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:**
**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).
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 γ, 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

Absolute nuclear size

Relative nuclear size (N/C ratio)

B

Absolute nuclear size

Relative nuclear size (N/C ratio)
**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.
**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.
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).
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 Parbendazole, Astemizole and Paroxetin (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.
A  CELL INVASION
CHROMATIN EFFECTS
smaller nucleus
epithelia
larger nucleus
epithelia

NUCLEOSKELETAL EFFECTS
smaller nucleus
epithelia
larger nucleus
epithelia

B  CELL MOTILITY
normal nucleus
epithelia
nuclear size change
epithelia

Tollis et al. Figure S9
**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:**

| Metric   | Analysis strategy | % of 1-rep hits with p<0.05 | % of 2-rep hits with p<0.05 | % of 3-rep hits with p<0.05 |
|----------|-------------------|-----------------------------|-----------------------------|-----------------------------|
| 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                         |
| 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 | Betonicine | - | - | - | - | - | - | - | - |
| Plate09F02 | Fillaibin | - | - | - | - | - | - | - | - |
| Plate07A02 | Sarotonin hydrochloride | Neurotransmitter | SHT agonist | - | - | - | - | - | - |
| Plate09C09 | Skimmianine | Sedative | SHT ligand | - | - | - | - | - | - |
| Plate07D02 | Fluoxetine hydrochloride | Antidepressant | SHT uptake inhibitor | - | - | - | - | - | - |
| Plate09F03 | Citralopram hydrobromide | Antidepressant | SHT uptake inhibitor | - | - | - | - | - | - |
| Plate11F02 | Paroxetine hydrochloride | Antidepressant | SHT uptake inhibitor | - | - | - | - | - | - |
| Plate13F05 | Sertraline | Antidepressant | SHT uptake inhibitor | - | - | - | - | - | - |
| Plate06B03 | Anisomycin | Antiprotozoal | Acetylcholine esterase inhibitor | - | - | - | - | - | - |
| Plate14E03 | (-)-Eseroline fumarate salt | Potent analgesic | Acetylcholine esterase inhibitor | - | - | - | - | - | - |
| Plate10E09 | Vidarabine | Antiviral | Adenosine antimetabolite | + | + | - | - | - | - |
| Plate10D02 | Tetrahydrozoline hydrochloride | Vasoconstrictor | Alpha adrenergic agonist | - | - | - | - | - | - |
| Plate09G02 | Metaproterenol sulfate, orciprenaline sulfate | Bronchodilator | Beta adrenergic agonist | + | + | - | - | - | - |
| Plate03D08 | Metaraminol bitartrate | Vasoconstrictor | alpha Adrenergic agonist | + | + | - | - | - | - |
| Plate13H02 | Halofantrine hydrochloride | Antimalarial | Antimalarial | - | - | - | - | - | - |
| Plate07A04 | Azathioprine, 6 | Anticancer | Antimetabolite | - | - | - | - | - | - |
| Plate14G11 | Parbendazole | Anthelmintic (VET) | Anthelmintic | - | - | - | - | - | - |
| Plate13H11 | Pyrvinium pamoate | Anthelmintic (Nematodes, enterobiasis) | Anthelmintic | - | - | - | - | - | - |
| Plate10A02 | Althiazide | Antihypertensor | Antihypertensor | - | - | - | - | - | - |
| Plate09F03 | Tetrahydrozoline hydrochloride | Vasoconstrictor | Alpha adrenergic ligand | - | - | - | - | - | - |
| Plate09D09 | Serotonin hydrochloride | Neurotransmitter | SHT agonist | - | - | - | - | - | - |
| Plate14E03 | (+,-)-Synephrine | Adrenergic | Adrenergic | + | + | - | - | - | - |
| Plate03D08 | Metaraminol bitartrate | Vasoconstrictor | alpha Adrenergic agonist | + | + | - | - | - | - |
| Plate13H02 | Halofantrine hydrochloride | Antimalarial | Antimalarial | - | - | - | - | - | - |
| Plate07A04 | Azathioprine, 6 | Anticancer | Antimetabolite | - | - | - | - | - | - |
| Plate14G11 | Parbendazole | Anthelmintic (VET) | Anthelmintic | - | - | - | - | - | - |
| Plate13H11 | Pyrvinium pamoate | Anthelmintic (Nematodes, enterobiasis) | Anthelmintic | - | - | - | - | - | - |
| Plate10A02 | Althiazide | Antihypertensor | Antihypertensor | - | - | - | - | - | - |
| Plate09F03 | Tetrahydrozoline hydrochloride | Vasoconstrictor | Alpha adrenergic ligand | - | - | - | - | - | - |
| Plate09D09 | Serotonin hydrochloride | Neurotransmitter | SHT agonist | - | - | - | - | - | - |
| Plate14E03 | (+,-)-Synephrine | Adrenergic | Adrenergic | + | + | - | - | - | - |
| Plate03D08 | Metaraminol bitartrate | Vasoconstrictor | alpha Adrenergic agonist | + | + | - | - | - | - |
| Plate13H02 | Halofantrine hydrochloride | Antimalarial | Antimalarial | - | - | - | - | - | - |
| Plate07A04 | Azathioprine, 6 | Anticancer | Antimetabolite | - | - | - | - | - | - |
| Plate14G11 | Parbendazole | Anthelmintic (VET) | Anthelmintic | - | - | - | - | - | - |
| Plate13H11 | Pyrvinium pamoate | Anthelmintic (Nematodes, enterobiasis) | Anthelmintic | - | - | - | - | - | - |
| Plate10A02 | Althiazide | Antihypertensor | Antihypertensor | - | - | - | - | - | - |
| Plate09F03 | Tetrahydrozoline hydrochloride | Vasoconstrictor | Alpha adrenergic ligand | - | - | - | - | - | - |
| Plate | Compound | Class | Action | Notes |
|-------|-----------|-------|--------|-------|
| 14F08 | (-)-Isoproterenol hydrochloride | Bronchodilator | Beta adrenergic agonist | + |
| 05D03 | Dobutamine hydrochloride | Bronchodilator | Beta adrenergic agonist (beta1) | + |
| 05H02 | Terbutaline hemisulfate | Bronchodilator | Beta adrenergic agonist (beta2) | + |
| 12G06 | Salmeterol | Bronchodilator | Beta adrenergic agonist (beta2) | + |
| 05C10 | Ritalidine hydrochloride | Tocolytic | Beta adrenergic agonist (beta2) | + |
| 12G10 | (+,-)-Octopamine hydrochloride | Adrenergic | Beta adrenergic agonist (beta3) | + |
| 05C10 | Betaxolol hydrochloride | Antihypertensor | Beta adrenergic antagonist | - |
| 14A04 | Salmeterol | Bronchodilator | Beta adrenergic agonist (beta2) | + |
| 05C10 | Ritodrine hydrochloride | Tocolytic | Beta adrenergic agonist (beta2) | + |
| 12G06 | Propranolol hydrochloride | Antihypertensor | Beta adrenergic antagonist | - |
| 05D03 | (R)-(+)-Atenolol | Antihypertensor | Beta adrenergic blocker (beta1) | - |
| 12H03 | Oxprenolol hydrochloride | Antihypertensor | Beta adrenergic blocker | - |
| 05C10 | Fenspiride hydrochloride | Antiinflammatory | Bradykinin antagonist | - |
| 14B08 | Osprenolol hydrochloride | Antihypertensor | Beta adrenergic blocker | + |
| 12H04 | Debrisoquin sulfate | Antihypertensor | Catecholamine depletor | + |
| 03F04 | Fenspiride hydrochloride | Antiinflammatory | Bradykinin antagonist | + |
| 12G02 | (+)-Isoproterenol (+)-bitartrate salt | Bronchodilator | Bronchodilator | + |
| 05E09 | Bepranol hydrochloride | Antiinflammatory | Ca2+ channel blocker | - |
| 09D03 | Tetrahydrodibergainine | Sedative | Ca2+ channel blocker | - |
| 04E07 | Perhexiline maleate | Vasodilator | Ca2+ channel blocker | - |
| 06H09 | Felodipine | Antihypertensor | Ca2+ channel blocker (L-Type) | - |
| 07H11 | Prenylamine lactate | Vasodilator | Ca2+ channel stimulation | - |
| 13C07 | Proscillaridin A | Cardiotonic | Cardiac glycoside | + |
| 05F03 | Debrisoquin sulfate | Antihypertensor | Catecholamine depletor | + |
| 07G02 | Ciclopirox ethanolate | Antifungal | Cell membrane proteins synthesis inhibitor | + |
| 14H09 | Cefepime | Antibacterial | Cell wall destruction agent | + |
| 06G11 | Ceforanide | Antibacterial | Cell wall synthesis inhibitor | - |
| 14D09 | Benzylpenicillin sodium | Antibacterial | Cell wall synthesis inhibitor | + |
| 10A06 | Defensamine mesylate | Chelating agent | Chelating agent | + |
| 03E03 | Trinitrobenzene-3,3',5'-trifluorotoluidine | Hypocholesteremic drug | Cholesterol downregulation | + |
| 12H09 | Urocol | Anticholesterogenic | Cholesterol regulation | + |
| 07B02 | Metaxime hydrochloride | Antiparkinsonian | Cholinergic inhibition | - |
| 09G02 | Trihexyphenidyl-D,L | Antiparkinsonian | Cholinergic inhibition | - |
| 02C08 | Tomatine | Antifungal | Cholinergic inhibition | - |
| 0C02 | Nadide | - | CoA reductase inhibitor (HMG CoA) | - |
| 07D07 | Lovastatin | Antihypercholesterolemic drug | Cholesterol downregulation | + |
| 13A10 | 3-Acetamidomobacunarin | Antiinflammatory | coumarin | - |
| 03E04 | Flufenamic acid | Analgesic | cyclooxygenase inhibition | + |
| 03E06 | Tolfenamic acid | Antiinflammatory | cyclooxygenase inhibition | - |
| 07C09 | Resveratrol | Antiinflammatory | cyclooxygenase inhibition | - |
| 10A03 | Isopyrin hydrochloride | Antiinflammatory | cyclooxygenase inhibition | + |
| 10B11 | Ebselen | Antiinflammatory | cyclooxygenase inhibition | - |
| 10H02 | (R)-Naproxen sodium salt | Antiinflammatory | cyclooxygenase inhibition | + |
| 11B07 | Suprofen | Antiinflammatory | cyclooxygenase inhibition | - |
| 11D07 | Indoprofen | Antiinflammatory | cyclooxygenase inhibition | - |
| 11F07 | Tolmetin sodium salt dihydrate | Antiinflammatory | cyclooxygenase inhibition | - |
| Plate   | Compound                              | Activity                          | Other Effects                        |
|---------|---------------------------------------|-----------------------------------|--------------------------------------|
| 13E04   | Azapropazone                          | Anti-inflammatory                 | cyclooxygenase inhibition            |
| 14A10   | Oxyphenbutazone                       | Anti-inflammatory                 | cyclooxygenase inhibition            |
| 09G06   | Methylbenzethonium chloride           | Antibacterial                     | Detergent                            |
| 09G09   | Benzethonium chloride                 | Antibacterial                     | Detergent                            |
| 10F08   | Alexidine dihydrochloride             | Antibacterial                     | Detergent                            |
| 10H03   | Propidium iodide                      | Antibacterial                     | Detergent                            |
| 02G09   | Carbenoxolonic acid potassium salicylate | Anti-inflammatory   | cyclooxygenase synthase inhibitor  |
| 02G04   | Chlorhexidine                         | Bacteriostatic                    | Detergent                            |
| 12E06   | Theronium bromide                     | Detergent                         |                                      |
| 14F05   | Sulfadoxine                           | Antibacterial                     | Dihydropteroate synthase inhibitor   |
| 09G06   | Canrenoic acid potassium sodium salt | Antihypercholesteremic            |                                      |
| 02G09   | Niclosamide                           | Anthelmintic                      |                                      |
| 09G03   | Succinylsulfathiazole                 | Antibacterial                     | Folic acid synthesis inhibition      |
| 09H02   | Alfaxalone                            | In combination with alfadolone acetate and alfadolone acetate as anesthetic (intravenous) | GABA receptor stimulation           |
| 09G03   | Alfaxalone                            | In combination with alfadoxone acetate and alfadoxone acetate as anesthetic (intravenous) | GABA receptor stimulation           |
| 09G03   | Alfadolone acetate                    | In combination with alfadoxone acetate and alfadoxone acetate as anesthetic (intravenous) | GABA receptor stimulation           |
| 07D09   | Budesonide                            | Anti-inflammatory                 | Glucocorticoid                       |
| 04D10   | Methylprednisolone 6-alpha            | Glucocorticoid                    |                                      |
| 09A06   | Fluoradrenolol                        | Glucocorticoid                    |                                      |
| 09G09   | Fluorometholone                       | Glucocorticoid                    |                                      |
| Plate     | Compound                  | Molecular Function | Structural Function |
|-----------|---------------------------|--------------------|---------------------|
| 10G02     | Clobetasol propionate     | Glucocorticoid     | –                   |
| 14A05     | Prednicarbide             | Glucocorticoid (topical) | Glucocorticoid |
| 08B03     | Mometasone furoate        | Antiinflammatory   | glucocorticoid receptor | agonist |
| 10F02     | Alclometasone dipropionate| Anti-inflammatory  | glucocorticoid receptor | agonist |
| 03F08     | Beclometasone phosphate   | Parasite suppressor| Glucose transport inhibitor ? |
| 02E07     | Mefoquine hydrochloride   | Antimalarial       | Heme polymerase inhibitor |
| 06G07     | Prednisolone              | Antimalarial       | Heme polymerase inhibitor |
| 10H08     | Methotrexate sodium maleate salt | Analgesic, Histamine antagonist |
| 10H04     | Cloterahydrochloride      | Antiinflammatory   | Histamine antagonist |
| 07C11     | Cyloheximide              | Antiinflammatory   | Histamine antagonist (H1) |
| 02F07     | Ketotifen hydrochloride   | Antihistaminic     | Histamine antagonist (H1) |
| 07C04     | Cetirizine dihydrochloride| Antihistaminic     | Histamine antagonist (H1) |
| 13F04     | Dextropine citrate        | Antihistaminic     | Histamine antagonist (H1) |
| 06E09     | Roxatidine dihydrochloride| Antiulcerative     | Histamine antagonist (H2) |
| 14D05     | Cyproterone acetate       | Antiandrogen       | hormone antiandrogen |
| 09E09     | Estropipate               | Estrogen           | Hormone estrogen |
| 10D07     | Diethylstilbestrol        | Estrogen           | Hormone estrogen |
| 11E07     | Ethynylestradiol 3-methyl ether | Estrogen, Hormone estrogen |
| 05H08     | Clomiphene citrate        | Antineoplastic     | hormone estrogen, Estrogen, hormone estrogen agonist |
| 02C06     | Danazol                   | Antagonadotropin   | hormone estrogen antagonist |
| 12H07     | Megestrol acetate         | Progestogen        | Hormone progestogen |
| 07H07     | Mycophenolic acid         | Antineoplastic     | Inosine monophosphate dehydrogenase inhibitor |
| 02E03     | Metamphetamine hydrochloride DL | Isoferrenaline uptake inhibitor extraneuronal |
| 07H05     | Tolazamide                | Antidiabetic       | K+ channel blocker (ATP-dependent channels) |
| 03C11     | Tolbutamide               | Hypoglycemic       | K+ channel blocker (ATP-dependent channels) |
| 08F03     | Harmol hydrochloride      | Antiepileptic      | Liver conjugation probe |
| 11H07     | Arcaine sulfate           | Lower blood sugar  | – |
| 12A04     | Digoxigenin               | Antimalarial       | Mainly used as a non-isotopic label for DNA |
| 03A11     | Phenelzine sulfate        | Antidepressant     | MAO inhibitor |
| 10H06     | Isocarboxazid             | Antidepressant     | MAO inhibitor |
| 08F04     | Harmine hydrochloride     | Antihistaminic     | MAO inhibitor |
| 04H09     | Quinacrine dihydrochloride dihydrate | Antimalarial | MAO inhibitor |
| 07G11     | Parthenolide              | Antineoplastic     | MAPK inhibitor |
| 06B05     | Apigenin                  | Antiproliferative  | MAPK inhibitor |
| 12D03     | Monobenzone               | Depigmentor        | melanin inhibition |
| 09A07     | Helveticoside             | Cardiotoxic        | membrane ATP inhibitor |
| 10C09     | Monensin sodium salt      | Antibacterial      | Membrane ionophores producer |
| 03E11     | Fenbendazole              | Anthelmintic       | microtubule polymerisation inhibitor |
| 05E04     | Colchicine                | Antiinflammatory   | microtubule polymerisation inhibitor |
| 02B11     | Nocodazole                | Antiproliferative  | microtubule polymerisation inhibitor |
| 02H06     | Paclitaxel                | Antiproliferative  | microtubule polymerisation inhibitor |
| Plate | Chemical Name                  | Category                                      | Action                                                                 |
|-------|--------------------------------|-----------------------------------------------|----------------------------------------------------------------------|
| 04A08 | Albendazole                    | Antihelmintic                                 | Neuronal nicotinic acetylcholine receptor ligand                        |
| 10G03 | Podophyllotoxin                | Antitumor                                     | Mammalian cytoskeleton microtubule polymerisation inhibitor             |
| 12H08 | Desoxytocoricoesterone         | Antiviral                                     | Mammalian cytoskeleton microtubule polymerisation inhibitor             |
| 03G03 | Antimycin A                    | Antifungal                                    | Mammalian mitochondrial electron transport inhibitor                    |
| 14C05 | Meprobamate                    | Local anesthetic                              | Mammalian cytoskeleton microtubule polymerisation inhibitor             |
| 09D07 | Beta-escin                     | Peripheral vascular disorder                  | Mammalian cytoskeleton microtubule polymerisation inhibitor             |
| 14B06 | Piperidine hydrochloride       | Anti-analgesic                                | Mammalian cytoskeleton microtubule polymerisation inhibitor             |
| 09H03 | Benzocaine                     | Anesthetic                                    | Na+ channel blocker                                                   |
| 10E02 | Butamben                      | Anesthetic                                    | Na+ channel blocker                                                   |
| 03D10 | Prilocaine hydrochloride       | Local anesthetic                              | Na+ channel blocker                                                   |
| 10G09 | Hexylcaine hydrochloride       | Local anesthetic                              | Na+ channel blocker                                                   |
| 09H07 | Pramoxine hydrochloride        | Local anesthetic (voltage-dependent)          | Na+ channel blocker                                                   |
| 12H10 | Proparacaine hydrochloride     | Topical anesthetic (ophthalmic)               | Na+ channel blocker                                                   |
| 01B04 | Hydroflumethiazide             | Antihypertensive                              | Na+ Cl- transport inhibitor                                           |
| 03F11 | Indapamide                     | Antihypertensive                              | Na+ Cl- transport inhibitor                                           |
| 06D07 | Diltiazem                      | Cardiotoxic                                   | Na+ K+ ATPase inhibitor                                               |
| 06D08 | Digoxin                        | Cardiotoxic                                   | Na+ K+ ATPase inhibitor                                               |
| 06H02 | Strophantin octahydrate        | Cardiotoxic                                   | Na+ K+ ATPase inhibitor                                               |
| 09B07 | Lanatoside C                   | Cardiotoxic                                   | Na+ K+ ATPase inhibitor                                               |
| 03F53 | Pyrantel tartrate              | Anthelmintic                                  | Neuronal nicotinic acetylcholine receptor ligand                        |
| 09E03 | beta-Belladonrin dichloroethylate | Muscle relaxant                              | Nicotinic receptor ligand                                             |
| 11A07 | Trimipramine maleate salt      | Antidepressant                                | Noradrenaline uptake inhibitor                                         |
| 09G04 | Famprofazone                   | Analgesic                                     | NSAI                                                                 |
| 14G05 | Clonixin Lysinate              | Analgesic                                     | NSAI                                                                 |
| 09B09 | Suxibuzone                     | Antiinflammatory                              | NSAI                                                                 |
| 11C07 | Oxalamine citrate salt         | Antiinflammatory                              | NSAI                                                                 |
| 09F10 | Hexestrol                      | Estrogen antiinflammatory                     | Nuclear receptor ligand                                               |
| 10H09 | Dienestrol                     | Non-steroidal estrogen                        | Nuclear receptor ligand                                               |
| 13G06 | Letrozole                      | Antineoplastic                                | P450 inhibitor                                                        |
| 10F09 | Prednisone hydrochloride       | Local anesthetic                              | P450 inhibitor (mono- oxygenases)                                    |
| 05G10 | Ketoconazole                   | Antifungal                                    | P450 inhibitor (P450x17)                                              |
| 08C08 | Cilostazol                     | Antithrombotic                                | Phosphodiesterase inhibitor                                           |
| 14H05 | Saquinavir mesylate            | Antiviral (HIV)                               | Protease inhibitor                                                    |
| 02G07 | Tamoxifen citrate              | Anticancer                                    | Protein kinase C inhibitor                                            |
| 08A11 | Emetine dihydrochloride        | Antiasthmatic                                  | Protein synthesis inhibitor                                           |
| 10G11 | Cyclohexamide                  | Antibacterial                                  | Protein synthesis inhibitor                                           |
| 09E02 | Lycorine hydrochloride         | Antitumor                                     | Protein translation inhibitor                                          |
| 13E09 | Gabexate mesilate              | Severe acute pancreatitis                     | Proteinase inhibitor                                                  |
| 05H05 | Kanamycin A sulfate            | Antibacterial                                  | Ribosomal protein synthesis inhibitor                                 |
| 10D09 | Ribostamycin sulfate salt      | Antibacterial                                  | Ribosomal protein synthesis inhibitor                                 |
| 12H02 | Crotamiton                     | Sebacide                                      | Sebacide                                                             |
| 13F10 | Tribenoside                    | Sclerosing agent                              | Sclerosing agent                                                      |
| 12A06 | Cantharidin                    | Rubefiant                                     | Serine protease releaser                                              |
| 05G08 | Carbamazepine citrate          | Antiepileptic                                  | Serine protease releaser                                              |
| 10G10 | Drotaverine hydrochloride      | Spasmolytic                                   | Spasmolytic                                                          |
| 02E08 | Isoniazide                     | Antibacterial                                  | Sterol 14-demethylase inhibitor                                       |

S29
| Plate | Name                  | Function                  | Enzyme Inhibitor | Topoisomerase I Inhibitor | Topoisomerase II Inhibitor | Additional Properties |
|-------|-----------------------|---------------------------|-----------------|---------------------------|---------------------------|-----------------------|
| 03D11 | Camptothecine (S+)+   | Antitumor agent           | Topoisomerase I | +                         | +                         | +                     |
| 14F09 | Kaempferol            | Anti-inflammatory         | Topoisomerase I | +                         |                           |                       |
| 05G06 | Mitoxantrone dihydrochloride | Antineoplastic            | Topoisomerase II Inhibitor | +                         |                           | +                     |
| 05H07 | Etoposide             | Antineoplastic            | Topoisomerase II Inhibitor | +                         | +                         | +                     |
| 09F11 | Cefmetazole sodium salt | Antibacterial             | Transpeptidase Inhibitor (bacterial) | -                         |                           |                       |
| 14G06 | Verteporfin           | Treatment of age-related macular degeneration | Treatment of age-related macular degeneration | +                         |                           |                       |
| 11H10 | Capsaicin             | Topical analgesic         | Vanilloid receptor ligand | +                         |                           |                       |
| 06C02 | Suloctidil            | Vasodilator               | Vasodilator     | -                         |                           |                       |
| 12B07 | N-Acetyl-L-leucine    | Vertigo                   | Vertigo         | +                         |                           |                       |
| 08H05 | Riboflavin            | Vitamin                   | Vitamin         | +                         |                           |                       |
| 06F10 | Menadione             | Vitamin K3                | Vitamin precursor | +/-                       |                           |                       |
| 09F08 | 3-alpha-Hydroxy-5-beta-androstan-17-one | | | | | |
| 14D11 | Methiazole            |                           |                 | -                         |                           |                       |
| 14E05 | Leucomosine           |                           |                 | -                         |                           |                       |
| 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   | Yohimbine acid monohydrate     | -                        | -                                | +          |            |               |               |             |             |
| Plate09A09   | Betonicine                     | -                        | -                                |            |            |               |               |             |             |
| Plate09F02   | Filafbin                       | -                        | -                                | +          | +          |               |               | +           |             |
| Plate07D11   | Sulfasalazine                  | Treatment of ulcerative colitis | 15-hydroxydehydrogenase inhibitor | -          |            |               |               |             |             |
| Plate09H08   | Finasteride                    | Antialopecia agent       | 5A-reductase inhibitor           | +          |            |               |               |             |             |
| Plate05F06   | Methochepine maleate           | -                        | 5HT antagonist                   |            |            |               |               |             |             |
| Plate04F08   | Benzylamine hydrochloride      | Analgesic                | 5HT antagonist                   | -          |            |               |               |             |             |
| Plate13D03   | Pizotifen maleate              | Antimigraine             | 5HT antagonist                   | +          | +          |               |               |             |             |
| Plate02C04   | Cyproheptadine hydrochloride   | Antipruritic              | 5HT antagonist                   | -          |            |               |               |             |             |
| Plate06C11   | Cisapride                      | Peristaltic stimulant    | 5HT antagonist                   | +          |            |               |               |             |             |
| Plate09C09   | Skimmianine                    | Sedative                 | 5HT ligand                       |            |            |               |               |             |             |
| Plate05E05   | Metergoline                    | Antiprolactin             | 5HT antagonist (5HT1)            |            |            |               |               |             |             |
| Plate07F02   | Premperone                     | -                        | 5HT antagonist (5HT2)            |            |            |               |               |             |             |
| Plate14B09   | Ondansetron Hydrochloride      | Antiemetic               | 5HT antagonist (5HT3)            | +          |            |               |               |             |             |
| Plate09C09   | Piroxetine Hydrochloride       | Sedative                 | 5HT ligand                       |            |            |               |               |             |             |
| Plate02B03   | Zimelidine hydrochloride       | Antidepressant           | 5HT uptake inhibitor             | +          |            |               |               |             |             |
| Plate07A09   | Dosulepin hydrochloride        | Antidepressant           | 5HT uptake inhibitor             | -          |            |               |               |             |             |
| Plate07D02   | Fluoxetine hydrochloride       | Antidepressant           | 5HT uptake inhibitor             | -          |            |               |               |             |             |
| Plate09F03   | Citralopram 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 tartrate salt    | Potent analgesic         | Acetylcholine esterase inhibitor | +          | +          |               |               |             |             |
| Plate10E04   | Meclotenoxate hydrochloride    | Cerebral stimulant       | Acetylcholine precursor          | -          | +          |               |               |             |             |
| Plate10E09   | Vidarabine                     | Antiviral                | Adenosine antimetabolite         | -          |            |               |               |             |             |
| Plate11H05   | Theobromine                    | Bronchodilator           | Adenosine receptor antagonist    | -          |            |               |               |             |             |
| Plate03D02   | Dilazep dihydrochloride        | Vasodilator              | Adenosine uptake inhibitor       | -          |            |               |               |             |             |
| Plate11B04   | Bucladesine sodium             | Cardiotonic              | Adenylate cyclase modulator      | -          | +          |               |               |             |             |
| Plate01E08   | Ticlopidine Hydrochloride      | Platelet antagonist      | AOP antagonist                    | +          |            |               |               |             |             |
| Plate04C04   | Dextrin hydrochloride          | Anticonvulsant            | Adrenaline uptake inhibitor      | -          |            |               |               |             |             |
| Plate09C11   | Tetrandrine                    | Analgesic                | Alkaloid                          | +          | -          | -             | -             |             |             |
| Plate09D09   | Ricinine                       | Alkaloid                 |                                  |            |            |               |               |             |             |
| Plate06E05   | Piperlongumine                 | Antifungal               | Alkaloid                          | +          | +/*        |               |               |             |             |
| Plate08E07   | (-)-Cinchonidine               | Antimarial               | Alkaloid                          | +          |            |               |               |             |             |
| Plate08E08   | Eburnamone (-)                | Cerebral vasodilator     | Alkaloid                          | +          |            |               |               |             |             |
| Plate08F02   | Hamamelidol dihydrochloride    | Vasoactive               | Alkaloid                          | -          |            |               |               |             |             |
| Plate03D02   | Mildronate hydrochloride       | Hypotensor               | Alpha adrenergic                  | -          |            |               |               |             |             |
| Plate14E09   | (-)-Synephrine                 | Adrenergic               | Alpha adrenergic                  | -          | -          | -             |              | +           |             |
| Plate03F05   | Gentiobiose                    | Antihyperlipoproteinemia | Alpha adrenergic                  | -          |            |               |               |             |             |
| Plate07F06   | Methoxamine hydrochloride      | Antihypotensive          | Alpha Adrenergic                  | -          |            |               |               |             |             |
| Plate05A05   | Phenylalanostinin hydrochloride| Decoagulant              | Alpha Adrenergic                  | -          |            |               |               |             |             |
| Plate03D08   | Metaraminol bitartrate         | Vasocostructor           | Alpha Adrenergic                  | -          | -          |               |               |             |             |
| Plate | Compound                        | Class                      | Effects                                      |
|-------|---------------------------------|----------------------------|----------------------------------------------|
| 13F08 | Etilefrine hydrochloride        | Antihypotensive            | Alpha Adrenergic agonist (alpha1)            |
| 13H09 | Methylpropanol hydrochloride    | Vasoconstrictor            | Alpha Adrenergic agonist (alpha2)            |
| 10B10 | Levonordefrin                   | Vasoconstrictor            | Alpha Adrenergic agonist (alpha2)            |
| 01E03 | Moxisylyte hydrochloride        | Vasoconstrictor            | Alpha adrenergic antagonist                   |
| 01F11 | Tolazoline hydrochloride        | Vasoconstrictor            | Alpha adrenergic antagonist                   |
| 02G02 | Verapamil hydrochloride         | Antihypertensive            | Alpha adrenergic agonist (alpha2)            |
| 01H05 | Moxisylyte hydrochloride        | Vasoconstrictor            | Alpha adrenergic antagonist                   |
| 04C03 | Amitryptiline hydrochloride     | Antihypertensive            | Alpha Adrenergic agonist (alpha1)            |
| 05A03 | Alfuzosin hydrochloride         | Antihypertensive            | Alpha Adrenergic antagonist                   |
| 08B08 | Rauwolfia hydrochloride         | Antihypertensive            | Alpha adrenergic antagonist                   |
| 09F09 | Tetrahydrozoline hydrochloride  | Vasoconstrictor            | Alpha adrenergic ligand                      |
| 08H03 | Diprylflur hydrochloride        | Vasoconstrictor            | Alpha adrenergic agonist (alpha1)            |
| 10D03 | Seneciphylline monohydrate      | Antihypertensive            | Antiarrhythmic                               |
| 07E03 | Thiostrpton                     | Antiarrhythmic              | Antiarrhythmic                               |
| 12H06 | Flortenicol                     | Antiarrhythmic              | Antiarrhythmic                               |
| 13D11 | Lymecycline                     | Antiarrhythmic              | Antiarrhythmic                               |
| 13A11 | Roxarsonate                     | Antiarrhythmic              | Antiarrhythmic                               |
| 08D10 | Senecephylline                  | Antiarrhythmic              | Antiarrhythmic                               |
| 10H07 | Lithocholic acid                | Cholagogue                  | Antiarrhythmic                               |
| 09A03 | Epicatechin                     | Antihypertensive            | Antidiarrhoeic                               |
| 13A04 | Eloniconazole                   | Antiarrhythmic              | Antiarrhythmic                               |
| 14G11 | Parbendazole                    | Antiarrhythmic (VET)        | Antiarrhythmic                               |
| 13H11 | Pynvinium pamoate               | Antiarrhythmic              | Antiarrhythmic                               |
| 14D07 | Ciprofibrate                    | Antiarrhythmic              | Antiarrhythmic                               |
| 01H02 | Todralazine hydrochloride       | Antiarrhythmic              | Antiarrhythmic                               |
| 01A02 | Althiazide                      | Antiarrhythmic              | Antiarrhythmic                               |
| 13H02 | Halofantrine hydrochloride      | Antiarrhythmic              | Antiarrhythmic                               |
| 05C08 | Thioquanoxide                   | Antiarrhythmic              | Antiarrhythmic                               |
| 11G07 | Azacytidine-5                   | Antiarrhythmic              | Antiarrhythmic                               |
| 06H11 | Puromycin dihydrochloride       | Antiarrhythmic              | Antiarrhythmic                               |
| 02B05 | Azathiopeprine                   | Antiarrhythmic              | Antiarrhythmic                               |
| 07A11 | Iobenguane sulfate              | Antiarrhythmic              | Antiarrhythmic                               |
| 10E06 | Ethoxyquin                      | Antiarrhythmic              | Antiarrhythmic                               |
| 06A05 | Tocopherol (R,S)                | Antiarrhythmic              | Antiarrhythmic                               |
| 06B04 | Carbamsone                      | Antiarrhythmic              | Antiarrhythmic                               |
| 12C07 | Fluspirilen                     | Antiarrhythmic              | Antiarrhythmic                               |
| 14A09 | Piperacetazine                   | Antiarrhythmic              | Antiarrhythmic                               |
| 14B05 | Levopropoxyphene naptsylate      | Antiarrhythmic              | Antiarrhythmic                               |
| 07D04 | Norcyclobenzaprine              | Antiarrhythmic              | Antiarrhythmic                               |
| 06H10 | Methoxy-8-nsoralen              | Antiarrhythmic              | Antiarrhythmic                               |
| 09G11 | Strophanthin                     | Antiarrhythmic              | Antiarrhythmic                               |
| 07B08 | Vancomycin hydrochloride        | Antiarrhythmic              | Antiarrhythmic                               |
| 08G02 | Methoxy-6-harmaline              | Antiarrhythmic              | Antiarrhythmic                               |
| 03D09 | Salbutamol                      | Antiarrhythmic              | Antiarrhythmic                               |
| 04E03 | Fenoterol hydrochloride         | Antiarrhythmic              | Antiarrhythmic                               |
| 05C06 | Cibembutol hydrochloride        | Antiarrhythmic              | Antiarrhythmic                               |
| Plate   | Compound                        | Category            | Effect                      |
|---------|---------------------------------|---------------------|-----------------------------|
| 07C06   | Metaproterenol sulfate, orciprenaline sulfate | Bronchodilator       | Beta adrenergic agonist     |
| 10C10   | Isoethaline mesylate salt       | Bronchodilator       | Beta adrenergic agonist     |
| 14F08   | (-)-Isoproterenol hydrochloride | Bronchodilator       | Beta adrenergic agonist     |
| 01G09   | Ilosauvurine hydrochloride      | Vasodilator          | Beta adrenergic agonist     |
| 05D03   | Dobutamine hydrochloride        | Bronchodilator       | Beta adrenergic agonist     |
| 05H02   | Terbutaline hemisulfate         | Bronchodilator       | Beta adrenergic agonist     |
| 12G06   | Salmeterol                     | Bronchodilator       | Beta adrenergic agonist     |
| 05C10   | Ritodrine hydrochloride         | Tocolytic            | Beta adrenergic agonist     |
| 12G10   | (+,-)-Octopamine hydrochloride  | Adrenergic           | Beta adrenergic agonist     |
| 02A11   | Pindolol                        | Antiarrhythmic       | Beta adrenergic antagonist  |
| 07B10   | Propranolone hydrochloride      | Antiarrhythmic       | Beta adrenergic antagonist  |
| 10B04   | Metoprolol-(+,-) (+)-tartrate salt | Antihypertensor    | Beta adrenergic antagonist  |
| 14A04   | Penbutolol sulfate              | Antihypertensor      | Beta adrenergic antagonist  |
| 01G10   | Acebutolol hydrochloride        | Antiarrhythmic       | Beta adrenergic antagonist  |
| 04A11   | Alprenolol hydrochloride        | Antihypertension     | Beta adrenergic antagonist  |
| 04D08   | Labetalol hydrochloride         | Antihypertension     | Beta adrenergic antagonist  |
| 03A10   | Hydralazine dihydrochloride     | Antihypertension     | Beta adrenergic antagonist  |
| 12H03   | Propranolol hydrochloride       | Antihypertensive     | Beta adrenergic blocker     |
| 07F07   | (S)-(-)-Atenolol                | Antihypertensive     | Beta adrenergic blocker     |
| 14B08   | Osprenolol hydrochloride        | Antihypertensive     | Beta adrenergic blocker     |
| 14D06   | (R)-Propranolol hydrochloride   | Antihypertensive     | Beta adrenergic blocker     |
| 12H04   | (R)-(+)-Atenolol                | Antihypertensive     | Beta adrenergic blocker     |
| 05C04   | Desipramine hydrochloride       | Antidepressant       | Beta Adrenergic transport inhibitor |
| 07G10   | Trimazadidine dihydrochloride   | Antianoxic           | Beta-oxidation inhibition   |
| 13A02   | Denatonium benzoate             | Bittering agent      | Prevent poisoning           |
| 03F04   | Fenopride hydrochloride         | Antiinflammatory     | Bradykinin antagonist       |
| 12D02   | (+)-Isoproterenol (+)-tartrate salt | Bronchodilator     | Bronchodilator             |
| 02G05   | Loperamide hydrochloride        | Antidiarrhoeic       | Ca2+ channel antagonist     |
| 01H09   | Thioridazine hydrochloride      | Neuroleptic          | Ca2+ channel antagonist     |
| 05D07   | Adenosine 5'-monophosphate monohydrate | Nutrient             | Ca2+ channel blocker       |
| 09D03   | Tetrahydroidberberin            | Sedative             | Ca2+ channel blocker       |
| 04E07   | Perhexiline maleate             | Vasodilator          | Ca2+ channel blocker       |
| 08D06   | Calycanthine                    | Ca2+ channel blocker |
| 03A06   | Ethosuximide                    | Anticonvulsant       | Ca2+ channel inhibitor      |
| 07D06   | Trimethadione                    | Anticonvulsant       | Ca2+ channel inhibitor      |
| 07H11   | Prenylamine lactate             | Vasodilator          | Ca2+ channel stimulation   |
| 01G04   | Nifedipine                      | Antihypertensive     | Ca2+ channels blocker      |
| 11G04   | Lidocaine acid disodium salt    | Calcium regulator    | Calcium regulator          |
| 01A05   | Metformin hydrochloride         | Antidiabetic         | cAMP/PKA                   |
| 05E06   | Brinzolamide                    | Antiglaucoma drug    | Carbonic anhydrase inhibitor |
| 14H07   | Dorzolamide hydrochloride       | Antiglaucoma drug    | Carbonic anhydrase inhibitor |
| Plate | Compound                        | Class               | Effect                                           | +  | -  | +  |
|-------|--------------------------------|---------------------|-------------------------------------------------|----|----|----|
| 01A04 | Acetazolamide                  | Diuretic            | Carbonic anhydrase inhibitor                     | +  |    | +  |
| 11A03 | Methazolamide                  | Diuretic            | Carbonic anhydrase inhibitor                     | -  |    |    |
| 13C07 | Proscillaridin                 | Cardiotonic         | Cardiac glycoside                                | +  |    | +  |
| 14E08 | 2-Chloropyrazine               | Cardiotonic         | Cardiotonic                                      | -  |    | +  |
| 08A05 | Syrosingopine                  | -                   | Catecholamine depolar                         | -  |    |    |
| 05F03 | Debrisquin sulfate             | Antihypertensive    | Catecholamine depolar                         | +  |    | -  |
| 11H06 | Reserpine                      | Neuroleptic         | Catecholamine pump inhibitor                    | +  |    |    |
| 07G02 | Ciclopirox ethanolamine        | Antifungal          | Cell membrane proteins synthesis inhibitor      | -  |    |    |
| 07A10 | Cefazidime pentahydrate        | Antibacterial       | Cell wall destruction agent                     | +  |    |    |
| 07E07 | Ethionamide                    | Antibacterial       | Cell wall destruction agent                     | +  |    |    |
| 13E10 | Pivampicillin                  | Antibacterial       | Cell wall destruction agent                     | +  |    | +  |
| 13F02 | Flucloxacillin sodium          | Antibacterial       | Cell wall destruction agent                     | +  |    |    |
| 13G09 | Benzathine benzylpenicillin    | Antibacterial       | Cell wall destruction agent                     | +  |    |    |
| 14H09 | Cefipime hydrochloride         | Antibacterial       | Cell wall destruction agent                     | -  |    |    |
| 06G11 | Ceforanide                     | Antibacterial       | Cell wall synthesis inhibitor (bacterial)       | +  |    | -  |
| 06H04 | Cefotetan                      | Antibacterial       | Cell wall synthesis inhibitor (bacterial)       | -  |    | +  |
| 14E07 | D-cycloserine                  | Antibacterial       | Cell wall synthesis inhibitor (bacterial)       | -  |    | +  |
| 14E10 | (S)-(-)-Cycloserine            | Antibacterial       | Cell wall synthesis inhibitor (bacterial)       | -  |    | +  |
| 14G07 | Meropenem                      | Antibacterial       | Cell wall synthesis inhibitor (bacterial)       | +  |    |    |
| 07C05 | Etifenin                       | Diagnostic agent    | Chelating agent                                  | -  |    |    |
| 12G02 | Pentetic acid                  | Chelating agent (iron) | Chelating agent, chymotrypsin-like proteasome activity inhibitor | -  |    | +  |
| 12A07 | Clioquinol                     | Anti-infective      | Chelating agent                                  | -  |    |    |
| 02E04 | Dehydrocholic acid             | Choleretic          | Choleretic                                       | -  |    |    |
| 05G05 | Prebucol                       | Antihyperlipoproteinic | Cholesterol downregulation                   | +  |    |    |
| 06A03 | Arecoline hydrobromide         | Antihelmintic       | Cholinergic                                       | +  | -  | +  |
| 06E10 | Pilocarpine nitrate            | Antiglaucoma drug   | Cholinergic                                      | +  |    | +  |
| 03H04 | Hyoscyamine (L)                | Antispasmodic       | Cholinergic                                       | +  |    |    |
| 09A08 | Myosmine                       | Cholinergic         | Cholinergic                                       | +  |    |    |
| 02A04 | Edrophonium chloride           | Myasthenia Gravis test | Cholinergic                                     | +  |    |    |
| 01F03 | Carbamazapine                  | Anticonvulsant      | Cholinergic antagonist                           | -  |    |    |
| 09E11 | Napeline                       | Antiarrhythmic      | cholinergic inhibition                           | +  |    |    |
| 04F05 | Pimethixene maleate            | Antihistaminic      | cholinergic inhibition                           | -  |    |    |
| 07B02 | Metixene hydrochloride         | Antiparkynic        | cholinergic inhibition                           | +  |    | +  |
| 10H10 | Pridinol methanesulfonate salt | Antiparkinsonian    | cholinergic inhibition                           | +/+|    |    |
| 01E09 | Dicyclomine hydrochloride      | Antispasmodic       | cholinergic inhibition                           | +  |    |    |
| 14A03 | Trichloethy chloride           | Antispasmodic       | cholinergic inhibition                           | +  |    |    |
| 04E08 | Oxbytynin chloride             | Spasmolytic         | cholinergic inhibition                           | -  |    |    |
| 10H05 | Eucatropine hydrochloride      | cholinergic inhibition | cholinergic inhibition                           | +  |    | -  |
| 02A03 | Cotinine (-)                   | Antidepressant      | cholinergic inhibition (and nicotinic inhibition)| +  |    |    |
| 05H04 | Homocholinium bromide          | Anticholinergic     | Cholinergic inhibition (partial, Acetylcholine stores depolar) | +  |    |    |
| 02C08 | Tomatine                       | Antifungal          | Cholinergic inhibition (pH-dependent competitive inhibition of the enzyme acetylcholinesterase) | -  |    | -  |
| 01F02 | Trichlorfon                    | Antihelminthic      | Cholinergic inhibition Cholinesterase inhibitor | +  |    | -  |
| Plate | Compound Name | Category | Action | Additional Information |
|-------|---------------|----------|--------|------------------------|
| 05A10 | Tacrine hydrochloride hydrate | Cognition enhancer | Cholinesterase inhibitor | - |
| 12A03 | Bemegride | CNS stimulant | CNS stimulant | + |
| 10C02 | Nadide | CoA nicotinamide adenine dinucleotide | CoA reductase inhibitor (HMG CoA) | - |
| 11G06 | Simvastatin | Antihyperlipidemic | CoA synthesis precursor | - |
| 06H03 | Pantethinic acid calcium salt monohydrate | Nutritional factor | CoA synthesis role | - |
| 04H05 | Eralapril maleate | Antihypertension | Converting enzyme inhibitor | + |
| 14G08 | Ramipril | Antihypertension | Converting enzyme inhibitor | + |
| 13A10 | 3-Acetamidocoumarin | Antiinflammatory | coumarin | - + |
| 13A03 | Scopoletin | Antispasmodic | Coumarin | + |
| 08A02 | Tubocurarine chloride pentahydrate (+) | Muscle relaxant | Curarising | + |
| 01C10 | Antipyrine | Analgesic | cyclooxygenase inhibition | + |
| 09E04 | Flufenamic acid | Analgesic | cyclooxygenase inhibition | - |
| 09H04 | Dipyrone | Analgesic | cyclooxygenase inhibition | + - |
| 11B06 | Fosfosal | Analgesic | cyclooxygenase inhibition | - |
| 01E06 | Naproxen | Antiinflammatory | cyclooxygenase inhibition | + |
| 01F05 | Mefenamic acid | Antiinflammatory | cyclooxygenase inhibition | - |
| 01H04 | Sulindac | Antiinflammatory | cyclooxygenase inhibition | + |
| 02B09 | Acetylsalicylsalicylic acid | Antiinflammatory | cyclooxygenase inhibition | - |
| 03E06 | Tolfenamic acid | Antiinflammatory | cyclooxygenase inhibition | + |
| 03E07 | Medoflamamic acid sodium monohydrate | Antiinflammatory | cyclooxygenase inhibition | - |
| 03F09 | Fenbufen | Antiinflammatory | cyclooxygenase inhibition | - |
| 03F10 | Ketsoprofen | Antiinflammatory | cyclooxygenase inhibition | - |
| 07C09 | Resveratrol | Antiinflammatory | cyclooxygenase inhibition | + - +/+ |
| 07E08 | Tenoxicam | Antiinflammatory | cyclooxygenase inhibition | + |
| 10A03 | Isopyrin hydrochloride | Antiinflammatory | cyclooxygenase inhibition | - + + |
| 10B11 | Ebselen | Antiinflammatory | cyclooxygenase inhibition | - + - |
| 10H02 | (R)-Naproxen sodium salt | Antiinflammatory | cyclooxygenase inhibition | + - + |
| 11B07 | Suprofen | Antiinflammatory | cyclooxygenase inhibition | - |
| 11D07 | Indoprofen | Antiinflammatory | cyclooxygenase inhibition | + |
| 11F07 | Tolmetin sodium salt dihydrate | Antiinflammatory | cyclooxygenase inhibition | = + |
| 10A11 | Balsalazine Sodium | Anti-inflammatory | cyclooxygenase inhibition | - |
| 13E04 | Azapropazone | Anti-inflammatory | cyclooxygenase inhibition | + - + |
| 14A10 | Oxphenbutazone | Anti-inflammatory | cyclooxygenase inhibition | - - + + + |
| 14B11 | Oxsaprozin | Anti-inflammatory | cyclooxygenase inhibition | + |
| 01C11 | Antipyrine, 4-hydroxy | Anti-inflammatory | cyclooxygenase inhibition | + |
| 09G06 | Methyl benzethonium chloride | Antibacterial | Detergent | - + - - + |
| 09G09 | Benzethonium chloride | Antibacterial | Detergent | - - +/+ |
| 10F08 | Alexidene dihydrochloride | Antibacterial | Detergent | - - - + +/+ |
| 10H03 | Propridium iodide | Antibacterial | Detergent | + + + |
| 04E06 | Chenodiol | Anticholelithogenic | Detergent | - |
| 02G04 | Chlorhexidine | Bacteriostatic | Detergent | - |
| Plate | Compounds | Targets | Actions | Notes |
|-------|-----------|---------|---------|-------|
| 12E06 | Thonzonium bromide | Detergent | + | - |
| 13D10 | Preguaniol hydrochloride | Antimalarial | dihydrofolate reductase inhibitor | + |
| 14F05 | Sulfoxamine | Antibacterial | dihydropropanate synthase inhibitor | +/- + |
| 09A05 | N-Acetyl- DL-thioleucine Thiolactone | Expectorant | Disulfide bridge breaker | - |
| 02A10 | Uric acid | Diuretic | Diuretic | - |
| 02A02 | Metronidazole | Antibacterial | DNA damage (bacterial) | - + |
| 07B03 | Nitrofurazone | Antibacterial | DNA damage (bacterial) | + - |
| 07D06 | Nitrofurantoin | Urinary antiseptic | DNA damage (bacterial) | + |
| 07H06 | Nitrofurantoin | Anthelmintic | DNA intercalating agent | - |
| 08C06 | Furaltadone | Antiprotozoal | DNA intercalating agent | - |
| 09A05 | N-Acetyl-DL-homocysteine Thiolactone | Thiolactone | Expectorant | Disulfide bridge breaker | - |
| 08G05 | Ellipticine | Anticancer | DNA Intercalating agent | - |
| 07D09 | Doxorubicin | Antineoplastic | DNA intercalating agent | - |
| 08D07 | Tinidazole | Antiprotozoal | DNA intercalating agent | - |
| 08E02 | Daunorubicin | Antineoplastic | DNA intercalating agent | - |
| 08F05 | Perhexiline mesylate | Antipsychotic | DNA intercalating agent | + |
| 08G09 | Pimozide | Antipsychotic | DNA intercalating agent | - |
| 09F04 | Chlorpromazine | Antipsychotic | Dopamine antagonist | - |
| 07C10 | Amoxapine | Antidepressant | Dopamine antagonist | - |
| 07E10 | Mesoridazine besylate | Antipsychotic | Dopamine antagonist | + |
| 09F04 | Promazine hydrochloride | Antipsychotic | Dopamine antagonist | + |
| 04H04 | Trifluoperazine dihydrochloride | Antipsychotic | Dopamine antagonist | + |
| 01F04 | Trihexyphenidyl | Antipsychotic | Dopamine antagonist | + |
| 01H11 | Trimethobenzamide hydrochloride | Antipsychotic | Dopamine antagonist | + |
| 01F07 | Sulpiride | Antipsychotic | Dopamine antagonist | +/+ |
| 05C09 | Chlorpromazine dihydrochloride | Neuroleptic | Dopamine antagonist | - |
| 07H10 | DO 895/99 | Antipsychotic | Dopamine antagonist | - |
| 04G09 | Pimozide | Antipsychotic | Dopamine antagonist | - |
| 02B08 | Disulfiram | Alcohol deterrent | Dopamine beta hydroxylase inhibitor | - |
| 02C03 | Amoxapine | Antidepressant | Dopamine uptake inhibitor | - |
| 05G07 | GBF 1286 | Antidepressant | Dopamine uptake inhibitor | - |
| Plate | Compound                     | Activity                  | Effectivity |
|-------|------------------------------|---------------------------|-------------|
| 09E10 | Ungerine nitrate             | Sedative                  |             |
| 06H05 | Piperine                     | Antidiarrheic             |             |
| 06A09 | Butoconazole nitrate         | Antifungal                |             |
| 06A11 | Amphotericin B               | Antibacterial             |             |
| 01G11 | Tolnaftate                   | Antifungal                |             |
| 11A11 | Sulconazole nitrate          | Antifungal                |             |
| 01F07 | Guaifenesin                  | Expectorant               |             |
| 03E09 | Trimethoprim                 | Antibacterial             |             |
| 01D06 | Dapsone                      | Antiinflammatory          |             |
| 01D08 | Pyrimethamine                | Folic acid antagonist     |             |
| 09G02 | Succinylsulfinilfate          | Antibacterial             |             |
| 09H06 | Sulfabenzamide               | Antifungal                |             |
| 10B02 | Sulfaguanoxaline sodium salt | Antibacterial             |             |
| 10E10 | Sulfamer                     | Folic acid synthesis      | ++/–         |
| 10F06 | Sulfamethazine sodium salt   | Antibacterial             |             |
| 01B05 | Sulfanilamide                | Antifungal                |             |
| 01G02 | Morantel tartrate            | Anthelmintic              |             |
| 08A10 | Dihydroergotoxine mesylate   | Anticonvulsant GABA A receptor CI channel high affinity | ++/–         |
| 13B03 | THIP Hydrochloride           | GABA Agonist              |             |
| 06D11 | Epiandrosterone              | Anabolic steroid          |             |
| 07F10 | Thiococclidioside            | Muscle relaxant GABA agonist ? | +/–        |
| 03A03 | Pentylenetetrazole           | CNS stimulant             |             |
| 11E02 | Securinine                   | CNS stimulant             |             |
| 09C03 | Gelsemine                    | Tumour inhibitor          |             |
| 08C10 | Bicuculline (+)              | Convulsant GABA antagonist (GABAa) | +          |
| 09B03 | PicROTOXIN                   | Analeptic                 |             |
| 14A02 | Etomocide                    | Hypnotic GABA receptor (GABAa) | +          |
| 11G02 | Gabapentin                   | Anticonvulsant GABA receptor ligand | +          |
| 13B07 | Tracecolate hydrochloride    | GABA receptor ligand      |             |
| 12F02 | Propofol                     | Anesthetic (intravenous)  |             |
| 13E03 | Alfalexone                   | GABA receptor stimulation |             |
| 13E02 | Alfadolone acetate           | GABA receptor stimulation |             |
| 09B11 | Avermectin B1                | Antihelmic GABA receptors ligand | –          |
| 01D09 | Hexamethonium dibromide dihydrochloride | Antihypertensor Ganglion blocker | +          |
| 14H02 | Mocamamine hydrochloride     | Antihypertensor Ganglion blocker | –          |
| 05A04 | Chloropramide                | Antidiabetic Glucagon secretogen | –          |
| 13D08 | Fluticasone propionate       | Antiallergic glucocorticoid |             |
| 13F11 | Rimexolone                   | Anti-inflammatory (local) Glucocorticoid | +          |
| 04D10 | Methylprednisolone, 6-alpha  | Glucocorticoid Glucocorticoid | –          |
| Plate         | Substance                                      | Category                     | Subcategory                                      |
|---------------|------------------------------------------------|------------------------------|-------------------------------------------------|
| 09A04         | Flunisolide                                    | Glucocorticoid               | Glucocorticoid                                  |
| 09A06         | Flurandrenolide                                | Glucocorticoid               | Glucocorticoid                                  |
| 09H09         | Flumethasone                                   | Glucocorticoid               | Glucocorticoid                                  |
| 10A06         | Flurandrenolide                                | Glucocorticoid               | Glucocorticoid                                  |
| 10H09         | Fluorometholone                                | Glucocorticoid               | Glucocorticoid                                  |
| 10H05         | Flucinonide                                    | Glucocorticoid               | Glucocorticoid                                  |
| 10G02         | Flumethasone                                   | Glucocorticoid               | Glucocorticoid                                  |
| 10B05         | Clobetasol propionate                          | Glucocorticoid               | Glucocorticoid                                  |
| 10F05         | Prednicarbate (topical)                        | Glucocorticoid               | Glucocorticoid                                  |
| 10F02         | Alclometasone dipropionate                     | Anti-inflammatory             | glucocorticoid receptor agonist                 |
| 03F08         | Evoxine                                        | Sedative                     | Glycine receptor antagonist                     |
| 07B04         | Omeprazole                                     | Analgesic                    | Histamine antagonist                            |
| 04D11         | Quinidine hydrochloride dihydrochloride        | Antiarhythmic                | Histamine antagonist                            |
| 02E07         | Mefloquine hydrochloride                       | Antimalarial                 | Histamine antagonist                            |
| 04G10         | Amodiaquin dihydrochloride dihydrate           | Antimalarial                 | Histamine antagonist                            |
| 06F07         | Primacrine diphasate                           | Antimalarial                 | Histamine antagonist                            |
| 07G09         | Chloroquine diphasate                          | Antimalarial                 | Histamine antagonist                            |
| 06E04         | Trimeprazine tartrate                          | Antimalarial                 | Histamine antagonist                            |
| 07C11         | Cycloizine hydrochloride                       | Antimalarial                 | Histamine antagonist                            |
| 01C08         | Dicyclazine succinate                          | Antimalarial                 | Histamine antagonist                            |
| 01F10         | Pheniramine maleate                            | Antimalarial                 | Histamine antagonist                            |
| 01G06         | Diphenhydramine maleate male salt             | Analgesic                    | Histamine antagonist                            |
| 09G07         | Chlorcyclizine hydrochloride                   | Antihistaminic               | Histamine antagonist                            |
| 11E03         | Triprazepam tartrate                           | Antipruritic                 | Histamine antagonist                            |
| 10H04         | Ciprofazine hydrochloride                      | Antifusive                   | Histamine antagonist                            |
| 07C11         | Cycloizine hydrochloride                       | Antieptic                    | Histamine antagonist (H1)                       |
| 01C08         | Dicyclazine succinate                          | Antihistaminic               | Histamine antagonist (H1)                       |
| 01F10         | Pheniramine maleate                            | Antihistaminic               | Histamine antagonist (H1)                       |
| 01G06         | Diphenhydramine hydrochloride                  | Antihistaminic               | Histamine antagonist                            |
| 02F07         | Astemizole                                     | Antihistaminic               | Histamine antagonist (H1)                       |
| 04C03         | Triprolidine hydrochloride                     | Antihistaminic               | Histamine antagonist (H1)                       |
| 04C06         | Dimenhydrinate                                 | Antihistaminic               | Histamine antagonist (H1)                       |
| 04E04         | Homochlorcyclizine dihydrochloride             | Antihistaminic               | Histamine antagonist (H1)                       |
| 04G07         | Clemastine fumarate                            | Antihistaminic               | Histamine antagonist (H1)                       |
| 06F06         | Methylhydroxymethylene 1,5-naphtalenedisulfona te | Antihistaminic               | Histamine antagonist (H1)                       |
| 06H06         | Brompheniramine maleate                        | Antihistaminic               | Histamine antagonist (H1)                       |
| 07C04         | Cetinazine hydrochloride                       | Antihistaminic               | Histamine antagonist (H1)                       |
| 11A08         | Chloropyramine hydrochloride                   | Antihistaminic               | Histamine antagonist (H1)                       |
| 12A09         | Promethazine hydrochloride                     | Antihistaminic               | Histamine antagonist (H1)                       |
| 06C09         | Roxatidine Aceate HCl                          | Antileptic                   | Histamine antagonist (H2)                       |
| 12E02         | Nizatidine                                     | Antileptic                   | Histamine antagonist (H2)                       |
| 09B10         | 6-Furfurylamino-2purine                       | Plant growth accelerator     | Hormone (plants)                                |
| 06B02         | Androsterone                                   | Antithyroid                  | Androgen                                         |
| 11F04         | Liothyronine                                   | Thyroidic drug               | Hormone (Thyroid)                               |
| 06A02         | Testosterone propionate                        | Androgen                     | hormone Androgen                                |
| 07G07         | Pregnenolone                                   | Androgen                     | hormone androgen receptor antagonist            |
| 03B11         | Flutamide                                      | Anticancer                   | hormone androgen receptor antagonist            |

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| Plate | Name                                      | Class          | Description                                      | Effect |
|-------|-------------------------------------------|----------------|--------------------------------------------------|--------|
| 14D05 | Cyproterone acetate                       | Antiandrogen   | Hormone antiandrogen                             | +      |
| 13E07 | Epitiostanol                               | Antineoplastic | Hormone antiestrogen                             | ±      |
| 09E09 | Estropipate                               | Estrogen       | Hormone estrogen                                 | ±      |
| 10D07 | Diethylstilbestrol                        | Estrogen       | Hormone estrogen                                  | ±      |
| 11E07 | Ethynylestradiol 3-methyl ether           | Estrogen       | Hormone estrogen                                  | ±      |
| 11E11 | Equin                                     | Estrogen       | Hormone estrogen                                  | ±      |
| 11G03 | Raloxifene hydrochloride                  | Estrogen       | Hormone estrogen (agonist)                       | ±      |
| 05H08 | Clomiphene citrate (Z,E)                  | Estrogen       | Hormone estrogen (agonist)                       | ±      |
| 02C06 | Danazol                                   | Antigonadotropin| Hormone estrogen (antagonist)                    | +      |
| 06H08 | Progestone                                | Progestogen    | Hormone progestogen                              | +      |
| 09D02 | Megestrol acetate                         | Progestogen    | Hormone progestogen                              | ±      |
| 09D06 | Hippoestrine hydrobromide                 | Hypotensor     | Hypotensor                                        | ±      |
| 06E06 | Nitamine hydrochioride                    | Hypotensor     | Hypotensor                                        | ±      |
| 11E06 | Amiprilose hydrochloride                   | Immunomodulator| Immunomodulator                                   | ±      |
| 03D03 | Thalidomide                               | Immunosuppressant| Immunosuppressant                                | ±      |
| 07H07 | Myocophenolic acid                        | Antineoplastic | Inosine monophosphate dehydrogenase inhibitor    | ±      |
| 02E03 | Metanephrine hydrochloride DL             | Adrenergic      | Isoprenaline uptake inhibitor extraneuronal      | ±      |
| 01B11 | Minoxidil                                 | Antihypertensor| K+ channel activator                              | +      |
| 02C07 | Nicorandil                                | Antihypertensor| K+ channel agonist (ATP-dependent channels)      | ±      |
| 13A07 | Sotalol hydrochloride                     | Antianginal    | K+ channel antagonist (ATP-dependent channels)   | ±      |
| 07H05 | Tolazamide                                | Antidiabetic    | K+ channel blocker (ATP-dependent channels)      | ±      |
| 01F06 | Acetohexamide                             | Antidiabetic (type II, noninsulin-dependent) | K+ channel blocker (ATP-dependent channels) | ±/±    |
| 05G09 | Dequalinium dichloride                    | Antibacterial   | K+ channel blocker (Ca2+-dependent channels, aparmp-sensitive small conductance) | ±      |
| 04D06 | Fenofibrate                               | Hypolipidemiant| Lipoprotein lipase activator                      | ±      |
| 10G04 | Clofibric acid                            | Antihyperlipoproteinemia | Lipoprotein lipase activator                    | ±      |
| 04E05 | Diethylcarbamazine citrate                | Anthelmintic    | Lipoygenase inhibitor                            | ±      |
| 07C08 | Quercetine dihydrate                      | Antimalarial    | Lipoygenase inhibitor                            | ±      |
| 08F03 | Harmol hydrochloride monohydrate          | Anxiolytic      | Liver conjugation probe                          | ±      |
| 11H07 | Arcaine sulfate                           | Bronchodilator  | Lowsers blood sugar                              | ±/±    |
| 12A04 | Digoxigenin                               | Diagnosis       | Mainly used as a non-isotopic label for DNA      | ±/±    |
| 03A11 | Phenezine sulfate                         | Antidepressant  | MAO inhibitor                                     | ±      |
| 10H06 | Isooxazole                                | Antidepressant  | MAO inhibitor                                     | ±      |
| 14F10 | Nialamide                                 | Antidepressant  | MAO inhibitor                                     | ±      |
| 08F04 | Harmine hydrochloride                     | Anthelminthic   | MAO inhibitor                                     | ±      |
| 04H09 | Quinacrine dihydrochloride dihydrate      | Antimalarial    | MAO inhibitor                                     | ±      |
| 13B04 | Pirinidole mesylate                       | Highly selective| Reversable inhibitor of monoamine oxidase type A | MAO inhibitor | ±      |
| 07H03 | Selegine hydrochloride                    | Antiparkinsonian| MAO inhibitor                                     | ±      |
| 07G11 | Parthenolide                              | Antiinflammatory| MAPK inhibitor                                    | ±      |
| 11H04 | Theophylline monohydrate                  | Bronchodilator  | Mastocyte degranulation inhibitor in vitro        | ±      |
| Plate     | Compound                        | Class                  | Effect                                      |
|-----------|---------------------------------|------------------------|---------------------------------------------|
| 12D03    | Monobenzone                     | Depigmentor            | melanin inhibition                          |
| 09A07    | Helvetoside                     | Cardiotonic            | membrane ATP inhibitor                       |
| 10C09    | Monensin sodium salt            | Antibacterial          | Membrane ionophores producer                 |
| 07D08    | Nystatine                       | Antifungal             | Membrane ionophores producer                 |
| 04B11    | Praziquantel                    | Anthelmintic           | Membrane permeability modulator             |
| 03E11    | Fenbendazole                    | Anthelmintic           | microtubule polymerisation inhibitor         |
| 05E04    | Colchicine                      | Antiinflammatory       | microtubule polymerisation inhibitor         |
| 02B11    | Nocodazole                      | Antineoplastic         | microtubule polymerisation inhibitor         |
| 02H06    | Paclitaxel                      | Antineoplastic         | microtubule polymerisation inhibitor         |
| 04A08    | Albendazole                     | Antineoplastic         | microtubule polymerisation inhibition        |
| 10G03    | Podophyllotoxin                 | Antiviral              | Microtubule polymerization                   |
| 12H08    | Desoxycorticosterone            | Mineralocorticoid      | Mineralocorticoid                           |
| 03G03    | Antimycin A                     | Antifungal             | Mitochondrial electron transport inhibitor   |
| 14C05    | Meptylcarine hydrochloride      | Local anesthetic       | Monoamine transport inhibition               |
| 11D08    | Carbexolone disodium salt       | Antulcerative          | Mucus stimulating synthesis                  |
| 11E05    | Procyclidine hydrochloride      | Antiparkinsonian       | Muscarinic antagonist                        |
| 01G03    | Homatropine hydrobromide (RLS)  | Antispasmodic          | Muscarinic antagonist                        |
| 11C11    | Ethanerine hydrochloride        | Antispasmodic          | Muscarinic antagonist                        |
| 03H05    | Chlorphenoxcarbamide            | Muscle relaxant        | Muscle relaxant                             |
| 09H03    | Benzocaine                      | Anesthetic             | Na+ channel blocker                         |
| 01B02    | Meticrane                       | Antihypertensor        | Na+ channel blocker                         |
| 01E02    | Precaine hydrochloride          | Local anesthetic       | Na+ channel blocker                         |
| 01E10    | Amyline hydrochloride           | Local Anesthetic       | Na+ channel blocker                         |
| 01E11    | Lidocaine hydrochloride         | Local anesthetic       | Na+ channel blocker                         |
| 01F08    | Benzoxinate hydrochloride       | Local anesthetic       | Na+ channel blocker                         |
| 01F09    | Chlortazine                     | Local anesthetic       | Na+ channel blocker                         |
| 04G06    | Dipexetine hydrochloride        | Local anesthetic       | Na+ channel blocker                         |
| 09H07    | Pramexine hydrochloride         | Local anesthetic       | Na+ channel inhibitor (voltage-dependent)    |
| 12H10    | Proparacaine hydrochloride      | Topical anesthetic     | Na+ channel inhibitor (voltage-dependent)    |
| 10G05    | Bendrofullumethiazide           | Antihypertensor        | Na+ Cl+ transport inhibitor                 |
| 01A10    | Hydrochlorothiazide             | Diuretic               | Na+ Cl+ transport inhibitor                 |
| 03F11    | Indapamide                      | Antihypertensor        | Na+ Cl+ uptake inhibitor                    |
| 05C02    | Furosemide                      | Diuretic               | Na+ Cl+ uptake inhibitor                    |
| 14A11    | Quinethazone                    | Diuretic               | Na+ Cl+ uptake inhibitor                    |
| 13C08    | Sanguinarine                    | Antimicrobial drug     | Na+ K+ ATPase inhibitor                      |
| 06D07    | Digoxigenin                     | Cardiotonic            | Na+ K+ ATPase inhibitor                      |
| 06D08    | Digoxin                         | Cardiotonic            | Na+ K+ ATPase inhibitor                      |
| 06H02    | Strophantin octahydrate         | Cardiotonic            | Na+ K+ ATPase inhibitor                      |
| 09B07    | Lanatoside C                    | Cardiotonic            | Na+ K+ ATPase inhibitor                      |
| 13G08    | Tocainide hydrochloride         | Antirhythmic           | Na+ K+ transport inhibitor                  |
| 13G11    | Torsemide                       | Diuretic               | Na+ uptake inhibitor                         |
| 14A08    | Piretanide                      | Diuretic               | Na+ uptake inhibitor                         |
| Plate | Drug Name | Category | Action | Notes |
|-------|-----------|----------|--------|-------|
| 01A06 | Atracurium besylate | Neuromuscular blocking agent | Curarizing agent | - |
| 03F03 | Pyrantel tartrate | Anthelmintic | Neuronal blocking agent | - |
| 13A09 | Decamethonium bromide | Muscle relaxant (skeletal) | Neuronal blocking agent | + |
| 08H04 | Thiophan | Neuronal blocking agent | Anticonvulsant | + |
| 09D10 | Delsoline | Anticonvulsant | Neuronal blocking agent | + |
| 09C10 | Anabasine | Anticonvulsant | Neuronal blocking agent | - |
| 09E03 | beta-Belladonna dichloroethylate | Anticonvulsant | Neuronal blocking agent | - |
| 09H05 | Isoniazid | Anticonvulsant | Neuronal blocking agent | + |
| 05E07 | Ambroxol hydrochloride | Expectorant | Neuronal blocking agent | - |
| 07G08 | Meclizine | Vasodilator | Neuronal blocking agent | + |
| 13B09 | Memantine hydrochloride | Antidepressant | Neuronal blocking agent | + |
| 14F02 | Spasmolytic | Antispasmodic | Neuronal blocking agent | - |
| 12C10 | Diclofenac sodium | Analgesic | Neuronal blocking agent | + |
| 07F08 | Piracetam | Nootropic | Neuronal blocking agent | - |
| 01B06 | Heptaminol hydrochloride | Antihypotensive | Neuronal blocking agent | + |
| 12C11 | Nicotexine hydrochloride | Antihypotensive | Neuronal blocking agent | - |
| 04C10 | Clopropramide hydrochloride | Antidepressant | Neuronal blocking agent | - |
| 05C07 | Mapropramide hydrochloride | Antidepressant | Neuronal blocking agent | - |
| 11A07 | Trimipramine maleate salt | Antidepressant | Neuronal blocking agent | - |
| 04B05 | Nortriptyline hydrochloride | Antidepressant | Neuronal blocking agent | - |
| 01D03 | Epizole | Analgesic | Neuronal blocking agent | - |
| 09G04 | Fampridine | Analgesic | Neuronal blocking agent | + |
| 14G05 | Clonipramine | Antidepressant | Neuronal blocking agent | + |
| 09F10 | Hexestrol | Estrogen | Neuronal blocking agent | + |
| 10H09 | Dienestrol | Non-steroidal estrogen | Neuronal blocking agent | - |
| 01B09 | Idoxuridine | Antiviral | Neuronal blocking agent | - |
| 02D02 | Nafoxidine hydrochloride | Antiviral | Neuronal blocking agent | + |
| 05D10 | Dextrimethorphan hydrobromide monohydrate | Antiviral | Neuronal blocking agent | - |
| 13E05 | Meptazinol hydrochloride | Analgesic (narcotic) | Neuronal blocking agent | + |
| 14G04 | Quinidine | Antiepileptic | Neuronal blocking agent | + |
| 13G06 | Letrozole | Antineoplastic | Neuronal blocking agent | + |
| 02E05 | Hesperetin | Antineoplastic | Neuronal blocking agent | - |
| 10F09 | Proadilan hydrochloride | Local anesthetic | Neuronal blocking agent | - |
| 05G10 | Ketoconazole | Antifungal | Neuronal blocking agent | + |
| 04A03 | Flavoxate hydrochloride | Antispasmodic | Phosphodiesterase inhibitor | + |
| 08C08 | Clofibric acid | Antithrombotic | Phosphodiesterase inhibitor | - |
| 01D04 | Diprophylline | Cardiac analgetic | Phosphodiesterase inhibitor | + |
| 03B03 | Estetiphenine | Cardiac analgetic | Phosphodiesterase inhibitor | - |
| 04C09 | Vinpocetine | Antistroke | Phosphodiesterase inhibitor | + |
| 13F03 | Trapidil | Vasodilator (coronary) | Phosphodiesterase inhibitor | + |
| 09A02 | Sulmazole | Cardiotonic | Phosphodiesterase inhibitor (III) | + |
| 10H11 | Aniracetam | Cardiotonic | Phosphodiesterase inhibitor (III) | + |
| 13B08 | Zardaverine | Hemostatic | Phosphodiesterase inhibitor (III) | + |
| 12H11 | Aminocaproic acid | Antistroke | Phosphodiesterase inhibitor | + |
| 12D10 | Bacitracin | Antibacterial | Neuronal blocking agent | + |
| 01A03 | Allantoin | Vulnerary | Neuronal blocking agent | + |
| Plate | Compound | Class | Function | Interaction |
|-------|----------|-------|----------|-------------|
| 01C05 | Norethynodrel | Progestogen | Progesterone receptor agonist | - |
| 04C02 | Ethisterone | Progestogen | Progesterone receptor agonist | - |
| 02G02 | Bromocriptine mesylate | Antiparkinsonian | Prolactin inhibitor | + |
| 13F09 | Alprostadil | Vasodilator | Prostaglandine E1 receptor ligand | + |
| 04B06 | Niflumic acid | Analgesic | Prostaglandine synthesis inhibitor | + |
| 06F11 | Dinoprost trometamol | Smooth muscle activator | Prostaglandin agonist | - |
| 14H05 | Saquinavir mesylate | Antiviral (HIV) | Protease inhibitor | - + |
| 02G07 | Tamoxifen citrate | Anticancer | Protein kinase C inhibitor | + |
| 08A11 | Ethamide dihydrochloride | Antineoplastic | Protein synthesis inhibitor | + + + + |
| 10G11 | Cycloheximide | Antimicrobial | Protein synthesis inhibitor | + - + + |
| 13A05 | Methacycline hydrochloride | Antimicrobial | Protein synthesis inhibitor | + + |
| 09E07 | Lycorine hydrochloride | Antitumoral | Protein translation inhibitor | - + + + |
| 13E09 | Gabexate mesilate | Severe acute pancreatitis | Proteinase inhibitor | + + + + |
| 03F06 | Mefenamic acid | Antipyretic | Nonsteroidal anti-inflammatory drug | - |
| 01A02 | Azaguanine-8 | Antineoplastic | Purine antimetabolite | + + + + |
| 11H02 | Iopamidol | Diagnostic aid | Radiocontrast agent | + + + + |
| 12F10 | Iodipamide | Diagnostic aid | Radiocontrast agent | + + + + |
| 12A05 | Meglumine | Expectorant | Radiocontrast agent | + + + + |
| 11H03 | Isopromide | Expectorant | Radiocontrast agent | + + + + |
| 03C10 | Aminopurine, 6-benzyl | Respiratory kinase inhibitor (plants) | + + + + |
| 13H08 | Zalcitabine | Antiviral (HIV) | Reverse transcriptase inhibitor | - + |
| 01D02 | Chloramphenicol | Antibacterial | Ribosomal peptidyltransferase inhibitor | + + + + |
| 01C06 | Thiamphenicol | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 02H02 | Erythromycin | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 02H03 | Oleandomycin phosphate | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 04H06 | Minocycline hydrochloride | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 05A02 | Streptomycin sulfate | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 05H05 | Kanamycin A sulfate | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 07C07 | Sisomicin sulfate | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 07H08 | Dithromycin | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 09A11 | Butoxetine disulfate salt | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 10D04 | Demeclocycline hydrochloride | Antibacterial | Ribosomal protein synthesis inhibitor | + + + + |
| 11F05 | Rifampicin | Antimicrobial | RNA polymerase inhibitor | + + + + |
| 07E06 | Rifampicin | Antimicrobial | RNA polymerase inhibitor | + + + + |
| 13D04 | Ribavirin | Antiviral | RNA synthesis inhibitor (viral) | + + + + |
| 12H02 | Crotamiton | Scabicide | Scabicide | + + + + |
| 13F10 | Tribenoside | Sclerosing agent | Sclerosing agent | + + + + |
| 12A06 | Carbenoxolone | Anticancer | Protease inhibitor | + + + + |
| 02G11 | Dihydroergotamine tartrate | Antimigraine | Serotonin antagonist | + + + + |
| 12E11 | Protriptyline hydrochloride | Antidepressant | Serotonin reuptake inhibitor | + + + + |
| 13D06 | Fluoxetine maleate | Antidepressant | Serotonin reuptake inhibitor | + + + + |
| 05G08 | Carbamazepine citrate | Anticonvulsant | Sigma1 receptor ligand | + + + + |
| 12G03 | Breyelin tosylate | Antidiuretic | SNS inhibition | + + + + |
| 10G10 | Diterene hydrochloride | Spasmolytic | Spasmolytic | + + + + |
| 02E08 | Ilosone | Antibacterial | Sterol 14-demethylase inhibitor | + + + + |
| Plate | Drug Name       | Category               | Effect                          | Plate | Drug Name       | Category               | Effect                          |
|-------|----------------|------------------------|--------------------------------|-------|----------------|------------------------|--------------------------------|
| 07B06 | Terconazole    | Antifungal             | Sterol 14-demethylase inhibitor | 14E11 | Homosalate     | Tool for uv screen     |                                |
| 01B03 | Benzonatate    | Antitussive            | Stretch receptor sensitivity decrease | 09F06 | Acacetin       | Anti-oxidant           | Topoisomerase I inhibitor      |
| 01A09 | Amprolum hydrochloride | Cocciidostatic     | Thiamine transport inhibitor   | 03D11 | Camptothecine (S,) | Antitumor agent       | Topoisomerase I inhibitor      |
| 14F09 | Kaempferol     | Anti-inflammatory      | Topoisomerase I inhibitor      | 03D04 | Oxolinic acid  | Antibacterial          | Topoisomerase II inhibitor     |
| 05G06 | Mitoxantrone dihydrochloride | Antineoplastic | Topoisomerase II inhibitor     | 05H07 | Etoposide      | Antineoplastic         | Topoisomerase II inhibitor     |
| 07H04 | Pentamidine isethionate | Antiparasitic      | Topoisomerase inhibition       | 14H11 | Nadifloxacin   | Antibacterial          | Topoisomerase inhibitor (topoisomerase II) |
| 03H06 | Metampicillin sodium salt | Antitumor agent    | Transpeptidase inhibitor (bacterial) | 06E11 | Dicloxacillin sodium salt | Antibacterial | Transpeptidase inhibitor (bacterial) |
| 07A06 | Cefadroxil     | Antibacterial          | Transpeptidase inhibitor (bacterial) | 07D10 | Imipenem       | Antibacterial          | Transpeptidase inhibitor (bacterial) |
| 09H10 | Cephalothin sodium salt | Antibacterial | Transpeptidase inhibitor (bacterial) | 09H11 | Cefuroxime sodium salt | Antibacterial | Transpeptidase inhibitor (bacterial) |
| 10A04 | Phenethicillin potassium salt | Antibacterial | Transpeptidase inhibitor (bacterial) | 13E11 | Talampicillin hydrochloride | Antibacterial | Transpeptidase inhibitor (bacterial) |
| 14G06 | Verteporfin    | Treatment of age-related macular degeneration | Treatment of age-related macular degeneration | 06E06 | Cytobenzaprin hydrochloride | Muscle relaxant | Tricyclic antidepressant |
| 01B08 | Levodopa       | Antiparkinsonian       | Tyrosine aminotransferase inhibitor | 11H10 | Capsaicin      | Topical analgesic      | Vanilloid receptor ligand      |
| 12B07 | N-Acetyl-L-leucine | Vertigo            | Vertigo                         | 06A08 | Adamanitamine fumarate | Antiviral             | Viral assembly inhibition (and uncoating inhibition) |
| 06F11 | Vitamin K2     | Dietary factor for controlling blood pressure | Vitamin                         | 06C10 | Cholecalciferol | Vitamin              |                                 |
| 06D04 | Cyanocobalamine | Vitamin              | Vitamin                         | 08G04 | Pyridoxine hydrochloride | Vitamin              |                                 |
| 13E08 | Fursultiamine hydrochloride | Vitamin (enzyme cofactor) | Vitamin                         |       | Phloroxyzine | Antiviral              | Vitamin (enzyme cofactor)      |
| 07E11 | Trolox         | Vitamin E analog      | Vitamin                         | 07F09 | Phenindione    | Anticoagulant          | Vitamin K inhibition           |
| 09F08 | Phenindione    | Anticoagulant          | Vitamin K inhibition            | 13A08 | 6-Hydroxytropinone | +                          |                                 |
| 14D02 | Imidurea       |                       |                                 | 14D08 | Tropine        |                         |                                 |
| 14D11 | Methazolone    | + +                   |                                 | 14E05 | Leucomin       |                         |                                 |

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| 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 | Yohimbinic acid monohydrate | - | - | + | + |
| Plate09A09 | Betonicine | - | - | - | - |
| 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 uptake inhibitor | - | - |
| Plate02B03 | Zimelidine dihydrochloride monohydrate | Antidepressant | 5HT uptake inhibitor | - | - |
| Plate07D02 | Fluoxetine hydrochloride | Antidepressant | 5HT uptake inhibitor | - | - |
| Plate11F02 | Paroxetine hydrochloride | Antidepressant | 5HT uptake inhibitor | - | - |
| Plate06B03 | Anisomycin | Antiprotozoal | Acetylcholine esterase inhibitor | - | - |
| Plate14E09 | (-)-Eseroline fumarate salt | Potent analgesic | Acetylcholine esterase inhibitor | - | - |
| Plate01D05 | Triamterene | Diuretic | Aldosterone antagonist (non competitive) | + | + |
| Plate10D02 | Terazosin hydrochloride | Antihypertensive | Alpha adrenergic antagonist | - | - |
| Plate07B05 | Dipivefrin hydrochloride | Adrenergic (ophthalmic) | alpha beta Agrenergic agonist | - | - |
| Plate04F04 | Glafenine hydrochloride | Analgesic | Analgesic | + | + |
| Plate01B10 | Captopril | Antihypertensive | Angiotensin converting enzyme inhibitor | - | - |
| Plate10G08 | Merbromin | Antibacterial | Antibacterial | + | + |
| Plate13A11 | Roxarsone | Antibacterial | Antibacterial | - | - |
| Plate09A03 | Epicatechin-(-) | Antidiarrhoeic | Antidiarrhoeic | - | - |
| Plate12F09 | Benserazide hydrochloride | In combination with levodopa as antiparkinsonian | amino acid decarboxylase inhibitor (L-aromatic a.a) | - | - |
| Plate14G11 | Parbendazole | Anthelmintic (VET) | Anthelmintic | +/+ | - | - |
| Plate13H11 | Pyruvinozide | Anthelmintic (Nematodes, enterobiasis) | Anthelmintic | - | - |
| Plate10A02 | Althiazide | Antihypertensive | Antihypertensive | - | - |
| Plate13H02 | Halofantrine hydrochloride | Antimalarial | Antimalarial | - | - |
| Plate07B05 | Propylthiouracil | Antihyperthyroid | Antimetabolite | + | + |
| Plate11G07 | Azacytidine-5' | Antineoplastic | Antimetabolite | - | - |
| Plate06H11 | Piroxylen dinehydrochloride | Antiprotozoal | Antimetabolite | - | - |
| Plate | Chemical Name | Category | Activity 1 | Activity 2 |
|-------|---------------|----------|------------|------------|
| Plate01E06 | Ethoxyquin | Antifungal | | |
| Plate03G11 | Strophanthidin | Cardiotonic | ATPase inhibitor | + + |
| Plate08G02 | Methoxy-6-hamalan | Psoriasis treatment | Benzodiazepine receptor ligand | + |
| Plate03D09 | Salbutamol | Bronchodilator | Beta adrenergic agonist | + |
| Plate04E03 | Fenoterol hydrobromide | Cardiotonic | + |
| Plate05C06 | Clobutinol hydrochloride | Bronchodilator | Beta adrenergic agonist | + |
| Plate10C10 | Isocathinone mesylate salt | Bronchodilator | Beta adrenergic agonist | + |
| Plate14F08 | (-)-Isoproterenol hydrochloride | Bronchodilator | Beta adrenergic agonist | + |
| Plate05C10 | Dobutamine hydrochloride | Bronchodilator | Beta adrenergic agonist (beta1) | + |
| Plate05E03 | Dobutamine hydrochloride | Bronchodilator | Beta adrenergic agonist (beta2) | - |
| Plate05E02 | Dobutamine hydrochloride | Bronchodilator | Beta adrenergic agonist (beta2) | + |
| Plate05H02 | Dobutamine hydrochloride | Bronchodilator | Beta adrenergic agonist (beta2) | - |
| Plate12G06 | Terbutaline hemisulfate | Bronchodilator | Beta adrenergic agonist (beta2) | + |
| Plate05C10 | Ritodrine hydrochloride | Bronchodilator | Beta adrenergic agonist (beta2) | + |
| Plate12G10 | (+,-)-Octopamine hydrochloride | Adrenergic | Beta adrenergic agonist (beta3) | + |
| Plate05C06 | Enoxime hydrochloride | Tocolytic | Beta adrenergic agonist (beta2) | + |
| Plate05E02 | Dobutamine hydrochloride | Antihypertensor | Beta adrenergic antagonist | - |
| Plate04A11 | Dobutamine hydrochloride | Antihypertensor | Beta adrenergic antagonist (beta1) | + |
| Plate04D08 | Dobutamine hydrochloride | Antihypertensor | Beta adrenergic antagonist (beta1) | + |
| Plate03A10 | Dobutamine hydrochloride | Antihypertensor | Beta adrenergic antagonist (could be, not shown) | + |
| Plate07F07 | (S)-(-)-Atenolol | Antihypertensor | Beta adrenergic blocker | + |
| Plate14B08 | Dobutamine hydrochloride | Antihypertensor | Beta adrenergic blocker | +/=/ |
| Plate | Compound | Function | Mode of Action |
|-------|----------|----------|----------------|
| 05G05 | Probucol | Antihyperproteic | Cholesterol downregulation |
| 03E03 | Triacetin, 3:3:5-triiodothyroacetic acid | Hypcholesterolemic drug | Cholesterol downregulation |
| 02A04 | Edrophonium chloride | Myasthenia Gravis test | Cholinergic |
| 01F03 | Carbamazepine | Anticonvulsant | Cholinergic antagonist |
| 01H06 | Adipheneridine hydrochloride | Local anesthetic | Cholinergic inhibition |
| 10H05 | Eucatropine hydrochloride | | Cholinergic inhibition |
| 02A03 | Cotinine ( - ) | Antidepressant | Cholinergic inhibition (and nicotinic inhibition) |
| 02C08 | Tomatine | Antifungal | Cholinergic inhibition |
| 10C02 | Nadolol |  | CoA nicotinamide adenine dinucleotide |
| 07D07 | Lovastatin | Antihypercholesteremic | |
| 13A10 | 3-Acetamidocoumarin | Antiinflammatory | coumarin |
| 03E04 | Flufenamic acid | Analgesic | Cyclooxygenase inhibition |
| 01D10 | Diffunisal | Antiinflammatory | Cyclooxygenase inhibition |
| 02B09 | Acetylsalicylic acid | Antiinflammatory | Cyclooxygenase inhibition |
| 07C09 | Reseveratrol | Antiinflammatory | Cyclooxygenase inhibition |
| 10B11 | Ebselen | Antiinflammatory | Cyclooxygenase inhibition |
| 10H32 | (R)-Naproxen sodium salt | Antiinflammatory | Cyclooxygenase inhibition |
| 11B07 | Suprofen | Antiinflammatory | Cyclooxygenase inhibition |
| 11F07 | Tolmetin sodium salt dihydrate | Antiinflammatory | Cyclooxygenase inhibition |
| 13E04 | Azapropazone | Anti-inflammatory | Cyclooxygenase inhibition |
| 14A10 | Oxphenbutazone | Anti-inflammatory | Cyclooxygenase inhibition |
| 09G06 | Methyl benzethonium chloride | Antibacterial | Detergent |
| 09G09 | Benzethonium chloride | Antibacterial | Detergent |
| 10F08 | Alexidine hydrochloride | Antibacterial | Detergent |
| 10H03 | Procidium iodide | Antibacterial | Detergent |
| 02G04 | Chlorhexidine | Bacteriostatic | Detergent |
| 12E06 | Thoronizum bromide | | Detergent |
| 02A02 | Metronidazole | Antibacterial | DNA damage (bacterial) |
| 07B03 | Nitrofurantoin | Antibacterial | DNA damage (bacterial) |
| 07H06 | Nitrofurazone | Antibacterial | DNA damage (bacterial) |
| 02A05 | Moroxydine hydrochloride | Antiviral | DNA damage (viral DNA RNA) |
| 05D06 | Hydroxycholine | Anthelmintic | DNA intercalating agent |
| 06D09 | Dorosorbic acid hydrochloride | Antibacterial | DNA intercalating agent |
| 08F55 | Ellipticine | Anticancer | DNA Interlacing agent |
| 07A08 | Daunorubicin hydrochloride | Antineoplastic | DNA intercalating agent |
| 14B07 | Trifluridine | Antiviral (ophthalmic) | DNA replication inhibitor (viral) |
| 07F05 | Atovaquone | Antineoplastic | DNA synthesis inhibitor (antiprotozoa) |
| 13B11 | Pinleodil hydrochloride | Vasodilator (peripheral) | Dopamine agonist |
| 02C02 | R(-) Apomorphine hydrochloride hemihydrate | Emetic | Dopamine agonist (D1) |
| 06F52 | Alizapride HCI | Antieptic | Dopamine antagonist |
| 08E02 | Scualnine | Antieptic | Dopamine antagonist |
| 02F03 | Loxapine succinate | Anxiolytic | Dopamine antagonist |
| Plate | Chemical Name | Class | Function | Notes |
|-------|---------------|-------|----------|-------|
| 01F04 | Triflupromazine hydrochloride | Antipsychotic | Dopamine antagonist | + |
| 01F27 | Sulpiride | Antipsychotic | Dopamine antagonist (D2) | + |
| 02B08 | Disulfiram | Alcohol deterrent | Dopamine beta hydroxylase inhibitor | +/− |
| 13D09 | Zuclopenthixol hydrochloride | Antipsychotic | Dopamine receptor blocker | + |
| 13H06 | Molindone hydrochloride | Antipsychotic | Dopamine receptor ligand | − |
| 05G07 | GB 12909 dihydrochloride | Antidepressant | Dopamine uptake inhibitor | + |
| 03G07 | Griseofulvin | Antifungal | Enzymatic inductor | − |
| 11A11 | Sulconazole nitrate | Antifungal | Ergosterol synthesis inhibition | − |
| 11G11 | Luteolin | Antioxidant | Flavonoid | + |
| 03E09 | Trimethoprim | Antibacterial | Folic acid antagonist | + |
| 01D08 | Pyrimethamine | Antiprotozoal | Folic acid antagonist | +/− |
| 08B02 | Sulfaguanidine sodium salt | Antibacterial | Folic acid synthesis inhibition | − |
| 08A10 | Dihydropyridine mesylate | Anticonvulsant | GABA A receptor Cl− channel high affinity | − |
| 07F10 | Thiocolchicoside | Muscle relaxant | GABA antagonist | + |
| 11E02 | Securinine | CNS stimulant | GABA antagonists | + |
| 09C03 | Gelserine | Tumor inhibitor | GABA antagonist | − |
| 09B03 | Picrotoxinin | Analeptic | GABA channel blocker | − |
| 09B11 | Avermectin B1 | Antihelminthic | GABA receptors ligand | + |
| 05A04 | Chlorpropamide | Antihypertensive | Glucose transport inhibitor | + |
| 02D11 | Triamcinolone | Anti-inflammatory | Glucocorticoid | + |
| 07D09 | Budesonide | Anti-inflammatory | Glucocorticoid | + |
| 01H08 | Prednisone | Glucocorticoid | Glucocorticoid | + |
| 04D10 | Methylprednisolone-6 α | Glucocorticoid | Glucocorticoid | + |
| 05E03 | Betamethasone | Glucocorticoid | Glucocorticoid | + |
| 09A04 | Flurisamide | Glucocorticoid | Glucocorticoid | + |
| 09A06 | Flurandrenolide | Glucocorticoid | Glucocorticoid | + |
| 09H09 | Fluorometholone | Glucocorticoid | Glucocorticoid | + |
| 10B05 | Flumethasone | Glucocorticoid | Glucocorticoid | + |
| 10F05 | Fluocinonide | Glucocorticoid | Glucocorticoid | + |
| 10G02 | Clobetasol propionate | Glucocorticoid | Glucocorticoid | − |
| 14H10 | Docortione pivalate | Glucocorticoid | Glucocorticoid | + |
| 08B03 | Mometasone furoate | Anti-inflammatory | Glucocorticoid receptor agonist | + |
| 10F02 | Allocortone dipropionate | Anti-inflammatory | Glucocorticoid receptor agonist | + |
| 05E08 | Benfluoride | Hypolipidemic | Glucose transport enhancer | − |
| 03F08 | Mebendazole | Parasite suppressor | Glucose transport inhibitor? | + |
| 02E07 | Metbazine hydrochloride | Antimalarial | Heme polymerase inhibitor | − |
| 06H07 | Primidone diprophosphate | Antimalarial | Heme polymerase inhibitor | − |
| 10H09 | Methohexizine maleate salt | Analgesic | Histamine antagonist | + |
| 09G07 | Chlorcyclizine hydrochloride | Antihistaminic | Histamine antagonist | + |
| 10H04 | Clopanserine hydrochloride | Antitussive | Histamine antagonist | − |
| 02F07 | Astemizole | Antihistaminic | Histamine antagonist (H1) | − |
| 11A08 | Chlorpromazine hydrochloride | Antihistaminic | Histamine antagonist (H1) | − |
| 13H10 | Levocabastine hydrochloride | Antihistaminic | Histamine antagonist (H1) | − |
| 03E02 | Ranitidine hydrochloride | Antulcerative | Histamine antagonist (H2) | − |
| 06C09 | Rosazine maleate HCl | Antulcerative | Histamine antagonist (H2) | − |
| 09E09 | Estropipate | Estrogen | Hormone estrogen | − |
| 10D07 | Diethylstilbestrol | Estrogen | Hormone estrogen | + |
| 11E07 | Ethynylestradiol 3-methyl ether | Estrogen | Hormone estrogen | − |
| Plate | Compound | Biological Activity | Action | Label |
|-------|----------|---------------------|--------|-------|
| 05H08 | Clomiphene citrate (Z,E) | Antineoplastic hormone Estrogen agonist | - | - |
| 02C06 | Danazol | Antigonadotropin hormone Estrogen antagonist | +/- | - |
| 07H07 | Mycophenolic acid | Antineoplastic Insine monophosphate dehydrogenase inhibitor | +/- | + |
| 02E03 | Metanephrine hydrochloride DL | Isoprorenaline uptake inhibitor extraneuronal | - | + |
| 07H05 | Tolazamide | Antidiabetic K+ channel blocker (ATP-dependent channels) | - | - |
| 01F06 | Acetohexamide | Antidiabetic (type II, noninsulin-dependent) K+ channel blocker (ATP-dependent channels) | + | - |
| 02F02 | Glipizide | Hypoglycemic K+ channel blocker (ATP-dependent channels) | - | + |
| 03C11 | Tolbutamide | Hypoglycemic K+ channel blocker (ATP-dependent channels) | + | - |
| 04E05 | Diethylcarbamazine citrate | Antihelmintic Lipoxygenase inhibitor | + | - |
| 07C08 | Quercetine dihydrate | Antimalarial Lipoxygenase inhibitor | - | - |
| 08F03 | Harmel hydrochloride monohydrate | Anvolytic Liver conjugation probe | + | - |
| 11H07 | Arcaine sulfate | Lowers blood sugar | - | - |
| 12A04 | Digoxigenin | Diagnosis Mainly used as a non-isotopic label for DNA | - | + |
| 03A11 | Phenelzine sulfate | Antidepressant MAO inhibitor | - | - |
| 03B04 | Tranylcypromine hydrochloride | Antidepressant MAO inhibitor | - | - |
| 04H09 | Harmine hydrochloride dihydrate | Antihelmintic MAO inhibitor | + | - |
| 07G11 | Parthenolide | Antiflammatory MAPK inhibitor | - | + |
| 06B05 | Apigenin | Antiproliferative MAPK inhibitor | - | + |
| 12D03 | Monobenzone | Depigmentor melanin inhibition | - | - |
| 09A07 | Helveticoside | Cardiotonic membrane ATP inhibitor | - | - |
| 10C09 | Monensin sodium salt | Antibacterial Membrane ionophores producer | - | - |
| 03E11 | Fenbendazole | Antihelmintic microtubule polymerisation inhibitor | + | - |
| 05E04 | Colchicine | Antinflammatory microtubule polymerisation inhibitor | +/- | - |
| 02B11 | Nocodazole | Antineoplastic microtubule polymerisation inhibitor | +/- | - |
| 02H06 | Paclitaxel | Antineoplastic microtubule polymerisation inhibitor | +/- | - |
| 04A08 | Albindazole | microtubule polymerisation inhibitor | +/- | +/- |
| 10G03 | Podophyllotoxin | Antiviral microtubule polymerisation inhibitor | +/+, + | + |
| 03G03 | Antimycin A | Antifungal Mitochondrial electron transport inhibitor | - | + |
| 09D07 | Beta-escin | Peripheral vascular disorders Mucosamine transport inhibitor | - | - |
| 14B06 | Pipеридол-4-гидроксихлорид | Antispasmodic Muscarinic blocking agent | + | - |
| 09H03 | Benzocaine | Anesthetic Na+ channel blocker | - | - |
| 10E02 | Butamben | Anesthetic Na+ channel blocker | - | - |
| 01E10 | Amylamine hydrochloride | Local Anesthetic Na+ channel blocker | - | - |
| 03D10 | Prilocaine hydrochloride | Local anesthetic Na+ channel blocker | + | - |
| 04D06 | Fenofibrate | Hypolipidemiant Na+ channel blocker (voltage-dependent) | + | + |
| 10G05 | Bendroflumethiazide | Antihypertensor Na+ Cl- transport inhibitor | - | - |
| 03F11 | Indapamide | Antihypertensor Na+ Cl- uptake inhibitor | +/- | - |
| Plate | Chemical | Category | Action | Notes |
|-------|----------|----------|--------|-------|
| 02D03 | Metolazone | Diuretic | Na⁺ Cl⁻ uptake inhibitor | - |
| 14A11 | Quinethazone | Diuretic | Na⁺ Cl⁻ uptake inhibitor | - |
| 13C08 | Sanguinarine | Antimicrobial drug | Na⁺ K⁺ ATPase inhibitor | - |
| 06D07 | Digidoxin | Cardiotoxic | Na⁺ K⁺ ATPase inhibitor | + |
| 06D08 | Digosin | Cardiotoxic | Na⁺ K⁺ ATPase inhibitor | - |
| 06H02 | Strophantine octahydrate | Cardiotoxic | Na⁺ K⁺ ATPase inhibitor | + |
| 09B07 | Lanatoside C | Cardiotoxic | Na⁺ K⁺ ATPase inhibitor | + |
| 13A09 | Decamethonium bromide | Muscle relaxant (skeletal) | Neur muscular depolarizing agent | - |
| 09E03 | beta- Belladonna dichloroethylate | Muscle relaxant | Nicotinic receptor ligand | - |
| 11A07 | Tempranipine maleate salt | Antidepressant | Noradrenaline uptake inhibitor | - |
| 09B09 | Suxibuzone | Antiinflammatory | NSA | - |
| 11C07 | Chalazol citrate salt | Antiinflammatory | NSA | - |
| 10H09 | Dienestrol | Non-steroidal estrogen | Nuclear receptor ligand | - |
| 01B09 | Idoxuridine | Antiviral | Nucleic acid synthesis inhibitors | + |
| 13G06 | Letrozole | Anticancer | Protein kinase C inhibitor | + |
| 02E05 | Hesperetin | Antineoplastic | P450 inhibitor | + |
| 10F09 | Proadifen hydrochloride | Local anesthetic | P450 inhibitor (mono-oxygenases) | + |
| 04A03 | Flavoxate hydrochloride | Antispasmodic | Phosphodiesterase inhibitor | + |
| 08C08 | Clostazol | Antithrombotic | Phosphodiesterase inhibitor | + |
| 13F09 | Alprostadil | Vasodilator | Prostaglandine E1 receptor ligand | - |
| 14H05 | Saquinavir mesylate | Antiviral (HIV) | Protease inhibitor | - |
| 02G07 | Tamoxifen citrate | Anticancer | Protein kinase C inhibitor | + |
| 08A11 | Emetine dihydrochloride | Antiabetic | Protein synthesis inhibitor | - |
| 10G11 | Cycloheximide | Antibacterial | Protein synthesis inhibitor | - |
| 13A05 | Methacycline hydrochloride | Antibacterial | Protein synthesis inhibitor | - |
| 02H05 | Josophacin | Antibacterial | Ribosomal protein synthesis inhibitor | - |
| 05H05 | Kanamycin A sulfate | Antibacterial | Ribosomal protein synthesis inhibitor | + |
| 13F10 | Tribenoside | Sclerosing agent | Sclerosing agent | - |
| 12A06 | Cantharidin | Rubefiant | Serine protease releaser | - |
| 10G10 | Diphenylhydrochloride | Spasmolytic | Spasmolytic | - |
| 02E08 | Isoniazide | Antituberculosis | Sterol 14-demethylase inhibitor | - |
| 01G08 | Miconazole | Antifungal | Sterol 14-demethylase inhibitor | - |
| 03D11 | Camptothecine (S,+) | Antitumor agent | Topoisomerase I inhibitor | + |
| 03E05 | Flumequine | Antibacterial | Topoisomerase II inhibitor | + |
| 05G06 | Mitoxantrone ditydrochloride | Antineoplastic | Topoisomerase II inhibitor | - |
| 05H07 | Etoposide | Anticancer | Topoisomerase II inhibitor | + |
| 14H11 | Nadifloxacin | Antibacterial | Topoisomerase inhibitor (topoisomerase II) | - |
| 02D06 | Ampicillin trihydrate | Antibacterial | Transpeptidase inhibitor (bacterial) | - |
| 14G06 | Verteporfin | Treatment of age-related macular degeneration | Treatment of age-related macular degeneration | + |
| 11H10 | Capsaicin | Topical analgesic | Vanilloid receptor ligand | - |
| 06C02 | Sulodiazol | Vasodilator | Vasodilator | - |
| 12B07 | N-Acetyl-L-leucine | Vertigo | Vertigo | + |
| 06A08 | Adaptamantamine fumarate | Antituberculosis | Viral assembly inhibition (and uncoating inhibition) | + |
| 08H05 | Riboflavin | Vitamin | Vitamin | + |
| 07E11 | Trolox | Vitamin E analog | Vitamin | + |
| Plate06F10 | Menadione | Vitamin K3 | Vitamin precursor | +/- |   |   |
|------------|-----------|------------|------------------|-----|---|---|
| Plate14D11 | Methiazole |           |                   | -   |   |   |
| 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 | Betonicine    | -                 | -              | -         | -         | -            |             | -          | -           |
| Plate02B10 | Mianserin    | Antidepressant    | 5HT antagonist | -         | -         | -            |             | -          | -           |
| Plate02C04 | Cyproheptadine hydrochloride | Antipruritic | 5HT antagonist (5HT3) | -         | -         | -            |             | -          | -           |
| Plate06G02 | Dexamethasone acetate | Antinflammatory | 5HT antagonist effect doper | -         | -         | -            |             | -          | -           |
| Plate09C09 | Skimmianine | Sedative          | 5HT ligand    | -         | -         | -            |             | -          | -           |
| Plate01H03 | Imipramine hydrochloride | Antidepressant | 5HT transport inhibitor | -         | +         | -            |             | -          | -           |
| Plate02B03 | Zimelidine dihydrochloride monohydrate | Antidepressant | 5HT uptake inhibitor | -         | -         | -            |             | -          | -           |
| Plate02E11 | Dexamethasone acetate | Antiinflammatory | 5HT antagonist effect | -         | -         | -            |             | -          | -           |
| Plate02B03 | Paroxetine hydrochloride | Antidepressant | 5HT uptake inhibitor | -         | +         | -            |             | -          | -           |
| Plate06G02 | Tropisetron HCl | Antiemetic | 5HT antagonist (5HT3) | -         | -         | -            |             | -          | -           |
| Plate02E09 | (-)-Eseroline fumarate salt | Potent analgesic | Acetylcholine esterase inhibitor | -         | -         | -            |             | -          | -           |
| Plate07D02 | Dipyridamole | Platelet antiaggregant | Adenosine metabolism inhibitor | -         | -         | -            |             | -          | -           |
| Plate01E08 | Ticitopidine hydrochloride | Platelet antiaggregant | ADP antagonist | -         | -         | -            |             | -          | -           |
| Plate02E09 | Spironolactone | Diuretic | Aldosterone antagonist | -         | -         | -            |             | -          | -           |
| Plate01D05 | Triamterene | Diuretic | Aldosterone antagonist (non competitive) | -         | -         | -            |             | -          | -           |
| Plate09D09 | Ricinine | Alkaloid | -              | -         | -         | -            |             | -          | -           |
| Plate08E05 | Piperlongumine | Antifungal | Alkaloid | +         | +         | -            |             | -          | -           |
| Plate09B05 | Dacarbazine | Antineoplastic | Alkylating agent | +         | -         | -            |             | -          | -           |
| Plate02B07 | Guanabenz acetate | Antihypertenser | Alpha adrenergic agonist | -         | -         | -            |             | -          | -           |
| Plate02G08 | Nercine | Vasodilator | Alpha adrenergic agonist | +         | -         | -            |             | -          | -           |
| Plate12E07 | Idazoxan hydrochloride | Antiparkinsonian | Alpha adrenergic agonist (alpha2) | -         | -         | -            |             | -          | -           |
| Plate10B10 | Levonordefrin | Vasoconstrictor | Alpha Adrenergic agonist (alpha2) | -         | -         | -            |             | -          | -           |
| Plate01E03 | Moxisylyte hydrochloride | Vasodilator | Alpha adrenergic antagonist | -         | -         | -            |             | -          | -           |
| Plate01F11 | Tolazoline hydrochloride | Vasodilator | Alpha adrenergic antagonist | -         | -         | -            |             | -          | -           |
| Plate01H05 | Amitriptyline hydrochloride | Antidiabetic | Alpha Adrenergic antagonist (alpha1) | -         | -         | -            |             | -          | -           |
| Plate09F09 | Tetrahydrozoline hydrochloride | Vasoconstrictor | Alpha adrenergic ligand | -         | -         | -            |             | -          | -           |
| Plate01B10 | Captopril | Antihypertensor | Angiotensive converting enzyme inhibitor | -         | -         | -            |             | -          | -           |
| Plate13A11 | Roxarsone | Antibacterial | Antibacterial | -         | -         | -            |             | -          | -           |
| Plate09A03 | Ethoxyquin | Antifungal | Antioxidant | -         | -         | -            |             | -          | -           |
| Plate14G11 | Parbendazole | Anthelmintic (VET) | Anthelmintic | +         | -         | -            |             | -          | -           |
| Plate13H11 | Pyrvinium pamoate | Anthelmintic (Nematodes, enterobiasis) | Anthelmintic | -         | -         | -            |             | -          | -           |
| Plate01H02 | Tetralazine hydrochloride | Antihypertensor | Antihypertensor | -         | -         | -            |             | -          | -           |
| Plate13H02 | Halotranine hydrochloride | Antimalarial | Antimalarial | -         | -         | -            |             | -          | -           |
| Plate11G07 | Azacytidine-5 | Antineoplastic | Antimetabolite | +/−        | +         | -            |             | -          | -           |
| Plate06H11 | Puremycin dihydrochloride | Antiprotozoal | Antimetabolite | -         | -         | -            |             | -          | -           |
| Plate02B05 | Azathioprine | Immunosuppressant | Antimetabolite | -         | -         | -            |             | -          | -           |
| Plate10E06 | Ethoxyquin | Antifungal | Antioxidant | +/−        | -         | -            |             | -          | -           |
| Plate09G11 | Strophanthidin | Cardiotonic | ATPase inhibitor | +         | -         | -            |             | -          | -           |
| Plate10C10 | Isethathine mesylate salt | Bronchodilator | Beta adrenergic agonist | -         | -         | -            |             | -          | -           |
| Plate | Chemical Name | Class | Action | Notes |
|-------|---------------|-------|--------|-------|
| 01G09 | Isoxsuprine hydrochloride | Vasodilator | Beta adrenergic agonist | |
| 09G02 | Terbutaline hemisulfate | Bronchodilator | Beta adrenergic agonist (beta2) | |
| 01G10 | Acetabutol hydrochloride | Antianginal | Beta adrenergic antagonist (beta1) | |
| 14B08 | Oxprenolol hydrochloride | Antihypertensor | Beta adrenergic blocker | |
| 12D02 | (+)-Isoproterenol (+)-bitartrate salt | Bronchodilator | Bronchodilator | + |
| 02G05 | Loperamide hydrochloride | Antidiarrhoeic | Ca2+ channel antagonist | |
| 01G04 | Nifedipine | Antihypertensor | Ca2+ channels blocker (L type) | + |
| 01D10 | Diflunisal | Antiinflammatory | Cyclooxygenase inhibition | |
| 14H09 | Cotinine (-) | Antidepressant | Cholinergic inhibition (and nicotinic inhibition) | |
| 01C03 | Panthenol (D) | Vitamin | CoA synthesis precursor | |
| 02C08 | Tomatine | Antifungal | Cholinergic inhibition (pH-dependent competitive inhibition of the enzyme acetylcholinesterase) | |
| 01F02 | Trichlorfon | Antihelmintic | Cholinergic inhibition | |
| 01C33 | Panthenol (D) | Vitamin | CoA synthesis precursor | |
| 14H09 | Enalapril maleate | Antihypertensor | Converting enzyme inhibitor | |
| 03E06 | Toltenamic acid | Antiinflammatory | Cyclooxygenase inhibition | |
| 01E09 | Dicyclomine hydrochloride | Antispasmodic | Cholinergic inhibition | |
| 01H04 | Sulindac | Antiinflammatory | Cyclooxygenase inhibition | |
| 02B09 | Acetylsalicylic acid | Antiinflammatory | Cyclooxygenase inhibition | |
| 10H02 | (R)-Naproxen sodium salt | Antiinflammatory | Cyclooxygenase inhibition | +
| 03F10 | Ketoprofen | Antiinflammatory | Cyclooxygenase inhibition | |
| 07C09 | Resveratrol | Antiinflammatory | Cyclooxygenase inhibition | +
| 10B11 | Ebselen | Antiinflammatory | Cyclooxygenase inhibition | |
| Plate | Compound | Category | Inhibitory Effect |
|-------|----------|----------|------------------|
| 11F07 | Tolmetin sodium salt dihydrate | Antiinflammatory | cyclooxygenase inhibition |
| 01E05 | Isoxipam | Antiinflammatory | cyclooxygenase inhibition |
| 11B07 | Suprofen | Antiinflammatory | cyclooxygenase inhibition |
| 11D07 | Indoprofen | Antiinflammatory | cyclooxygenase inhibition |
| 13E04 | Azapropazone | Anti-inflammatory | cyclooxygenase inhibition |
| 14A10 | Antipyrine, 4-hydroxy | Antipyrine metabolite | cyclooxygenase inhibition |
| 01C11 | Antipyrine, 4-hydroxy | Antipyrine metabolite | cyclooxygenase inhibition |
| 10H03 | Propidium iodide | Antibacterial | Detergent |
| 09G09 | Benzethonium chloride | Antibacterial | Detergent |
| 10F08 | Alexidine dihydrochloride | Antibacterial | Detergent |
| 09G06 | Methyl benzethonium chloride | Antibacterial | Detergent |
| 02A10 | Ursolic acid | Diuretic | Detergent |
| 02A02 | Metronidazole | Antiinflammatory | DNA damage (bacterial) |
| 07B03 | Nitrofural | Antiinflammatory | DNA damage (bacterial) |
| 01D11 | Niclosamide | Antiinflammatory | DNA damage (Helminthic) |
| 02A05 | Metoxylidid hydrochloride | Antiinflammatory | DNA damage (viral DNA RNA) |
| 07A08 | Daunorubicin hydrochloride | Antiinflammatory | DNA intercalating agent |
| 14B07 | Trifluridine | Antiinflammatory | DNA replication inhibitor (viral) |
| 01G07 | Minaprine dihydrochloride | Antiinflammatory | Dopamine agonist |
| 02C02 | R(+) Apomorphine hydrochloride hemihydrate | Antiinflammatory | Dopamine agonist (D1) |
| 08G09 | Salicilol hydrobromide | Antiinflammatory | Dopamine analog |
| 01G05 | Chlorpromazine hydrochloride | Antiinflammatory | Dopamine antagonist |
| 08E02 | Scolerine | Antiinflammatory | Dopamine antagonist |
| 02D06 | Haloperidol | Antiinflammatory | Dopamine antagonist |
| 02E06 | Perphenazine | Antiinflammatory | Dopamine antagonist |
| 02G10 | Thiopeperazine dimesylate | Antiinflammatory | Dopamine antagonist |
| 02F03 | Loxapine succinate | Antiinflammatory | Dopamine antagonist |
| 01F04 | Trifluromethyldichloro | Antiinflammatory | Dopamine antagonist |
| 01H11 | Trimethobenzamide | Antiinflammatory | Dopamine antagonist (D2) |
| 01F07 | Sulpiride | Antiinflammatory | Dopamine antagonist (D2) |
| 08B07 | Acetazolamide maleate salt | Antiinflammatory | Dopamine antagonist |
| 02B08 | Disulfiram | Alcohol deterrent | Dopamine beta hydroxylase inhibitor |
| 05G07 | GBR 12909 dihydrochloride | Antiinflammatory | Dopamine uptake inhibitor |
| 02C03 | Amoxapine | Antiinflammatory | Dopamine uptake inhibitor |
| 02C09 | Nifensine maleate | Antiinflammatory | Dopamine uptake inhibitor |
| 02D10 | Picotamide monohydrate | Antiinflammatory | Eicosanoid receptor antagonist |
| 01G11 | Tolnaftate | Antiinflammatory | Eicosanoid synthesis inhibitor |
| 11A11 | Sulconazole nitrate | Antiinflammatory | Eicosanoid synthesis inhibitor |
| 01D06 | Dapsone | Antiinflammatory | Folic acid antagonist |
| 01D08 | Pyrimethamine | Antiinflammatory | Folic acid antagonist |
| 02F06 | Methotrexate | Antiinflammatory | Folic acid inhibitor |
| 09G03 | Sulconazole thioacetate | Antiinflammatory | Folic acid synthesis inhibitor |
| 01A11 | Sulfaguanidine | Antiinflammatory | Folic acid synthesis inhibitor |
| 01B05 | Sulfacetamide sodium hydrate | Antiinflammatory | Folic acid synthesis inhibitor |
| Plate | Chemical Name                  | Category        | Biological Activity                                                                 |
|------|-------------------------------|-----------------|-------------------------------------------------------------------------------------|
| 01B07| Sulfathiazole                  | Antibacterial   | Folic acid synthesis inhibitor                                                       |
| 01C02| Sulfaphenazole                 | Antibacterial   | Folic acid synthesis inhibitor                                                       |
| 01C04| Sulfadiazine                   | Antibacterial   | Folic acid synthesis inhibitor                                                       |
| 01G02| Morantel tartrate              | Anthelmintic    | Fumarate reductase inhibitor                                                         |
| 08A10| Dihydroergotoxine mesylate     | Anticonvulsant  | GABA A receptor CI-channel high affinity                                              |
| 07F10| Thioicolchicoside              | Muscle relaxant  | GABA agonist ?                                                                       |
| 09C03| Gelisemine                     | Tumour inhibitor| GABA antagonist                                                                      |
| 01G02| Gabapentin                     | Anticonvulsant  | GABA receptor ligand                                                                 |
| 02D11| Triamcinolone                  | Anti-inflammatory| Glucocorticoid                                                                       |
| 01A07| Isotretinoin                   | Anti-inflammatory| Glucocorticoid                                                                       |
| 09H09| Fluorometholone                | Anti-inflammatory| Glucocorticoid                                                                       |
| 01H08| Prednisone                     | Glucocorticoid  | Glucocorticoid                                                                       |
| 01G02| Clofibric acid propionate      | Glucocorticoid  | Glucocorticoid                                                                       |
| 14H10| Ciclosporine                   | Glucocorticoid  | Glucocorticoid                                                                       |
| 10F02| Alclometasone dipropionate     | Anti-inflammatory| glucocorticoid receptor agonist                                                      |
| 02E07| Mefloquine hydrochloride       | Antimalarial     | Heme polymerase inhibitor                                                            |
| 06H07| Primaquine diphosphate         | Antimalarial     | Heme polymerase inhibitor                                                            |
| 01E04| Betazole hydrochloride         | Gastric secretion stimulant| Histamine analog                                                                   |
| 11A08| Chlorpromazine hydrochloride   | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 01C08| Doxylamine succinate           | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 01F10| Pheniramine maleate            | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 01G06| Diphenhydramine hydrochloride  | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 02D08| Chlorpheniramine maleate       | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 02F04| Hydroxyzine hydrochloride      | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 02F07| Astemizole                     | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 02F09| Terfenadine                    | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 02B04| Azacyclonol                    | Antipsychotic    | Histamine antagonist (H1)                                                            |
| 01C07| Cimetidine                     | Antiulcer        | Histamine antagonist (H2)                                                            |
| 02C05| Famotidine                     | Antiulcer        | Histamine antagonist (H2)                                                            |
| 06C09| Roxatidine Acetate HCl         | Antiulcer        | Histamine antagonist (H2)                                                            |
| 03B11| Flutamide                      | Anticancer       | Hormone androgen receptor antagonist                                                  |
| 09E09| Estropipate                    | Estrogen         | Hormone estrogen                                                                     |
| 11E07| Ethynylestradiol 3-methyl ether| Estrogen        | Hormone estrogen                                                                      |
| 02C06| Danazol                        | Antagonadotropin | hormone Estrogen antagonist                                                            |
| 02B06| Lynestrenol                    | Progestagen      | hormone estrogen inhibition                                                           |
| 07H07| Mycophenolic acid              | Antineoplastic   | Inosine monophosphate dehydrogenase inhibitor                                         |
| 02E03| Metoprolol hydrochloride DL    | Isopropenalin uptake inhibitor extraneuronal                                          |
| 02C07| Nicorandil                     | Antihypertensor  | K+ channel agonist (ATP-dependent channels)                                           |
| 01F06| Acetohexamide                  | Antidiabetic      | K+ channel blocker (ATP-dependent channels)                                          |
| 02F02| Glipizide                      | Hypoglycemic     | K+ channel blocker (ATP-dependent channels)                                          |
| Plate05G09 | Dequalinium dichloride | Antibacterial | K+ channel blocker (Ca2+-dependent channels , apamin-sensitive small conductance) | + |
|----------|------------------------|--------------|-------------------------------------------------------------------------------|---|
| Plate11H07 | Arcaine sulfate | Lowers blood sugar | - |
| Plate12A04 | Digoxigenin | Diagnosis | Mainly used as a non-isotopic label for DNA |
| Plate03A11 | Phenelzine sulfate | Antidepressant | MAO inhibitor |
| Plate08F04 | Harmine hydrochloride | Antihelminthic | MAO inhibitor |
| Plate04H09 | Quinacrine dihydrochloride dihydrate | Antimalarial | MAO inhibitor |
| Plate07G11 | Parthenolide | Antiinflammatory | MAPK inhibitor |
| Plate09A07 | Helvetoside | Cardiotonic | membrane ATP inhibitor |
| Plate05E04 | Colchicine | Antiinflammatory | microtubule polymerisation inhibitor |
| Plate02B11 | Nocodazole | Antineoplastic | microtubule polymerisation inhibitor |
| Plate02H07 | Paclitaxel | Antineoplastic | microtubule polymerisation inhibitor |
| Plate04A08 | Albendazole | Antineoplastic | microtubule polymerisation inhibitor |
| Plate10G03 | Podophyllotoxin | Antiviral | Microtubule polymerisation inhibitor |
| Plate03G03 | Antimycin A | Antifungal | Mitochondrial electron transport inhibitor |
| Plate09D07 | Beta-Escin | Peripheral vascular disorders | Monoamine transport inhibition |
| Plate01G03 | Homatropine hydrobromide (R,S) | Antispasmodic | Muscarinic antagonist |
| Plate02E10 | Pirenzepine dihydrochloride | Antiulcerative | Muscarinic antagonist (M1) |
| Plate01B01 | Dibucaine | Local anesthetic | Na+ channel blocker |
| Plate01E02 | Procaine hydrochloride | Local anesthetic | Na+ channel blocker |
| Plate01E11 | Lidocaine hydrochloride | Local anesthetic | Na+ channel blocker |
| Plate01F08 | Benzocaine hydrochloride | Local anesthetic | Na+ channel blocker |
| Plate01F09 | Oxicamhydrocine | Local anesthetic | Na+ channel blocker |
| Plate01H07 | Oxethazaine | Local anesthetic | Na+ channel blocker |
| Plate01E10 | Amylene hydrochloride | Local Anesthetic | Na+ channel blocker |
| Plate01G05 | Bendroflumethiazide | Antihypertensor | Na+ Cl- transport inhibitor |
| Plate01B04 | Hydroflumethiazide | Antihypertensor | Na+ Cl- transport inhibitor |
| Plate02D03 | Metolazone | Diuretic | 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 |
| Plate13A09 | Decamethonium bromide | Muscle relaxant (skeletal) | Neuromuscular depolarizing agent |
| Plate09E03 | beta- Belladonnine dichloroethylate | Muscle relaxant | Nicotinic receptor ligand |
| Plate02C10 | Dizociline maleate | - | MDMA receptor probe |
| Plate01B06 | Heptamin hydrochloride | Antihypotensive | Noradrenaline increase |
| Plate11A07 | Trimipramine maleate salt | Antidepressant | Noradrenaline uptake inhibitor |
| Plate01D03 | Epirizole | Analgesic | NSAI |
| Plate09B09 | Suxibuzone | Antiinflammatory | NSAI |
| Plate11C07 | Oxalamine citrate salt | Antiinflammatory | NSAI |
| Plate01B09 | Idoxuridine | Antiinflammatory | Nucleic acid synthesis inhibitors |
| Plate01B08 | Meticrane | Antihypertensor | Na+ channel blocker |
| Plate01D03 | Epirizole | Analgesic | NSAI |
| Plate11C07 | Oxalamine citrate salt | Antiinflammatory | NSAI |
| Plate01B09 | Idoxuridine | Antiinflammatory | Nucleic acid synthesis inhibitors |
| Plate  | Name                                      | Category          | Property/Effect                        |
|--------|-------------------------------------------|-------------------|----------------------------------------|
| 02D07  | Naltrexone hydrochloride dihydrate        | Analgesic         | Opioid antagonist                       |
| 02D02  | Naloxone hydrochloride                    | Opioate antidote  | Opioid antagonist                       |
| 02D09  | Nalbuphine hydrochloride                  | Analgesic         | Opioid ligand                          |
| 02E05  | Hesperetin                                |                   | P450 inhibitor                          |
| 01F09  | Prolidam hydrochloride                    | Local anesthetic  | P450 inhibitor (mono-oxygenases)        |
| 05G10  | Ketoneonazole                             | Antifungal        | P450 inhibitor (P450c17)                |
| 08C08  | Cilostazol                                | Antithrombotic    | Phosphodiesterase inhibitor             |
| 01D04  | Diprophyline                              | Cardiac analgetic | Phosphodiesterase inhibitor             |
| 02B02  | Khellin                                   | Phototherapeutic agent | Phototherapeutic agent                  |
| 01A03  | Allantoin                                 | Vulnerary          | Precipitate proteins                    |
| 01C05  | Norhydrodrel                              | Progestogen       | Progesterone receptor agonist           |
| 02E02  | Bromocryptine mesylate                    | Antiparkinsonian  | Progesterone receptor agonist           |
| 02G07  | Tamoxifen citrate                         | Anticancer        | Protein kinase C inhibitor              |
| 08A11  | Emetine dihydrochloride                  | Antiamebic        | Protein synthesis inhibitor             |
| 10G11  | Cycloheximide                             | Antibacterial     | Protein synthesis inhibitor             |
| 09E07  | Lycorine hydrochloride                   | Antitumoral       | Ribosomal protein synthesis inhibitor   |
| 01D02  | Chloramphenicol                           | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 01C06  | Thiamicilocal                             | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 01D07  | Troelandomycin                            | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 02F08  | Cirandamycin hydrochloride                | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 02F11  | Tetracycline hydrochloride                | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 02G06  | Chlorotetracycline hydrochloride          | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 02H02  | Erythromycin                              | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 02H03  | Cleandamycin phosphate                    | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 02H09  | Neomycin sulfate                          | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 02H10  | Dihydrostreptomycin sulfate               | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 02H11  | Gentamicine sulfate                       | Antibacterial     | Ribosomal protein synthesis inhibitor   |
| 13F10  | Tribenoside                               | Sclerosing agent  | Sclerosing agent                        |
| 12A06  | Cantharidin                               | Rubefiant          | Serine protease release                 |
| 02G11  | Dihydroergotamine tartrate                | Antimigraine      | Serotonin antagonist                    |
| 05G08  | Carbetapentane citrate                    | Antilussive       | Signal receptor ligand                  |
| 02E08  | Isocoumarol                               | Antibacterial     | Sterol 14-demethylase inhibitor         |
| 01G08  | Miconazole                                | Antifungal        | Sterol 14-demethylase inhibitor         |
| 01B03  | Benzonatate                               | Antilussive       | Stretch receptor sensitivity decrease    |
| 01A09  | Amprolum hydrochloride                    | Coccidiostatic    | Thiamine transport inhibitor            |
| 02D04  | Ciprofloxacin hydrochloride               | Anti-bacterial    | Topoisomerase and gyrase inhibitor      |
| 03D11  | Camptothecine (S+)                        | Antitumor agent   | Topoisomerase I inhibitor               |
| 03E05  | Flumequine                                | Antibacterial     | Topoisomerase II inhibitor              |
| 05G06  | Mitoxantrone dihydrochloride              | Antineoplastic    | Topoisomerase II inhibitor              |
| 02D05  | Ampicillin trihydrate                     | Antibacterial     | Transpeptidase inhibitor (bacterial)    |
| 02F10  | Cefotaxime sodium salt                    | Antibacterial     | Transpeptidase inhibitor (bacterial)    |
| 01B08  | Levodopa                                  | Antiparkinsonian  | Tyrosine aminotransferase inhibitor     |
| 02C11  | Acenocoumarol                             | Anticoagulant     | Vitamin K antagonist                    |
| 06F10  | 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      | ![Structure](image) | 324.38285        | Anti-inflammatory | 25               | -       | -        | -          | -          | -          | -           |
| Paroxetine Hydrochloride | ![Structure](image) | 365.83552        | Antidepressant    | 25               | +       |          |            |            |            |             |
| Parbendazole         | ![Structure](image) | 247.29934        | Anthelmintic      | 4                | +       | +        | +          |            | +          |             |
| Piperlongumine       | ![Structure](image) | 317.34468        | Antifungal        | 20               | +       |          |            |            | +          |             |
| Digitoxigenin        | ![Structure](image) | 374.52503        | Cardiotonic       | >125             | +       |          |            |            | +          |             |