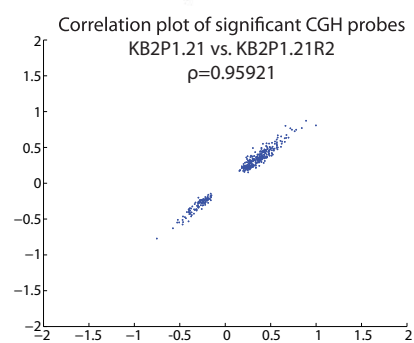
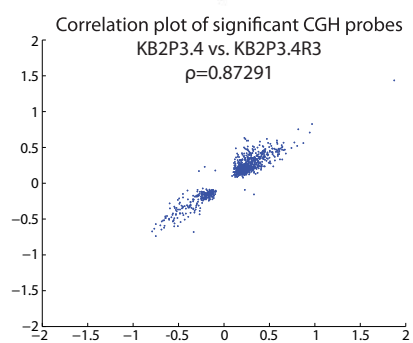
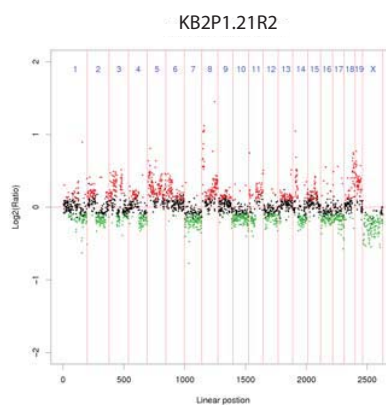
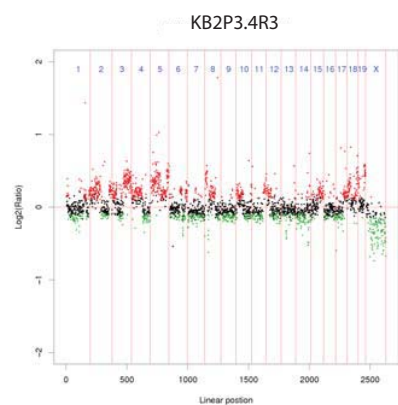
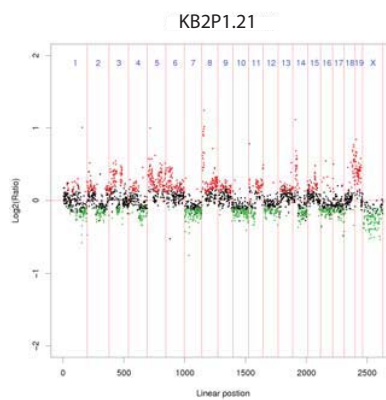
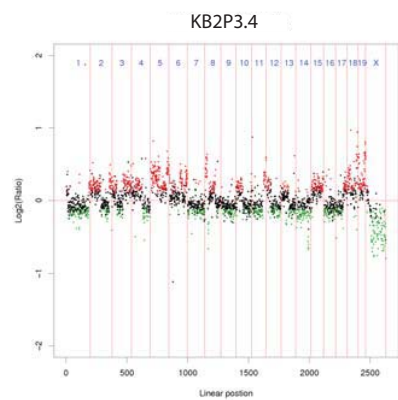




Supplementary table 1

| Drug name                                                | Description                                                                                                                                       | KB2P-3.4 IC50 | KB2P-3.4 r <sup>2</sup> | KP-3.33 IC50 | KP-3.33 r <sup>2</sup> | KB2P-3.4R3 IC50 | KB2P-3.4R3 r <sup>2</sup> | Combined Specificity Index |
|----------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|---------------|-------------------------|--------------|------------------------|-----------------|---------------------------|----------------------------|
| Chlorambucil                                             | DNA crosslinker; induces apoptosis                                                                                                                | 706           | 0.93                    | >50,000      | 1.00                   | >50,000         | 1.00                      | 3.70                       |
| Melphalan                                                | Antineoplastic; forms DNA intrastrand crosslinks by bifunctional alkylation in 5'-GGC sequences                                                   | 233           | 0.97                    | >50,000      | 1.00                   | 4,787           | 0.97                      | 3.64                       |
| Nimustine hydrochloride                                  | Antineoplastic; bifunctional nitrosourea alkylating anticancer agent                                                                              | 2,932         | 0.85                    | >50,000      | 1.00                   | >50,000         | 1.00                      | 2.46                       |
| 2-Cyclooctyl-2-hydroxyethylamine hydrochloride           | Inhibitor of phenylethanolamine N-methyltransferase (PNMT)                                                                                        | 3,480         | 0.92                    | >50,000      | 1.00                   | >50,000         | 1.00                      | 2.31                       |
| Carboplatin                                              | Antineoplastic                                                                                                                                    | 4,348         | 0.94                    | >50,000      | 1.00                   | >50,000         | 1.00                      | 2.12                       |
| SB 224289 hydrochloride                                  | Selective 5-HT1B serotonin receptor antagonist.                                                                                                   | 1,611         | 0.76                    | 3,372        | 0.71                   | >50,000         | 1.00                      | 1.81                       |
| (R)-(+)-Camptothecin                                     | DNA topoisomerase I inhibitor                                                                                                                     | 4             | 0.92                    | 10           | 0.98                   | 47              | 0.99                      | 1.49                       |
| Efliprone                                                | Cytochrome P450 (CYP1A1)and DNA topoisomerase II inhibitor                                                                                        | 63            | 0.97                    | 195          | 0.99                   | 326             | 0.98                      | 1.20                       |
| 3'-4'-Dichlorobenazamil                                  | Na <sup>+</sup> /Ca <sup>2+</sup> -exchanger inhibitor                                                                                            | 4,468         | 0.97                    | 6,433        | 0.94                   | 37,239          | 0.95                      | 1.08                       |
| 5-azacytidine                                            | DNA methyltransferase inhibitor                                                                                                                   | 1,522         | 0.79                    | 904          | 0.80                   | 26,463          | 0.80                      | 1.01                       |
| Thiothixene hydrochloride                                | Dopamine receptor antagonist; antipsychotic                                                                                                       | 2,214         | 0.75                    | 2,811        | 0.82                   | 17,796          | 0.90                      | 1.01                       |
| Methiothepin mesylate                                    | 5-HT1 Serotonin receptor antagonist; blocks serotonin autoreceptors                                                                               | 2,918         | 1.00                    | 7,580        | 1.00                   | 9,286           | 0.96                      | 0.92                       |
| 3HW 007 hydrochloride                                    | Selective antagonist of the cocaine site on the dopamine transporter.                                                                             | 3,377         | 0.97                    | 2,720        | 0.97                   | 30,767          | 0.98                      | 0.87                       |
| Taxol                                                    | Antitumor agent; promotes assembly of microtubules and inhibits tubulin disassembly process                                                       | 9             | 0.84                    | 31           | 0.94                   | 18              | 0.94                      | 0.81                       |
| Chlorprothixene hydrochloride                            | D2 dopamine receptor antagonist; blocks a subset of GABA-A receptors in rat cortex that is also blocked by clozapine                              | 14,214        | 0.99                    | 25,249       | 0.80                   | >50,000         | 1.00                      | 0.80                       |
| Bay 11-7085                                              | Inhibits cytokine induced iκB (inhibitor of NFκB) phosphorylation                                                                                 | 969           | 0.67                    | 2,029        | 0.68                   | 2,100           | 0.67                      | 0.66                       |
| Mevastatin                                               | Antibiotic; inhibits post-translational prenylation of proteins such as Ras and geranyl/geranylation of Rho                                       | 5,745         | 0.63                    | >50,000      | 1.00                   | 2,822           | 0.68                      | 0.63                       |
| Sertraline hydrochloride                                 | Selective serotonin reuptake inhibitor; antidepressant                                                                                            | 13,932        | 0.92                    | 15,374       | 0.99                   | >50,000         | 1.00                      | 0.60                       |
| beta-Lapachone                                           | Induces apoptosis in HL-60 cells; anticancer agent                                                                                                | 2,729         | 0.99                    | 3,880        | 1.00                   | 7,492           | 0.98                      | 0.59                       |
| Metergoline                                              | 5-HT1/5-HT2 Serotonin receptor antagonist; analgesic; antispasmodic                                                                               | 10,795        | 0.97                    | 9,076        | 0.98                   | >50,000         | 1.00                      | 0.59                       |
| (±)-Octoclohepin maleate                                 | D2 Dopamine receptor antagonist; serotonin receptor antagonist                                                                                    | 12,198        | 0.99                    | 11,414       | 0.91                   | >50,000         | 1.00                      | 0.58                       |
| Tamoxifen citrate                                        | Anti-estrogen; relatively selective protein kinase C inhibitor                                                                                    | 11,950        | 0.72                    | 10,869       | 0.91                   | >50,000         | 1.00                      | 0.58                       |
| Perphenazine                                             | D2 dopamine receptor antagonist; sigma receptor agonist; phenothiazine antipsychotic                                                              | 5,664         | 0.97                    | 6,262        | 0.98                   | 14,760          | 0.97                      | 0.46                       |
| NNC 55-0396                                              | Selective T-type calcium channel inhibitor.                                                                                                       | 8,075         | 0.94                    | 13,520       | 0.97                   | 12,554          | 0.93                      | 0.42                       |
| Vincristine sulfate                                      | Inhibitor of microtubule assembly                                                                                                                 | 342           | 0.95                    | 384          | 0.97                   | 759             | 0.95                      | 0.40                       |
| SJ 9516                                                  | Cyclin-dependent kinase-2 (Cdk-2) inhibitor; induces apoptosis in colon cancer cells                                                              | 4,054         | 0.61                    | 2,064        | 0.76                   | 18,806          | 0.49                      | 0.37                       |
| Caffeic acid phenethyl ester                             | NFκB inhibitor                                                                                                                                    | 1,211         | 0.57                    | 1,618        | 0.47                   | 1,995           | 0.75                      | 0.34                       |
| Prochlorperazine dimaleate                               | Antipsychotic agent; used in the treatment of spastic gastrointestinal disorders                                                                  | 4,948         | 0.75                    | 4,756        | 0.98                   | 10,825          | 0.94                      | 0.32                       |
| NSC 95397                                                | Selective, irreversible Cdc25 dual specificity phosphatase inhibitor.                                                                             | 1,503         | 0.97                    | 1,681        | 0.97                   | 2,451           | 0.99                      | 0.26                       |
| Idarubicin                                               | Antineoplastic                                                                                                                                    | 39            | 0.99                    | 35           | 0.99                   | 80              | 1.00                      | 0.25                       |
| Calcimycin                                               | Ca <sup>2+</sup> ionophore used to potentiate responses to NMDA, but not quisqualate glutamate receptors                                          | 1,121         | 0.98                    | 819          | 1.00                   | 2,708           | 0.98                      | 0.25                       |
| 2,4-Phe chloromethyl ketone                              | Bovine chymotrypsin A-gamma inhibitor                                                                                                             | 18,340        | 0.67                    | 11,668       | 0.63                   | >50,000         | 1.00                      | 0.24                       |
| Sanguinarine chloride                                    | Inhibitor of Mg <sup>2+</sup> - and Na <sup>+</sup> /K <sup>+</sup> -ATPase; isolated from the leaves and stems of Mackaya cordata and microcarpa | 2,172         | 0.90                    | 2,554        | 0.98                   | 3,180           | 0.92                      | 0.24                       |
| Mitoxantrone                                             | DNA synthesis inhibitor                                                                                                                           | 24            | 0.95                    | 28           | 0.98                   | 34              | 0.97                      | 0.22                       |
| Terfenadine                                              | Non-sedating H1 histamine receptor antagonist                                                                                                     | 2,488         | 0.86                    | 2,662        | 0.90                   | 3,853           | 0.89                      | 0.22                       |
| Cortexolone maleate                                      | D2 dopamine receptor antagonist                                                                                                                   | 15,082        | 0.97                    | 7,217        | 1.00                   | >50,000         | 1.00                      | 0.20                       |
| Sobuzoxane                                               | DNA topoisomerase II inhibitor; induces apoptosis.                                                                                                | 5,794         | 0.98                    | 1,064        | 0.91                   | >50,000         | 1.00                      | 0.20                       |
| cis-(2)-Flupenthixol dihydrochloride                     | Dopamine receptor antagonist; antipsychotic                                                                                                       | 10,561        | 0.67                    | 3,513        | 0.77                   | >50,000         | 1.00                      | 0.20                       |
| Amisacrine hydrochloride                                 | DNA topoisomerase II inhibitor                                                                                                                    | 34            | 0.97                    | 33           | 0.98                   | 54              | 0.98                      | 0.19                       |
| Vinblastine sulfate salt                                 | Inhibitor of microtubule assembly                                                                                                                 | 31            | 0.92                    | 43           | 0.94                   | 34              | 0.93                      | 0.19                       |
| 7-Chloro-4-hydroxy-2-phenyl-1,8-naphthyridine            | A1 adenosine receptor antagonist                                                                                                                  | 3,231         | 0.85                    | 3,456        | 0.93                   | 4,450           | 0.93                      | 0.17                       |
| Diphenyleneiodonium chloride                             | Endothelial nitric oxide synthase inhibitor                                                                                                       | 504           | 0.93                    | 376          | 0.95                   | 995             | 0.87                      | 0.17                       |
| Fluphenazine dihydrochloride                             | Dopamine receptor antagonist; antipsychotic                                                                                                       | 4,799         | 0.97                    | 4,102        | 0.99                   | 7,790           | 0.98                      | 0.14                       |
| GR 127935 hydrochloride                                  | Selective 5-HT1B/1D serotonin receptor antagonist.                                                                                                | 2,579         | 1.00                    | 2,485        | 0.99                   | 3,430           | 0.97                      | 0.11                       |
| Brefeldin A from Penicillium brefeldianum                | Fungal metabolite that disrupts the structure and function of the Golgi apparatus                                                                 | 398           | 0.98                    | 473          | 0.99                   | 414             | 1.00                      | 0.09                       |
| Dequalinium analog, C-14 linker                          | Protein kinase C-alpha (PKC-alpha) inhibitor                                                                                                      | 4,314         | 0.97                    | 6,276        | 0.99                   | 3,469           | 1.00                      | 0.07                       |
| Cantharidin                                              | Protein phosphatase 2A inhibitor                                                                                                                  | 22,295        | 0.66                    | 11,498       | 0.88                   | >50,000         | 1.00                      | 0.06                       |
| 4'-Chloro-3-alpha-(diphenylmethoxy)propane hydrochloride | Dopamine reuptake blocker.                                                                                                                        | 14,181        | 0.87                    | 4,300        | 0.95                   | >50,000         | 1.00                      | 0.03                       |
| Podophyllotoxin                                          | Antineoplastic glucoside; inhibitor of microtubule assembly                                                                                       | 22            | 0.92                    | 24           | 0.89                   | 21              | 0.87                      | 0.02                       |
| Cockchine                                                | Prevents tubulin polymerization                                                                                                                   | 38            | 0.94                    | 35           | 0.96                   | 43              | 0.94                      | 0.02                       |
| Etoposide                                                | Topoisomerase II inhibitor; induces apoptosis; cell cycle inhibitor                                                                               | 427           | 0.98                    | 350          | 1.00                   | 493             | 0.98                      | -0.02                      |
| 5-Fluorouracil                                           | Thymidylate synthetase inhibitor; leads to accumulation of cells in S phase                                                                       | 2,567         | 0.79                    | 2,227        | 0.93                   | 2,787           | 0.92                      | -0.03                      |
| 2-methoxyestradiol                                       | Inhibitor of angiogenesis and endothelial cell proliferation                                                                                      | 3,812         | 0.98                    | 3,406        | 1.00                   | 3,827           | 0.99                      | -0.05                      |
| Trifluoperazine dihydrochloride                          | Calmodulin antagonist; dopamine receptor antagonist; antipsychotic; sedative                                                                      | 14,357        | 0.72                    | 3,687        | 0.66                   | >50,000         | 1.00                      | -0.05                      |
| Iodoacetamide                                            | Alkylating reagent for cysteine and histidine residues in proteins; irreversible protein inhibitor                                                | 6,669         | 0.98                    | 6,291        | 0.97                   | 6,291           | 0.99                      | -0.05                      |
| Chelerythrine chloride                                   | PKC inhibitor; affects translocation of PKC from cytosol to plasma membrane                                                                       | 3,163         | 0.98                    | 2,319        | 0.99                   | 3,834           | 0.99                      | -0.05                      |
| N-Oleoyldopamine                                         | Endogenous vanilloid; weak CB1 cannabinoid receptor ligand.                                                                                       | 4,810         | 0.86                    | 4,313        | 0.92                   | 4,703           | 0.91                      | -0.06                      |
| Quinacrine dihydrochloride                               | Monoamine oxidase (MAO) inhibitor; antimalarial                                                                                                   | 3,279         | 1.00                    | 2,567        | 0.99                   | 3,593           | 1.00                      | -0.07                      |
| GGR-74514A hydrochloride                                 | Cdk1 inhibitor                                                                                                                                    | 1,085         | 0.96                    | 669          | 0.94                   | 1,443           | 0.94                      | -0.09                      |
| Dequalinium dichloride                                   | Selective blocker of apamin-sensitive K <sup>+</sup> channels                                                                                     | 16,453        | 0.99                    | 22,907       | 0.97                   | 9,658           | 0.97                      | -0.09                      |
| Pimozide                                                 | Ca <sup>2+</sup> channel antagonist; antipsychotic; D2 dopamine receptor antagonist                                                               | 28,289        | 0.96                    | 13,073       | 0.99                   | >50,000         | 1.00                      | -0.09                      |
| Methotrexate                                             | Folic acid antagonist                                                                                                                             | >50,000       | 1.00                    | 40,007       | 0.87                   | >50,000         | 1.00                      | -0.10                      |
| 2,3-Dimethoxy-1,4-naphthoquinone                         | Redox cycling agent used to study role of ROS (reactive oxygen species)                                                                           | 4,389         | 0.95                    | 2,536        | 0.99                   | 6,054           | 0.96                      | -0.10                      |
| 1,10-Phenanthroline monohydrate                          | Metalloprotease inhibitor; chelates iron, zinc and other divalent metals                                                                          | 2,731         | 0.75                    | 2,295        | 0.72                   | 2,375           | 0.85                      | -0.14                      |
| Ammonium pyrrolidinedithiocarbamate                      | Prevents induction of nitric oxide synthase (NOS) by inhibiting translation of NOS mRNA                                                           | 1,936         | 0.93                    | 1,291        | 0.97                   | 2,082           | 0.99                      | -0.14                      |
| Nicosamide                                               | Protonophoric anthelmintic; uncouples oxidative phosphorylation                                                                                   | 1,791         | 0.94                    | 718          | 1.00                   | 3,185           | 0.98                      | -0.15                      |
| Nocodazole                                               | Disrupts microtubules by binding to beta-tubulin                                                                                                  | 78            | 0.95                    | 68           | 0.98                   | 57              | 0.97                      | -0.20                      |
| Doxazosin mesylate                                       | alpha1 adrenoceptor blocker                                                                                                                       | >50,000       | 1.00                    | 29,404       | 0.93                   | >50,000         | 1.00                      | -0.23                      |
| Tetraethylthiuram disulfide                              | Alcohol dehydrogenase inhibitor                                                                                                                   | 276           | 0.74                    | 201          | 0.92                   | 221             | 0.97                      | -0.23                      |
| Emetine dihydrochloride hydrate                          | Apoptosis inducer; RNA-Protein translation inhibitor                                                                                              | 47            | 0.98                    | 31           | 0.99                   | 36              | 0.99                      | -0.31                      |
| Ancitabine hydrochloride                                 | Antineoplastic                                                                                                                                    | 869           | 0.97                    | 311          | 0.98                   | 1,179           | 0.99                      | -0.31                      |
| Rotenone                                                 | Inhibitor of mitochondrial electron transport                                                                                                     | 509           | 0.86                    | 225          | 0.96                   | 488             | 0.96                      | -0.37                      |
| Thapsigargin                                             | Potent, cell-permeable, IP3-independent intracellular calcium releaser                                                                            | 160           | 0.98                    | 163          | 0.97                   | 58              | 0.99                      | -0.43                      |
| SKF 96365                                                | Selective inhibitor of receptor-mediated and voltage-gated Ca <sup>2+</sup> entry                                                                 | 6,150         | 0.76                    | 4,119        | 0.74                   | 3,392           | 0.88                      | -0.43                      |
| L-Buthionine-sulfoximine                                 | Glutathione synthesis inhibitor                                                                                                                   | 33,996        | 0.72                    | >50,000      | 1.00                   | 7,848           | 0.98                      | -0.47                      |
| Chlorpromazine hydrochloride                             | Dopamine receptor antagonist; anti-emetic; antipsychotic                                                                                          | >50,000       | 1.00                    | 16,811       | 0.83                   | >50,000         | 1.00                      | -0.47                      |
| Cantharidin Acid                                         | Protein phosphatase 1 (PP1) and 2A (PP2A) inhibitor                                                                                               | >50,000       | 1.00                    | 16,295       | 0.78                   | >50,000         | 1.00                      | -0.49                      |
| Tyrphostin A9                                            | Selective PDGF tyrosine kinase receptor inhibitor                                                                                                 | 5,304         | 0.69                    | 2,604        | 0.77                   | 3,276           | 0.74                      | -0.52                      |
| Nifedipine                                               | L-type Ca <sup>2+</sup> channel blocker; vasodilator                                                                                              | >50,000       | 1.00                    | >50,000      | 1.00                   | 14,415          | 0.97                      | -0.54                      |
| Cytosine-1-beta-D-arabinofuranoside hydrochloride        | Selective inhibitor of DNA synthesis                                                                                                              | 398           | 0.97                    | 77           | 0.99                   | 564             | 0.98                      | -0.56                      |
| Cyclosporin A                                            | Calcineurin phosphatase inhibitor; immunosuppressant                                                                                              | >50,000       | 1.00                    | 9,940        | 0.96                   | >50,000         | 1.00                      | -0.70                      |
| SJ 6655                                                  | Selective Src family kinase inhibitor.                                                                                                            | >50,000       | 1.00                    | 7,921        | 0.90                   | >50,000         | 1.00                      | -0.80                      |
| Olanastine fumarate                                      | H1 Histamine receptor antagonist                                                                                                                  | >50,000       | 1.00                    | 7,912        | 0.82                   | >50,000         | 1.00                      | -0.80                      |
| Spermidine trihydrochloride                              | Binds to the polyamine modulatory site of the NMDA glutamate receptor                                                                             | >50,000       | 1.00                    | 7,323        | 0.99                   | >50,000         | 1.00                      | -0.83                      |
| L1'-294,002 hydrochloride                                | Specific phosphatidylinositol 3-kinase (PI3K) inhibitor.                                                                                          | >50,000       | 1.00                    | >50,000      | 1.00                   | 6,100           | 0.95                      | -0.91                      |
| Leflunomide                                              | Immunosuppressive; its metabolite inhibits dihydroorotate dehydrogenase and several protein tyrosine kinases                                      | >50,000       | 1.00                    | 5,981        | 0.97                   | >50,000         | 1.00                      | -0.92                      |
| Tyrphostin AG 1478                                       | Selective inhibitor of epidermal growth factor receptor (EGFR) protein                                                                            | >50,000       | 1.00                    | 4,934        | 0.91                   | >50,000         | 1.00                      | -1.01                      |
| Loratadine                                               | H1 Histamine receptor antagonist                                                                                                                  | >50,000       | 1.00                    | 4,323        | 0.94                   | >50,000         | 1.00                      | -1.06                      |
| GW2974                                                   | Dual EGFR and ErbB-2 receptor tyrosine kinase inhibitor                                                                                           | >50,000       | 1.00                    | 3,220        | 0.98                   | >50,000         | 1.00                      | -1.19                      |
| Prazosin hydrochloride                                   | Peripheral alpha1 adrenoceptor antagonist                                                                                                         | >50,000       | 1.00                    | 3,085        | 0.74                   | >50,000         | 1.00                      | -1.21                      |
| Parthenolide                                             | Inhibits serotonin release from platelets; inhibits production of leukotriene B4 and thromboxane B2                                               | >50,000       | 1.00                    | 10,436       | 0.99                   | 13,180          | 0.96                      | -1.26                      |
| Mibefradil dihydrochloride                               | T-type Ca <sup>2+</sup> channel blocker                                                                                                           | 16,858        | 0.53                    | 3,099        | 0.84                   | 3,281           | 0.78                      | -1.45                      |
| 4-Phenyl-3-furoxancarboxilic                             | Nitric oxide donor; activator of rat lung soluble guanylyl cyclase                                                                                | >50,000       | 1.00                    | 4,727        | 0.44                   | 4,199           | 0.67                      | -2.10                      |
| BIO                                                      | Potent, selective, reversible, and ATP-competitive glycogen synthase kinase 3alpha/beta (GSK-3alpha/beta) inhibitor.                              | >50,000       | 1.00                    | 3,888        | 0.78                   | 4,550           | 0.52                      | -2.15                      |
| 3-Phenylpropargylamine hydrochloride                     | Potent, time-dependent inhibitor of dopamine beta-hydroxylase (DBH)                                                                               | >50,000       | 1.00                    | 2,175        | 0.64                   | 7,692           | 0.70                      | -2.17                      |
| SB 228357                                                | Selective 5-HT2B/2C serotonin receptor antagonist                                                                                                 | >50,000       | 1.00                    | 2,931        | 0.97                   | 4,539           | 0.97                      | -2.27                      |
| IC 261                                                   | Casein kinase-1 (CK-1delta/epsilon) inhibitor.                                                                                                    | >50,000       | 1.00                    | 1,874        | 0.71                   | 2,815           | 0.86                      | -2.68                      |