**Table S7:** Compounds that were both active and annotated.

| Compound name | Concentration [µM] | Source | Broad ID | Structure |
| --- | --- | --- | --- | --- |
| (D,L)-TETRAHYDROBERBERINE | 2.95 | Prestwick Chemical Inc. | BRD-A69950438 | BRD-A69950438-001-04-5 |
| 2,5-DITERTBUTYLHYDROQUINONE | 11.24 | Biomol International Inc. | BRD-K95603879 | BRD-K95603879-001-03-4 |
| AG-879 | 7.90 | Biomol International Inc. | BRD-K59469039 | BRD-K59469039-001-04-9 |
| ANISOMYCIN | 9.42 | Biomol International Inc. | BRD-K91370081 | BRD-K91370081-001-04-6 |
| BAY 11-7082 | 12.06 | Biomol International Inc. | BRD-K15025317 | BRD-K15025317-001-04-5 |
| BW-B 70C | 7.90 | Biomol International Inc. | BRD-A55946879 | BRD-A55946879-001-02-9 |
| CA-074-ME | 6.29 | Biomol International Inc. | BRD-A56020723 | BRD-A56020723-001-02-0 |
| CELECOXIB | 5.00 | MicroSource Discovery Systems Inc. | BRD-K02637541 | BRD-K02637541-001-02-4 |
| CERULENIN | 11.20 | Biomol International Inc. | BRD-K52075040 | BRD-K52075040-001-02-2 |
| COLCHICINE | 2.50 | Prestwick Chemical Inc. | BRD-K00259736 | BRD-K00259736-001-06-5 |
| CYCLIZINE | 5.00 | MicroSource Discovery Systems Inc. | BRD-K79501723 | BRD-K79501723-001-02-0 |
| CYCLIZINE HYDROCHLORIDE | 3.30 | Prestwick Chemical Inc. | BRD-K79501723 | BRD-K79501723-003-03-4 |
| DAUNORUBICIN HYDROCHLORIDE | 1.77 | Prestwick Chemical Inc. | BRD-K43389675 | BRD-K43389675-003-02-7 |
| DIGITOXIN | 5.00 | MicroSource Discovery Systems Inc. | BRD-A93236127 | BRD-A93236127-001-02-9 |
| DIGOXIN | 5.00 | MicroSource Discovery Systems Inc. | BRD-A94756469 | BRD-A94756469-001-02-1 |
| DISULFIRAM | 3.37 | Prestwick Chemical Inc. | BRD-K32744045 | BRD-K32744045-001-05-6 |
| ELLIPTICINE | 4.06 | Prestwick Chemical Inc. | BRD-K85985071 | BRD-K85985071-001-03-3 |
| ESTRADIOL | 9.18 | Biomol International Inc. | BRD-K18910433 | BRD-K18910433-001-04-4 |
| ETHINYL ESTRADIOL | 5.00 | MicroSource Discovery Systems Inc. | BRD-A02367930 | BRD-A02367930-001-02-9 |
| ETOPOSIDE | 1.70 | Prestwick Chemical Inc. | BRD-K37798499 | BRD-K37798499-001-02-5 |
| FCCP | 9.84 | Biomol International Inc. | BRD-K14821540 | BRD-K14821540-001-02-1 |
| FENBENDAZOLE | 3.34 | Prestwick Chemical Inc. | BRD-K51318897 | BRD-K51318897-001-04-7 |
| FENDILINE HYDROCHLORIDE | 2.84 | Prestwick Chemical Inc. | BRD-A71033472 | BRD-A71033472-003-05-6 |
| FLUPHENAZINE | 5.00 | Biomol International Inc. | BRD-K55127134 | BRD-K55127134-001-01-7 |
| FLUPHENAZINE DIHYDROCHLORIDE | 1.96 | Prestwick Chemical Inc. | BRD-K55127134 | BRD-K55127134-300-05-4 |
| GBR 12935 | 5.00 | Biomol International Inc. | BRD-K50135270 | BRD-K50135270-001-01-9 |
| GENTIAN VIOLET | 5.00 | MicroSource Discovery Systems Inc. | BRD-K60025295 | BRD-K60025295-003-02-5 |
| GF-109203X | 6.06 | Biomol International Inc. | BRD-K31342827 | BRD-K31342827-001-05-4 |
| GO6976 | 6.61 | Biomol International Inc. | BRD-K59304176 | BRD-K59304176-001-02-5 |
| HYCANTHONE | 2.81 | Prestwick Chemical Inc. | BRD-K50406511 | BRD-K50406511-001-06-2 |
| HYDROCHLOROTHIAZIDE | 3.36 | Prestwick Chemical Inc. | BRD-K13078532 | BRD-K13078532-001-05-2 |
| KINETIN RIBOSIDE | 5.00 | MicroSource Discovery Systems Inc. | BRD-K94325918 | BRD-K94325918-001-02-0 |
| LANATOSIDE C | 5.00 | MicroSource Discovery Systems Inc. | BRD-A64242993 | BRD-A64242993-001-02-3 |
| LAPACHOL | 5.00 | MicroSource Discovery Systems Inc. | BRD-A06912736 | BRD-A06912736-001-02-4 |
| LEVAMISOLE HYDROCHLORIDE | 5.00 | MicroSource Discovery Systems Inc. | BRD-K73107279 | BRD-K73107279-003-03-4 |
| LY-294002 | 8.13 | Biomol International Inc. | BRD-K27305650 | BRD-K27305650-001-05-9 |
| LY-83583 | 9.99 | Biomol International Inc. | BRD-K62792802 | BRD-K62792802-001-02-8 |
| LYCORINE | 5.00 | MicroSource Discovery Systems Inc. | BRD-A10335634 | BRD-A10335634-001-02-5 |
| MCI-186 | 14.35 | Biomol International Inc. | BRD-K35458079 | BRD-K35458079-001-04-2 |
| MELPHALAN | 5.00 | MicroSource Discovery Systems Inc. | BRD-K87827419 | BRD-K87827419-001-02-8 |
| METOCLOPRAMIDE | 5.00 | Biomol International Inc. | BRD-K75641298 | BRD-K75641298-001-01-5 |
| METOCLOPRAMIDE MONOHYDROCHLORIDE | 2.97 | Prestwick Chemical Inc. | BRD-K75641298 | BRD-K75641298-003-05-2 |
| MITOXANTRONE DIHYDROCHLORIDE | 1.93 | Prestwick Chemical Inc. | BRD-K21680192 | BRD-K21680192-300-05-2 |
| NERIIFOLIN | 5.00 | MicroSource Discovery Systems Inc. | BRD-A31385885 | BRD-A31385885-001-02-1 |
| NIFLUMIC ACID | 8.86 | Biomol International Inc. | BRD-K98763141 | BRD-K98763141-001-06-8 |
| NITRENDIPINE | 6.94 | Biomol International Inc. | BRD-A02006392 | BRD-A02006392-001-06-5 |
| NOVOBIOCIN SODIUM | 5.00 | MicroSource Discovery Systems Inc. | BRD-K85307935 | BRD-K85307935-236-02-0 |
| NSC-95397 | 8.05 | Biomol International Inc. | BRD-K68143200 | BRD-K68143200-001-02-6 |
| OXIBENDAZOLE | 5.00 | MicroSource Discovery Systems Inc. | BRD-K52075715 | BRD-K52075715-001-02-6 |
| OXYPHENBUTAZONE | 3.08 | Prestwick Chemical Inc. | BRD-A33749298 | BRD-A33749298-001-05-0 |
| OXYQUINOLINE HEMISULFATE | 5.00 | MicroSource Discovery Systems Inc. | BRD-K66808046 | BRD-K66808046-065-01-1 |
| PACLITAXEL | 1.17 | Prestwick Chemical Inc. | BRD-K62008436 | BRD-K62008436-001-03-1 |
| PCA 4248 | 6.92 | Biomol International Inc. | BRD-A29289453 | BRD-A29289453-001-02-1 |
| PENICILLIN V POTASSIUM | 5.00 | MicroSource Discovery Systems Inc. | BRD-K43966364 | BRD-K43966364-237-02-2 |
| PENITREM A | 3.94 | Biomol International Inc. | BRD-K03842655 | BRD-K03842655-001-02-1 |
| PERUVOSIDE | 5.00 | MicroSource Discovery Systems Inc. | BRD-A57089740 | BRD-A57089740-001-02-3 |
| PHENACEMIDE | 5.00 | MicroSource Discovery Systems Inc. | BRD-K40905133 | BRD-K40905133-001-02-3 |
| PIPERLONGUMINE | 3.15 | Prestwick Chemical Inc. | BRD-K24132293 | BRD-K24132293-001-05-3 |
| PROCAINE HYDROCHLORIDE | 3.67 | Prestwick Chemical Inc. | BRD-K24616672 | BRD-K24616672-003-05-2 |
| PROPAFENONE | 7.32 | Biomol International Inc. | BRD-A26334849 | BRD-A26334849-001-02-1 |
| PROPAFENONE HYDROCHLORIDE | 2.65 | Prestwick Chemical Inc. | BRD-A26334849 | BRD-A26334849-003-05-0 |
| PROPIOMAZINE MALEATE | 5.00 | MicroSource Discovery Systems Inc. | BRD-A10471441 | BRD-A10471441-050-02-8 |
| QUINACRINE DIHYDROCHLORIDE DIHYDRATE | 1.96 | Prestwick Chemical Inc. | BRD-A45889380 | BRD-A45889380-336-03-4 |
| R(-)-APOMORPHINE | 5.00 | Biomol International Inc. | BRD-K76022557 | BRD-K76022557-001-01-3 |
| RESVERATROL | 10.95 | Biomol International Inc. | BRD-K80738081 | BRD-K80738081-001-06-2 |
| RO 31-8220 | 5.46 | Biomol International Inc. | BRD-K06543683 | BRD-K06543683-001-04-4 |
| SDZ-201106 | 5.36 | Biomol International Inc. | BRD-A64553394 | BRD-A64553394-001-02-8 |
| SKF-96365 | 6.82 | Biomol International Inc. | BRD-A72703248 | BRD-A72703248-001-02-7 |
| STAUROSPORINE | 5.36 | Biomol International Inc. | BRD-K17953061 | BRD-K17953061-001-02-8 |
| TACRINE HYDROCHLORIDE HYDRATE | 4.26 | Prestwick Chemical Inc. | BRD-K81473089 | BRD-K81473089-003-04-8 |
| TENIPOSIDE | 5.00 | MicroSource Discovery Systems Inc. | BRD-A35588707 | BRD-A35588707-001-02-2 |
| TERFENADINE | 2.12 | Prestwick Chemical Inc. | BRD-A06352418 | BRD-A06352418-001-03-6 |
| TETRAHYDROPALMATINE | 5.00 | MicroSource Discovery Systems Inc. | BRD-A43940795 | BRD-A43940795-001-03-6 |
| TETRANDRINE | 4.01 | Biomol International Inc. | BRD-K08078237 | BRD-K08078237-001-07-3 |
| THIMEROSAL | 5.00 | MicroSource Discovery Systems Inc. | BRD-K61443650 | BRD-K61443650-236-02-4 |
| TICLOPIDINE HYDROCHLORIDE | 3.33 | Prestwick Chemical Inc. | BRD-K00603606 | BRD-K00603606-003-03-4 |
| TRIFLUOPERAZINE | 5.00 | Biomol International Inc. | BRD-K89732114 | BRD-K89732114-001-03-4 |
| TRIFLUOPERAZINE DIHYDROCHLORIDE | 2.08 | Prestwick Chemical Inc. | BRD-K89732114 | BRD-K89732114-300-05-5 |
| TRIPTOLIDE | 6.94 | Biomol International Inc. | BRD-K39484304 | BRD-K39484304-001-02-5 |
| U-0126 | 5.00 | Biomol International Inc. | BRD-K18787491 | BRD-K18787491-001-04-5 |