plate10B10	Levonordefrin	Vasoconstrictor	Alpha Adrenergic agonist (alpha2)		+/-			+	
Plate10D02	Terazosin hydrochloride	Antihypertensor	Alpha adrenergic antagonist		-				
Plate01H05	Amityptiline hydrochloride	Antidiabetic	Alpha Adrenergic antagonist (alpha1)			+			
Plate12G08	Prazosin hydrochloride	Antihypertensor	Alpha Adrenergic antagonist (alpha1)		+				
Plate09F09	Tetrahydrozoline hydrochloride	Vasoconstrictor	Alpha adrenergic ligand			-			
Plate08H03	Dipivefrin hydrochloride	Adrenergic (ophthalmic)	alpha beta Agrenergic agonist					+	
Plate12F09	Benserazide hydrochloride	In combination with levodopa as antiparkinsonian	amino acid decarboxylase inhibitor (L-aromatic a.a)		-				
Plate04F04	Glafenine hydrochloride	Analgesic	Analgesic					+	
Plate01B10	Captopril	Antihypertensor	Angiotensive converting enzyme inhibitor			-			
Plate10G08	Merbromin	Antibacterial	Antibacterial			+			
Plate13A11	Roxarsone	Antibacterial	Antibacterial	-					
Plate09A03	Epicatechin(-)	Antidiarrhoeic	Antidiarrhoeic	-					
Plate14G11	Parabendazole	Anthelmintic (VET)	Anthelmintic		+/-		-		+/-
Plate13H11	Pyrvinium pamoate	Anthelmintic (Nematodes, enterobiasis)	Anthelmintic	-	-				
Plate10A02	Althiazide	Antihypertensor	Antihypertensor	-	-	+			
Plate13H02	Halofantrine hydrochloride	Antimalarial	Antimalarial		-	+	+		
Plate07B05	Propylthiouracil	Antihyperthyroid	Antimetabolite				+		
Plate11G07	Azacytidine-5	Antineoplastic	Antimetabolite	-					
Plate06H11	Puromycin dihydrochloride	Antiprotozoal	Antimetabolite		-		-		-

Plate10E06	Ethoxyquin	Antifungal	Antioxydant		-				
Plate09G11	Strophanthidin	Cardiotonic	ATPase inhibitor					+	+
Plate08G02	Methoxy-6-harmalan	Psoriasis treatment	Benzodiazepine receptor ligand					+	
Plate03D09	Salbutamol	Bronchodilatator	Beta adrenergic agonist					+	
Plate04E03	Fenoterol hydrobromide	Bronchodilatator	Beta adrenergic agonist					+	
Plate05C06	Clenbuterol hydrochloride	Bronchodilatator	Beta adrenergic agonist					+	
Plate10C10	Isoetharine mesylate salt	Bronchodilatator	Beta adrenergic agonist					+	
Plate14F08	(-)-Isoproterenol hydrochloride	Bronchodilatator	Beta adrenergic agonist					+	
Plate05D03	Dobutamine hydrochloride	Bronchodilatator	Beta adrenergic agonist (beta1)					+	
Plate05E02	Bambuterol hydrochloride	Bronchodilatator	Beta adrenergic agonist (beta2)		-				
Plate05H02	Terbutaline hemisulfate	Bronchodilatator	Beta adrenergic agonist (beta2)		-			+	
Plate12G06	Salmeterol	Bronchodilatator	Beta adrenergic agonist (beta2)					+	
Plate05C10	Ritodrine hydrochloride	Tocolytic	Beta adrenergic agonist (beta2)					+	
Plate12G10	(+,-)-Octopamine hydrochloride	Adrenergic	Beta adrenergic agonist (beta3)					+	
Plate14A04	Penbutolol sulfate	Antihypertensor	Beta adrenergic antagonist		-				
Plate04A11	Alprenolol hydrochloride	Antihypertensor	Beta adrenergic antagonist (beta1)		-				
Plate04D08	Labetalol hydrochloride	Antihypertensor	Beta adrenergic antagonist (beta1)					+	
Plate03A10	Hydralazine hydrochloride	Antihypertensor	Beta adrenergic antagonist (could be, not shown)		-				
Plate07F07	(S)-(-)-Atenolol	Antihypertensor	beta adrenergic blocker					+	
Plate14B08	Oxprenolol hydrochloride	Antihypertensor	Beta adrenergic blocker		+/-				
Plate03F04	Fenspiride hydrochloride	Antiinflammatory	Bradykinin antagonist					+	
Plate12D02	(+)-Isoproterenol (+)-bitartrate salt	Bronchodilatator	Bronchodilatator		-	+		+	
Plate08H11	Solanine alpha	Antifungal	Butyrylcholinesterase inhibitor		-				
Plate02G05	Loperamide hydrochloride	Antidiarrhoeic	Ca2+ channel antagonist						-
Plate05E09	Bepidil hydrochloride	Antianginal	Ca2+ channel blocker		-				
Plate04E07	Perhexiline maleate	Vasodilatator	Ca2+ channel blocker		-	-		-	+
Plate06H09	Felodipine	Antihypertensor	Ca2+ channel blocker (L-Type)		-				
Plate11C10	Dimethadione	Anticonvulsant	'Ca2+ channel inhibitor voltage dependant		-				
Plate04C11	Fendiline hydrochloride	Antianginal	Ca2+ channel stimulation		-				
Plate07H11	Prenylamine lactate	Vasodilatator	Ca2+ channel stimulation		-		-		+
Plate14C06	Milrinone	Cardiotonic	cAMP/PKA		-				
Plate01A04	Acetazolamide	Diuretic	Carbonic anhydrase inhibitor			+			
Plate11A10	Dichlorphenamide		Carbonic anhydrase inhibitor		-				
Plate13C07	Proscillaridin A	Cardiotonic	Cardiac glycoside					+	+
Plate05F03	Debrisoquin sulfate	Antihypertensor	Catecholamine depletor				+	+	
Plate07G02	Ciclopirox ethanolamine	Antifungal	Cell membrane proteins synthesis inhibitor				+		+
Plate14H09	Cefepime hydrochloride	Antibacterial	Cell wall destruction agent					+	
Plate09D03	(d,l)-Tetrahydroberberine	Sedative	Cell wall synthesis inhibitor		-				
Plate06G11	Ceforanide	Antibacterial	Cell wall synthesis inhibitor (bacterial)				+		
Plate14D09	Benzylpenicillin sodium	Antibacterial	Cell wall synthesis inhibitor (bacterial)					+	
Plate10A06	Deferoxamine mesylate		chelating agent				+		+
Plate12A07	Clioquinol	Anti-infective	Chelating agent, chymotrypsin-like proteasome activity inhibitor		-				
Plate02E04	Dehydrocholic acid	Choleretic	Choleretic		+				

Plate05G05	Probucol	Antihyperlipoproteinemic	Cholesterol downregulation				-		
Plate03E03	Tiratricol, 3,3',5-triiodothyroacetic acid	Hypocholesterolemic drug	Cholesterol downregulation					+	+
Plate02A04	Edrophonium chloride	Myasthenia Gravis test	Cholinergic						+
Plate01F03	Carbamazepine	Anticonvulsivant	Cholinergic antagonist			+			
Plate01H06	Adiphenine hydrochloride	Local anesthetic	cholinergic inhibition				+		
Plate10H05	Eucatropine hydrochloride		cholinergic inhibition				+		
Plate02A03	Cotinine (-)	Antidepressant	cholinergic inhibition (and nicotinic inhibition)						+
Plate02C08	Tomatine	Antifungal	Cholinergic inhibition (pH-dependent competitive inhibition of the enzyme acetylcholinesterase)	-	-	-	-		
Plate10C02	Nadide	-	CoA nicotinamide adenine dinucleotide				-		
Plate07D07	Lovastatin	Antihypercholesterolemic	CoA reductase inhibitor (HMG CoA)				-		
Plate13A10	3-Acetamidocoumarin	Antiinflammatory	coumarin	-					
Plate03E04	Flufenamic acid	Analgesic	cyclooxygenase inhibition						+
Plate01D10	Diflunisal	Antiinflammatory	cyclooxygenase inhibition				-		
Plate02B09	Acetylsalicylsalicylic acid	Antiinflammatory	cyclooxygenase inhibition			-			
Plate07C09	Resveratrol	Antiinflammatory	cyclooxygenase inhibition					-	
Plate10B11	Ebselen	Antiinflammatory	cyclooxygenase inhibition	-	-				
Plate10H02	(R) -Naproxen sodium salt	Antiinflammatory	cyclooxygenase inhibition			-			+
Plate11B07	Suprofen	Antiinflammatory	cyclooxygenase inhibition	-					
Plate11F07	Tolmetin sodium salt dihydrate	Antiinflammatory	cyclooxygenase inhibition	-					
Plate13E04	Azapropazone	Anti-inflammatory	cyclooxygenase inhibition			-			
Plate14A10	Oxyphenbutazone	Anti-inflammatory	cyclooxygenase inhibition	-	-	-	-		-
Plate09G06	Methyl benzethonium chloride	Antibacterial	Detergent	-					
Plate09G09	Benzethonium chloride	Antibacterial	Detergent				-		+
Plate10F08	Alexidine dihydrochloride	Antibacterial	Detergent	-	-	-	-	+/-	-
Plate10H03	Propidium iodide	Antibacterial	Detergent						+
Plate02G04	Chlorhexidine	Bacteriostatic	Detergent			-			+
Plate12E06	Thonzonium bromide		Detergent			-			
Plate02A02	Metronidazole	Antibacterial	DNA damage (bacterial)						+
Plate07B03	Nitrofurantoin	Antibacterial	DNA damage (bacterial)				-		
Plate07H06	Nifuroxazide	Antibacterial	DNA damage (bacterial)						+
Plate02A05	Moroxydine hydrochloride	Antiviral	DNA damage (viral DNA RNA)						-
Plate05D06	Hycanthone	Anthelmintic	DNA intercalating agent			+			
Plate06D09	Doxorubicin hydrochloride	Antibacterial	DNA intercalating agent			+		+	+
Plate08F05	Ellipticine	Anticancer	DNA Intercalating agent	+	+			+	+
Plate07A08	Daunorubicin hydrochloride	Antineoplastic	DNA intercalating agent			+/-			-
Plate14B07	Trifluridine	Antiviral (ophthalmic)	DNA replication inhibitor (viral)	+/-	+/-			+	+
Plate07F05	Atovaquone	Antipneumocystic	DNA synthesis inhibitor (antiprotozoa)			+			
Plate13B11	Piribedil hydrochloride	Vasodilator (peripheral)	Dopamine agonist	-					
Plate02C02	R(-) Apomorphine hydrochloride hemihydrate	Emetic	Dopamine agonist (D1)			+/-			
Plate06F02	Alizapride HCl	Antiemetic	Dopamine antagonist			+/-			
Plate08E02	Scoulerine	Antiemetic	Dopamine antagonist			+/-		-	+/-
Plate02F03	Loxapine succinate	Anxiolytic	Dopamine antagonist			-			

Plate01F04	Triflupromazine hydrochloride	Antipsychotic	Dopamine antagonist ?		-					+
Plate01F07	Sulpiride	Antipsychotic	Dopamine antagonist (D2)		+					
Plate02B08	Disulfiram	Alcohol deterrent	Dopamine beta hydroxylase inhibitor		+/-					-
Plate13D09	Zuclopenthixol hydrochloride	Antipsychotic	dopamine receptor blocker		+					
Plate13H06	Molindone hydrochloride	Antipsychotic	Dopamine receptor ligand		-					
Plate05G07	GBR 12909 dihydrochloride	Antidepressant	Dopamine uptake inhibitor	+						
Plate03G07	Griseofulvin	Antifungal	Enzymatic inductor					-		
Plate11A11	Sulconazole nitrate	Antifungal	Ergosterol synthesis inhibition	-				-		
Plate11G11	Luteolin	Expectorant	Flavonoid		+			+		
Plate03E09	Trimethoprim	Antibacterial	Folic acid antagonist						+	
Plate01D08	Pyrimethamine	Antiprotozoal	Folic acid antagonist		+/-			+		-
Plate10B02	Sulfaquinoxaline sodium salt	Antibacterial	Folic acid synthesis inhibition		-					
Plate08A10	Dihydroergotomine mesylate	Anticonvulsant	GABA A receptor Cl-channel high affinity		-					
Plate07F10	Thiocolchicoside	Muscle relaxant	GABA agonist ?					+		
Plate11E02	Securinine	CNS stimulant	GABA antagonist							+
Plate09C03	Gelsemine	Tumour inhibitor	GABA antagonist	-						
Plate09B03	Picrotoxinin	Analeptic	GABA channel blocker	-						
Plate09B11	Avermectin B1	Anthelmintic	GABA receptors ligand						+	
Plate05A04	Chlorpropamide	Antidiabetic	Glucagon secretogen					+		
Plate02D11	Triamcinolone	Antiinflammatory	glucocorticoid		+					
Plate07D09	Budesonide	Antiinflammatory	Glucocorticoid	+				+		
Plate01H08	Prednisone	Glucocorticoid	Glucocorticoid		-					
Plate04D10	Methylprednisolone, 6-alpha	Glucocorticoid	Glucocorticoid					+	+	
Plate05E03	Betamethasone	Glucocorticoid	Glucocorticoid	+						
Plate09A04	Flunisolide	Glucocorticoid	Glucocorticoid					+		
Plate09A06	Flurandrenolide	Glucocorticoid	Glucocorticoid					+		
Plate09H09	Fluorometholone	Glucocorticoid	Glucocorticoid					-		
Plate10B05	Flumethasone	Glucocorticoid	Glucocorticoid					+		
Plate10F05	Fluocinonide	Glucocorticoid	Glucocorticoid							+
Plate10G02	Clobetasol propionate	Glucocorticoid	Glucocorticoid		-			+		
Plate14H10	Clocortolone pivalate	Glucocorticoid	Glucocorticoid	+				+		
Plate08B03	Mometasone furoate	Antiinflammatory	glucocorticoid receptor agonist					+		
Plate10F02	Alclometasone dipropionate	Anti-inflammatory	glucocorticoid receptor agonist		-					
Plate05E08	Benfluorex hydrochloride	Hypolipemic	Glucose transport enhancer	-						
Plate03F08	Mebendazole	Parasite suppressor	Glucose transport inhibitor ?		+			+/-		+/-
Plate02E07	Mefloquine hydrochloride	Antimalarial	Heme polymerase inhibitor		-	-				
Plate06H07	Primaquine diphosphate	Antimalarial	Heme polymerase inhibitor		-					+/-
Plate10H08	Methotrimeprazine maleate salt	Analgesic	Histamine antagonist					+		
Plate09G07	Chlorcyclizine hydrochloride	Antihistaminic	Histamine antagonist						+	
Plate10H04	Cloperastine hydrochloride	Antitussive	Histamine antagonist		-					
Plate02F07	Astemizole	Antihistaminic	Histamine antagonist (H1)		-					
Plate11A08	Chloropyramine hydrochloride	Antihistaminic	Histamine antagonist (H1)					+		
Plate13H10	Levocabastine hydrochloride	Antihistaminic	Histamine antagonist (H1)	-						
Plate03E02	Ranitidine hydrochloride	Antiulcerative	Histamine antagonist (H2)					-		
Plate06C09	Roxatidine Acetate HCl	Antiulcerative	Histamine antagonist (H2)		-					-
Plate09E09	Estropipate	Estrogen	Hormone estrogen					-		
Plate10D07	Diethylstilbestrol	Estrogen	Hormone estrogen		+			-		
Plate11E07	Ethinylestradiol 3-methyl ether	Estrogen	Hormone estrogen	-						

Plate05H08	Clomiphene citrate (Z,E)	Antineoplastic	hormone Estrogen agonist		-				
Plate02C06	Danazol	Antigonadotropin	hormone Estrogen antagonist		+/-		-		-
Plate07H07	Mycophenolic acid	Antineoplastic	Inosine monophosphate dehydrogenase inhibitor		+/-				+
Plate02E03	Metanephrine hydrochloride DL		Isoprenaline uptake inhibitor extraneuronal		-	+			
Plate07H05	Tolazamide	Antidiabetic	K+ channel blocker (ATP-dependent channels)					+	
Plate01F06	Acetohexamide	Antidiabetic (type II, noninsulin-dependent)	K+ channel blocker (ATP-dependent channels)		+				
Plate02F02	Glipizide	Hypoglycemic	K+ channel blocker (ATP-dependent channels)			-			
Plate03C11	Tolbutamide	Hypoglycemic	K+ channel blocker (ATP-dependent channels)	+			+		+
Plate04E05	Diethylcarbamazine citrate	Anthelmintic	Lipoxygenase inhibitor					+	
Plate07C08	Quercetine dihydrate	Antimalarial	Lipoxygenase inhibitor				-		
Plate08F03	Harmol hydrochloride monohydrate	Anxiolytic	Liver conjugation probe					+	
Plate11H07	Arcaine sulfate		Lowers blood sugar	-		+			
Plate12A04	Digoxigenin	Diagnosis	Mainly used as a non-isotopic label for DNA				-	+	+
Plate03A11	Phenelzine sulfate	Antidepressant	MAO inhibitor	-					
Plate03B04	Tranylcypromine hydrochloride	Antidepressant	MAO inhibitor			-			
Plate08F04	Harmine hydrochloride	Anthelmintic	MAO inhibitor		+				
Plate04H09	Quinacrine dihydrochloride dihydrate	Antimalarial	MAO inhibitor						+
Plate07G11	Parthenolide	Antiinflammatory	MAPK inhibitor		-	+	-		+
Plate06B05	Apigenin	Antiproliferative	MAPK inhibitor		+			+	
Plate12D03	Monobenzone	Depigmentor	melanin inhibition		-		+		+
Plate09A07	Helveticoside	Cardiotonic	membrane ATP inhibitor					+	-
Plate10C09	Monensin sodium salt	Antibacterial	Membrane ionophores producer				-		
Plate03E11	Fenbendazole	Anthelmintic	microtubule polymerisation inhibitor		+		+/-		-
Plate05E04	Colchicine	Antiinflammatory	microtubule polymerisation inhibitor		+/-		-		-
Plate02B11	Nocodazole	Antineoplastic	microtubule polymerisation inhibitor		+/-		+/-		-
Plate02H06	Paclitaxel	Antineoplastic	microtubule polymerisation inhibitor		+/-		-	-	+/-
Plate04A08	Albendazole		microtubule polymerization inhibition		+/-		+/-		+/-
Plate10G03	Podophyllotoxin	Antiviral	Microtubule polymerization inhibitor	-	-		+/-		+/-
Plate03G03	Antimycin A	Antifungal	Mitochondrial electron transport inhibitor			-	+		+
Plate09D07	Beta-Escin	Peripheral vascular disorders	Momoamine transport inhibition		-				
Plate14B06	Piperidolate hydrochloride	Antispasmodic	Muscarinic blocking agent		+				
Plate09H03	Benzocaine	Anesthetic	Na+ channel blocker	-					
Plate10E02	Butamben	Anesthetic	Na+ channel blocker		-				
Plate01E10	Amyleine hydrochloride	Local Anesthetic	Na+ channel blocker			-			
Plate03D10	Prilocaine hydrochloride	Local anesthetic	Na+ channel blocker		+				+
Plate04D06	Fenofibrate	Hypolipidemiant	<b>Na+ channel inhibitor (voltage-dependent)</b>					+	
Plate10G05	Bendroflumethiazide	Antihypertensor	Na+ Cl- transport inhibitor			-			
Plate03F11	Indapamide	Antihypertensor	Na+ Cl- uptake inhibitor		+/-				



Plate02D03	Metolazone	Diuretic	Na+ Cl- uptake inhibitor		-				
Plate14A11	Quinethazone	Diuretic	Na+ Cl- uptake inhibitor	-					
Plate13C08	Sanguinarine	Antimicrobial drug	Na+ K+ ATPase inhibitor		+				
Plate06D07	Digitoxigenin	Cardiotonic	Na+ K+ ATPase inhibitor				+	+	
Plate06D08	Digoxin	Cardiotonic	Na+ K+ ATPase inhibitor				+		
Plate06H02	Strophantine octahydrate	Cardiotonic	Na+ K+ ATPase inhibitor				+	+	
Plate09B07	Lanatoside C	Cardiotonic	Na+ K+ ATPase inhibitor	-			+	+	
Plate13A09	Decamethonium bromide	Muscle relaxant (skeletal)	Neuromuscular depolarizing agent	-					
Plate09E03	beta- Belladonnine dichloroethylate	Muscle relaxant	Nicotinic receptor ligand	-					
Plate11A07	Trimipramine maleate salt	Antidepressant	Noradrenaline uptake inhibitor	-					
Plate09B09	Suxibuzone	Antiinflammatory	NSAI			-			
Plate11C07	Oxalamine citrate salt	Antiinflammatory	NSAI	-					
Plate10H09	Dienestrol	Non-steroidal estrogen	Nuclear receptor ligand		-		-		-
Plate01B09	Idoxuridine	Antiviral	Nucleic acid synthesis inhibitors		+				
Plate13G06	Letrozole	Antineoplastic	P450 inhibitor					+	
Plate02E05	Hesperetin		P450 inhibitor		+/-				
Plate10F09	Proadifen hydrochloride	Local anesthetic	P450 inhibitor (mono-oxygenases)	-	-				
Plate04A03	Flavoxate hydrochloride	Antispasmodic	Phosphodiesterase inhibitor				+		
Plate08C08	Cilostazol	Antithrombotic	Phosphodiesterase inhibitor		+/-		-		+/-
Plate13F09	Alprostadil	Vasodilator	Prostaglandine E1 receptor ligand	-					
Plate14H05	Saquinavir mesylate	Antiviral (HIV)	Protease inhibitor				-		
Plate02G07	Tamoxifen citrate	Anticancer	Protein kinase C inhibitor						+
Plate08A11	Emetine dihydrochloride	Antiamebic	Protein synthesis inhibitor		-		-		-
Plate10G11	Cycloheximide	Antibacterial	Protein synthesis inhibitor				-		
Plate13A05	Methacycline hydrochloride	Antibacterial	Protein synthesis inhibitor (bacteria)	-					
Plate02H05	Josamycin	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate05H05	Kanamycin A sulfate	Antibacterial	Ribosomal protein synthesis inhibitor				+		
Plate13F10	Tribenoside	Sclerosing agent	Sclerosing agent	-	-				
Plate12A06	Cantharidin	Rubefiant	Serine protease releaser		-		-		
Plate10G10	Drofenine hydrochloride	Spasmolytic	Spasmolytic				-		
Plate02E08	Isoconazole	Antibacterial	Sterol 14-demethylase inhibitor		-				
Plate01G08	Miconazole	Antifungal	Sterol 14-demethylase inhibitor		-				
Plate03D11	Camptothecine (S,+)	Antitumor agent	Topoisomerase I inhibitor		+/-		+		+
Plate03E05	Flumequine	Antibacterial	Topoisomerase II inhibitor					+	
Plate05G06	Mitoxantrone dihydrochloride	Antineoplastic	topoisomerase II inhibitor		-		+		+
Plate05H07	Etoposide	Antineoplastic	Topoisomerase II inhibitor	+	+		+/-		
Plate14H11	Nadifloxacin	Antibacterial	Topoisomerase inhibitor (topoisomerase II)	-					
Plate02D05	Ampicillin trihydrate	Antibacterial	transpeptidase inhibitor (bacterial)		-				
Plate14G06	Verteporfin	Treatment of age-related macular degeneration	Treatment of age-related macular degeneration					+	
Plate11H10	Capsaicin	Topical analgesic	Vanilloid receptor ligand		+				
Plate06C02	Suloctidil	Vasodilatator	Vasodilatator		-				
Plate12B07	N-Acetyl-L-leucine	Vertigo	Vertigo					+	
Plate06A08	Adamantamine fumarate	Antiviral	Viral assembly inhibition (and uncoating inhibition)				+		
Plate08H05	Riboflavine	Vitamin	Vitamin					+	
Plate07E11	Trolox	Vitamin E analog	Vitamin		+				

Plate06F10	Menadione	Vitamin K3	Vitamin precursor		<b>+/-</b>				
Plate14D11	Methiazole						-		-

Supplementary Table 5

Compound	Chemical name	Therapeutic group	Mechanism/class	Hit PC3 6h	Hit PC3 36h	Hit HCT116 6h	Hit HCT116 36h	Hit H1299 6h	Hit H1299 36h
Plate09A09	Betonidine	-	-			-			
Plate02B10	Mianserine hydrochloride	Antidepressant	5HT antagonist		-				
Plate02C04	Cyproheptadine hydrochloride	Antipruritic	5HT antagonist		-				
Plate06G02	Tropisetron HCl	Antiemetic	5HT antagonist (5HT3)			-			
Plate02E11	Dexamethasone acetate	Antiinflammatory	5HT antagonist effect doper		-				
Plate09C09	Skimmianine	Sedative	5HT ligand			-			
Plate01H03	Imipramine hydrochloride	Antidepressant	5HT transport inhibitor		-	+			
Plate02B03	Zimelidine dihydrochloride monohydrate	Antidepressant	5HT uptake inhibitor		-				
Plate07D02	Fluoxetine hydrochloride	Antidepressant	5HT uptake inhibitor		+				
Plate11F02	Paroxetine Hydrochloride	Antidepressant	5HT uptake inhibitor	+	-				
Plate13F05	Sertraline	Antidepressant	5HT uptake inhibitor	+			+		
Plate09F03	Citalopram Hydrobromide	Antidepressant	5HT uptake inhibitor	-					
Plate06B03	Anisomycin	Antiprotozoal	Acetylcholine esterase inhibitor		+/-	+	+		+
Plate14E03	(-)-Eseroline fumarate salt	Potent analgesic	Acetylcholine esterase inhibitor		-				
Plate02G03	Dipyridamole	Platelet antiagregant	Adenosine metabolism inhibitor		-				
Plate01E08	Ticlopidine hydrochloride	Platelet antiagregant	ADP antagonist	-	-				
Plate02E09	Spironolactone	Diuretic	Aldosterone antagonist		-				
Plate01D05	Triamterene	Diuretic	Aldosterone antagonist (non competitive)		-				
Plate09D09	Ricinine		Alkaloid			-			
Plate08E05	Piperlongumine	Antifungal	Alkaloid	+	+	+			+
Plate08B05	Dacarbazine	Antineoplastic	Alkylating agent			+			
Plate02B07	Guanabenz acetate	Antihypertensor	Alpha adrenergic agonist		-				
Plate02G08	Nicergoline	Vasodilatator	Alpha adrenergic agonist	-	-				
Plate12E07	Idazoxan hydrochloride	Antiparkinsonian	Alpha adrenergic agonist (alpha2)		+				
Plate10B10	Levonordefrin	Vasoconstrictor	Alpha Adrenergic agonist (alpha2)			-			
Plate01E03	Moxislyte hydrochloride	Vasodilatator	Alpha adrenergic antagonist		-				
Plate01F11	Tolazoline hydrochloride	Vasodilatator	Alpha adrenergic antagonist		-				
Plate01H05	Amitryptiline hydrochloride	Antidiabetic	Alpha Adrenergic antagonist (alpha1)		-	+			
Plate09F09	Tetrahydrozoline hydrochloride	Vasoconstrictor	Alpha adrenergic ligand			-			
Plate01E07	Naphazoline hydrochloride	Vasoconstrictor	alpha adrenergic ligand		-				
Plate01B10	Captopril	Antihypertensor	Angiotensive converting enzyme inhibitor			-			
Plate13A11	Roxarsone	Antibacterial	Antibacterial	-					
Plate09A03	Epicatechin(-)	Antidiarrhoeic	Antidiarrhoeic	-					
Plate14G11	Parbendazole	Anthelmintic (VET)	Anthelmintic	+	-				+
Plate13H11	Pyrvinium pamoate	Anthelmintic (Nematodes, enterobiasis)	Anthelmintic	+/-					
Plate01H02	Todralazine hydrochloride	Antihypertensor	Antihypertensor		-				
Plate13H02	Halofantrine hydrochloride	Antimalarial	Antimalarial		-	+			
Plate11G07	Azacytidine-5	Antineoplastic	Antimetabolite	+/-			+		+
Plate06H11	Puromycin dihydrochloride	Antiprotozoal	Antimetabolite		-				
Plate02B05	Azathioprine	Immunosuppressant	Antimetabolite		-				
Plate10E06	Ethoxyquin	Antifungal	Antioxydant		+/-				
Plate09G11	Strophanthidin	Cardiotonic	ATPase inhibitor				+		+
Plate10C10	Isoetharine mesylate salt	Bronchodilator	Beta adrenergic agonist			-			

Plate01G09	Isoxsuprine hydrochloride	Vasodilatator	Beta adrenergic agonist	-	-			
Plate05H02	Terbutaline hemisulfate	Bronchodilatator	Beta adrenergic agonist (beta2)		-			
Plate01G10	Acebutolol hydrochloride	Antianginal	Beta adrenergic antagonist (beta1)	-	-			
Plate14B08	Oxprenolol hydrochloride	Antihypertensor	Beta adrenergic blocker	-				
Plate12D02	(+)-Isoproterenol (+)-bitartrate salt	Bronchodilatator	Bronchodilatator	+			+	
Plate02G05	Loperamide hydrochloride	Antidiarrhoeic	Ca2+ channel antagonist	-				
Plate01H09	Thioridazine hydrochloride	Neuroleptic	Ca2+ channel antagonist	-				
Plate05E09	Bepidil hydrochloride	Antianginal	Ca2+ channel blocker	-				
Plate09D03	(d,l)-Tetrahydroberberine	Sedative	Ca2+ channel blocker	-				
Plate04E07	Perhexiline maleate	Vasodilatator	Ca2+ channel blocker	-	-	+		+
Plate02F05	Diltiazem hydrochloride	Antianginal	Ca2+ channel blocker (L-Type)	-				
Plate06H09	Felodipine	Antihypertensor	Ca2+ channel blocker (L-Type)	-				
Plate07H11	Prenylamine lactate	Vasodilatator	Ca2+ channel stimulation	+/-				+
Plate01G04	Nifedipine	Antihypertensor	Ca2+ channels blocker (L type)	-	+			
Plate01A05	Metformin hydrochloride	Antidiabetic	cAMP/PKA	-				
Plate01A04	Acetazolamide	Diuretic	Carbonic anhydrase inhibitor	-	+			
Plate13C07	Proscillaridin A	Cardiotonic	Cardiac glycoside			+		+
Plate14H09	Cefepime hydrochloride	Antibacterial	Cell wall destruction agent		-			
Plate06G11	Ceforanide	Antibacterial	Cell wall synthesis inhibitor (bacterial)	+				
Plate01C09	Ethambutol dihydrochloride	Antibacterial	Chelating agent	-				
Plate02E04	Dehydrocholic acid	Choleretic	Choleretic	-				
Plate05G05	Probucol	Antihyperlipoproteine mic	Cholesterol downregulation		-			
Plate02A04	Edrophonium chloride	Myasthenia Gravis test	Cholinergic					+
Plate01F03	Carbamazepine	Anticonvulsivant	Cholinergic antagonist	-				
Plate01E09	Dicyclomine hydrochloride	Antispasmodic	cholinergic inhibition	-				
Plate01H10	Diphepanil methylsulfate	Bronchodilatator	cholinergic inhibition	-				
Plate01H06	Adiphenine hydrochloride	Local anesthetic	cholinergic inhibition	-	+			
Plate02A03	Cotinine (-)	Antidepressant	cholinergic inhibition (and nicotinic inhibition)					+
Plate02C08	Tomatine	Antifungal	Cholinergic inhibition (pH-dependent competitive inhibition of the enzyme acetylcholinesterase)	-	-	-		
Plate01F02	Trichlorfon	Anthelminthic	cholinergic inhibition Cholinesterase inhibitor	-				
Plate01C03	Panthenol (D)	Vitamin	CoA synthesis precursor	-				
Plate04H05	Enalapril maleate	Antihypertensor	Converting enzyme inhibitor			+		
Plate01C10	Antipyrine	Analgesic	cyclooxygenase inhibition	-				
Plate03E06	Tolfenamic acid	Antiinflammatory	cyclooxygenase inhibition				+	
Plate01D10	Diflunisal	Antiinflammatory	cyclooxygenase inhibition	-				
Plate01E06	Naproxen	Antiinflammatory	cyclooxygenase inhibition	-				
Plate01F05	Mefenamic acid	Antiinflammatory	cyclooxygenase inhibition	-				
Plate01H04	Sulindac	Antiinflammatory	cyclooxygenase inhibition	-				
Plate02B09	Acetylsalicylic acid	Antiinflammatory	cyclooxygenase inhibition	-				
Plate10H02	(R) -Naproxen sodium salt	Antiinflammatory	cyclooxygenase inhibition	+				
Plate03F10	Ketoprofen	Antiinflammatory	cyclooxygenase inhibition	-				
Plate07C09	Resveratrol	Antiinflammatory	cyclooxygenase inhibition	+				
Plate10B11	Ebselen	Antiinflammatory	cyclooxygenase inhibition	-				

Plate11F07	Tolmetin sodium salt dihydrate	Antiinflammatory	cyclooxygenase inhibition	-					
Plate01E05	Isoxicam	Antiinflammatory	cyclooxygenase inhibition	-	-				
Plate11B07	Suprofen	Antiinflammatory	cyclooxygenase inhibition	+/-					
Plate11D07	Indoprofen	Antiinflammatory	cyclooxygenase inhibition	+/-					
Plate13E04	Azapropazone	Anti-inflammatory	cyclooxygenase inhibition			+			
Plate14A10	Oxyphenbutazone	Anti-inflammatory	cyclooxygenase inhibition	-	-	+/-	+		
Plate01C11	Antipyrine, 4-hydroxy	Antipyrine metabolite	cyclooxygenase inhibition		-				
Plate10H03	Propidium iodide	Antibacterial	Detergent						+
Plate09G09	Benzethonium chloride	Antibacterial	Detergent			-			
Plate10F08	Alexidine dihydrochloride	Antibacterial	Detergent		-	-		+	+
Plate09G06	Methyl benzethonium chloride	Antibacterial	Detergent	-					+
Plate02G09	Canrenoic acid potassium salt	Antihypercholesterolemic	Detergent		-				
Plate02G04	Chlorhexidine	Bacteriostatic	Detergent		-				+
Plate02A10	Ursolic acid	Diuretic	Diuretic		-				
Plate02A02	Metronidazole	Antibacterial	DNA damage (bacterial)		-				+
Plate07B03	Nitrofurural	Antibacterial	DNA damage (bacterial)	+					
Plate01D11	Niclosamide	Anthelmintic	DNA damage (Helminthic)		-				
Plate02A05	Moroxidine hydrochloride	Antiviral	DNA damage (viral DNA RNA)		-				
Plate07A08	Daunorubicin hydrochloride	Antineoplastic	DNA intercalating agent		-		+		+
Plate14B07	Trifluridine	Antiviral (ophthalmic)	DNA replication inhibitor (viral)		-				
Plate01G07	Minaprine dihydrochloride	Antidepressant	Dopamine agonist		-				
Plate02C02	R(-) Apomorphine hydrochloride hemihydrate	Emetic	Dopamine agonist (D1)		+				
Plate08G09	Salsolinol hydrobromide	-	Dopamine analog			-			
Plate01G05	Chlorpromazine hydrochloride	Antiemetic	Dopamine antagonist		-				
Plate08E02	Scoulerine	Antiemetic	Dopamine antagonist		-				+
Plate02D06	Haloperidol	Antipsychotic	Dopamine antagonist		-				
Plate02E06	Perphenazine	Antipsychotic	Dopamine antagonist		-				
Plate02G10	Thiopropazine dimesylate	Antipsychotic	Dopamine antagonist		-				
Plate02F03	Loxapine succinate	Anxiolytic	Dopamine antagonist		-				
Plate01F04	Triflupromazine hydrochloride	Antipsychotic	Dopamine antagonist ?		-				
Plate01H11	Trimethobenzamide hydrochloride	Antiemetic	Dopamine antagonist (D2)		-				
Plate01F07	Sulpiride	Antipsychotic	Dopamine antagonist (D2)		-				
Plate08B07	Acetopromazine maleate salt	Tranquilizer	Dopamine antagonist ?			+			
Plate02B08	Disulfiram	Alcohol deterrent	Dopamine beta hydroxylase inhibitor	+	-		+		+
Plate05G07	GBR 12909 dihydrochloride	Antidepressant	Dopamine uptake inhibitor				+		
Plate02C03	Amoxapine	Antidepressant	Dopamine uptake inhibitor		-				
Plate02C09	Nomifensine maleate	Antidepressant	Dopamine uptake inhibitor		-				
Plate02D10	Picotamide monohydrate	Antithrombotic	Eicosenoid receptor antagonist		-				
Plate01G11	Tolnaftate	Antifungal	Ergosterol synthesis inhibition		-				
Plate11A11	Sulconazole nitrate	Antifungal	Ergosterol synthesis inhibition	-					
Plate01D06	Dapsone	Antiinflammatory	Folic acid antagonist		-				
Plate01D08	Pyrimethamine	Antiprotozoal	Folic acid antagonist		-				
Plate02F06	Methotrexate	anticancer	Folic acid inhibitor		-				
Plate09G03	Succinylsulfathiazole	Antibacterial	Folic acid synthesis inhibition	-					
Plate01A11	Sulfaguandine	Antibacterial	Folic acid synthesis inhibitor		-				
Plate01B05	Sulfacetamide sodic hydrate	Antibacterial	Folic acid synthesis inhibitor		-				

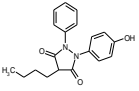
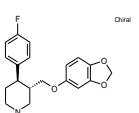
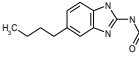
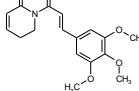
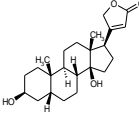
Plate01B07	Sulfathiazole	Antibacterial	Folic acid synthesis inhibitor		-				
Plate01C02	Sulfaphenazole	Antibacterial	Folic acid synthesis inhibitor		-				
Plate01C04	Sulfadiazine	Antibacterial	Folic acid synthesis inhibitor		-				
Plate01G02	Morantel tartrate	Anthelmintic	Fumarate reductase inhibitor		-	+			
Plate08A10	Dihydroergotoxine mesylate	Anticonvulsant	GABA A receptor Cl-channel high affinity	+					+
Plate07F10	Thiocolchicoside	Muscle relaxant	GABA agonist ?	+					
Plate09C03	Gelsemine	Tumour inhibitor	GABA antagonist	-					
Plate09B03	Picrotoxinin	Analeptic	GABA channel blocker	-					
Plate11G02	Gabapentin	Anticonvulsant	GABA receptor ligand	+					
Plate01D09	Hexamethonium dibromide dihydrate	Antihypertensor	Ganglion blocker		-				
Plate02D11	Triamcinolone	Antiinflammatory	glucocorticoid		-				
Plate01A07	Isoflupredone acetate	Anti-inflammatory	Glucocorticoid		-	+			
Plate09H09	Fluorometholone	Glucocorticoid	Glucocorticoid			-			
Plate01H08	Prednisone	Glucocorticoid	Glucocorticoid		+				
Plate10G02	Clobetasol propionate	Glucocorticoid	Glucocorticoid		-				
Plate14H10	Clocortolone pivalate	Glucocorticoid	Glucocorticoid		-				
Plate10F02	Alclometasone dipropionate	Anti-inflammatory	glucocorticoid receptor agonist			-			
Plate02E07	Mefloquine hydrochloride	Antimalarial	Heme polymerase inhibitor		+/-				
Plate06H07	Primaquine diphosphate	Antimalarial	Heme polymerase inhibitor		+/-	+	+		+
Plate01E04	Betazole hydrochloride	Gastric secretion stimulant	Histamine analog		-				
Plate11A08	Chloropyramine hydrochloride	Antihistaminic	Histamine antagonist (H1)			+			
Plate01C08	Doxylamine succinate	Antihistaminic	Histamine antagonist (H1)		-				
Plate01F10	Pheniramine maleate	Antihistaminic	Histamine antagonist (H1)		-				
Plate01G06	Diphenhydramine hydrochloride	Antihistaminic	Histamine antagonist (H1)		-				
Plate02D08	Chlorpheniramine maleate	Antihistaminic	Histamine antagonist (H1)		-				
Plate02F04	Hydroxyzine dihydrochloride	Antihistaminic	Histamine antagonist (H1)		-				
Plate02F07	Astemizole	Antihistaminic	Histamine antagonist (H1)		-				
Plate02F09	Terfenadine	Antihistaminic	Histamine antagonist (H1)		-				
Plate02B04	Azacyclonol	Anxiolytic	Histamine antagonist (H1)		-				
Plate01C07	Cimetidine	Antiulcer	Histamine antagonist (H2)		-				
Plate02C05	Famotidine	Antiulcerative	Histamine antagonist (H2)		-				
Plate06C09	Roxatidine Acetate HCl	Antiulcerative	Histamine antagonist (H2)	+	+/-		+		+
Plate03B11	Flutamide	Anticancer	hormone androgen receptor antagonist		-				
Plate09E09	Estropipate	Estrogen	Hormone estrogen			-			
Plate11E07	Ethinylestradiol 3-methyl ether	Estrogen	Hormone estrogen	+/-					
Plate02C06	Danazol	Antigonadotropin	hormone Estrogen antagonist		-				
Plate02B06	Lynestrenol	Progestogen	hormone estrogen inhibition		-				
Plate07H07	Mycophenolic acid	Antineoplastic	Inosine monophosphate dehydrogenase inhibitor		+/-				+
Plate02E03	Metanephine hydrochloride DL		Isoprenaline uptake inhibitor extraneuronal		-				
Plate02C07	Nicorandil	Antihypertensor	K+ channel agonist (ATP-dependent channels)		-				
Plate01F06	Acetohexamide	Antidiabetic (type II, noninsulin-dependent)	K+ channel blocker (ATP-dependent channels)		-				
Plate02F02	Glipizide	Hypoglycemic	K+ channel blocker (ATP-dependent channels)		-				



Plate02D07	Naltrexone hydrochloride dihydrate	Analgesic	Opioid antagonist		-				
Plate02D02	Naloxone hydrochloride	Opiate antidote	Opioid antagonist		-				
Plate02D09	Nalbuphine hydrochloride	Analgesic	Opioid ligand		-				
Plate02E05	Hesperetin		P450 inhibitor		-				
Plate10F09	Proadifen hydrochloride	Local anesthetic	P450 inhibitor (mono-oxygenases)	-	-				
Plate05G10	Ketoconazole	Antifungal	P450 inhibitor (P450c17)				+		
Plate08C08	Cilostazol	Antithrombotic	Phosphodiesterase inhibitor	+	+		+		+
Plate01D04	Diprophylline	Cardiac analeptic	Phosphodiesterase inhibitor		-				
Plate02B02	Khellin	Phototherapeutic agent	Phototherapeutic agent		-				
Plate01A03	Allantoin	Vulnerary	Precipitate proteins				+		
Plate01C05	Norethynodrel	Progestogen	Progesterone receptor agonist		-				
Plate02E02	Bromocryptine mesylate	Antiparkinsonian	Prolactin inhibitor		-				
Plate02G07	Tamoxifen citrate	Anticancer	Protein kinase C inhibitor		-				+
Plate08A11	Emetine dihydrochloride	Antiamebic	Protein synthesis inhibitor	+	+/-		+		+
Plate10G11	Cycloheximide	Antibacterial	Protein synthesis inhibitor	+			+		+
Plate09E07	Lycorine hydrochloride	Antitumoral	Protein translation inhibitor	+			+		+
Plate01D02	Chloramphenicol	Antibacterial	Ribosomal peptidyltransferase inhibitor		-				
Plate01C06	Thiamphenicol	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate01D07	Troleandomycin	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate02F08	Clindamycin hydrochloride	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate02F11	Tetracycline hydrochloride	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate02G06	Chlortetracycline hydrochloride	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate02H02	Erythromycin	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate02H03	Oleandomycin phosphate	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate02H09	Neomycin sulfate	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate02H10	Dihydrostreptomycin sulfate	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate02H11	Gentamicine sulfate	Antibacterial	Ribosomal protein synthesis inhibitor		-				
Plate13F10	Tribenoside	Sclerosing agent	Sclerosing agent	-	-				
Plate12A06	Cantharidin	Rubefiant	Serine protease releaser				+	+	
Plate02G11	Dihydroergotamine tartrate	Antimigraine	Serotonin antagonist		-				
Plate05G08	Carbetapentane citrate	Antitussive	Sigma1 receptor ligand				+		
Plate02E08	Isoconazole	Antibacterial	Sterol 14-demethylase inhibitor		-				
Plate01G08	Miconazole	Antifungal	Sterol 14-demethylase inhibitor		-				
Plate01B03	Benzonatate	Antitussive	Stretch receptor sensitivity decrease		-				
Plate01A09	Amprolium hydrochloride	Cocciostatic	Thiamine transport inhibitor		-				
Plate02D04	Ciprofloxacin hydrochloride	Anti-bacterial	topoisomerase and gyrase inhibitor		-				
Plate03D11	Camptothecine (S,+)	Antitumor agent	Topoisomerase I inhibitor				+		
Plate03E05	Flumequine	Antibacterial	Topoisomerase II inhibitor					+	
Plate05G06	Mitoxantrone dihydrochloride	Antineoplastic	topoisomerase II inhibitor				+		+
Plate02D05	Ampicillin trihydrate	Antibacterial	transpeptidase inhibitor (bacterial)		-				
Plate02F10	Cefotaxime sodium salt	Antibacterial	transpeptidase inhibitor (bacterial)		-				
Plate01B08	Levodopa	Antiparkinsonian	Tyrosine aminotransferase inhibitor		-				
Plate02C11	Acenocoumarol	Anticoagulant	Vitamin K antagonist		-				
Plate06F10	Menadione	Vitamin K3	Vitamin precursor		-				



## Supplementary Table 7

Compound name	Structure	Molecular Weight	Therapeutic group	Solubility mg/ml	PC3 6 h	PC3 36 h	H1299 6 h	H1299 36 h	HCT116 6 h	HCT116 36 h
Oxyphenbutazone		324.38285	Anti-inflammatory	25	-	-	-	-	-	-
Paroxetine Hydrochloride		365.83552	Antidepressant	25	Æ	+	Æ	Æ	Æ	Æ
Parbendazole		247.29934	Anthelmintic	4	Æ	+	Æ	+	Æ	+
Piperlongumine		317.34468	Antifungal	20	Æ	Æ	Æ	+	Æ	+
Digitoxigenin		374.52503	Cardiotonic	>125	Æ	Æ	Æ	+	Æ	+

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