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| Table S10. Prediction of drugs. | | |  |  |  |
| Rank | Score | Type | ID | Name | Description |
| 59 | 99.54 | cp | BRD-A17535965 | gelsemine | Acetylcholine receptor antagonist |
| 78 | 99.33 | cp | BRD-A24191444 | ifenprodil | Adrenergic receptor antagonist |
| 87 | 99.22 | cp | BRD-K21283037 | riluzole | Glutamate inhibitor |
| 90 | 99.19 | cp | BRD-A99411506 | esculin | Antioxidant |
| 92 | 99.19 | cp | BRD-K65417056 | meprylcaine | Local anesthetic |
| 97 | 99.15 | cp | BRD-K43736954 | cortisone | Glucocorticoid receptor agonist |
| 100 | 99.13 | cp | BRD-A44008656 | doxylamine | Histamine receptor antagonist |
| 110 | 99.04 | cp | BRD-A25569250 | KI-16425 | Lysophosphatidic acid receptor antagonist |
| 111 | 99.03 | cp | BRD-K45330754 | diethylstilbestrol | Estrogen receptor agonist |
| 116 | 99.02 | cp | BRD-A84327315 | calcitriol | Vitamin D receptor agonist |
| 8419 | -99.05 | cp | BRD-K37516142 | idebenone | Calcium channel modulator |
| 8422 | -99.08 | cp | BRD-K83636919 | entacapone | Catechol O methyltransferase inhibitor |
| 8423 | -99.08 | cp | BRD-K80527266 | triacsin-c | Adrenergic receptor antagonist |
| 8424 | -99.09 | cp | BRD-K59633790 | VU-0420363-1 | SARS coronavirus 3C-like protease inhibitor |
| 8435 | -99.15 | cp | BRD-A31800922 | procyclidine | Acetylcholine receptor antagonist |
| 8440 | -99.19 | cp | BRD-A50157456 | terbutaline | Adrenergic receptor agonist |
| 8442 | -99.21 | cp | BRD-K33483813 | actarit | Interleukin receptor agonist |
| 8445 | -99.22 | cp | BRD-K44084986 | Y-27632 | Rho associated kinase inhibitor |
| 8447 | -99.26 | cp | BRD-K06878038 | deferiprone | Chelating agent |
| 8453 | -99.3 | cp | BRD-K27351809 | nomegestrol | Progesterone receptor agonist |
| 8454 | -99.31 | cp | BRD-A22769835 | homochlorcyclizine | Antihistamine |
| 8460 | -99.33 | cp | BRD-K39569857 | avrainvillamide-analog-3 | nucleophosmin inhibitor |
| 8465 | -99.37 | cp | BRD-A36267905 | buphenine | Adrenergic receptor agonist |
| 8475 | -99.44 | cp | BRD-K22009844 | phenprobamate | Muscle relaxant |
| 8478 | -99.47 | cp | BRD-K63630713 | etacrynic-acid | Sodium/potassium/chloride transporter inhibitor |
| 8485 | -99.52 | cp | BRD-K85133207 | HDAC1-selective | HDAC inhibitor |
| 8486 | -99.54 | cp | BRD-K71103788 | duloxetine | Serotonin reuptake inhibitor |
| 8490 | -99.58 | cp | BRD-A37052580 | physostigmine | Acetylcholinesterase inhibitor |
| 8491 | -99.58 | cp | BRD-K40782193 | QX-222 | Sodium channel blocker |
| 8501 | -99.65 | cp | BRD-K73824630 | skatole | Thrombin inhibitor |
| 8503 | -99.66 | cp | BRD-K20313525 | rosmarinic-acid | GABA transaminase inhibitor |
| 8508 | -99.68 | cp | BRD-K37130656 | rivaroxaban | Coagulation inhibitor |
| 8512 | -99.72 | cp | BRD-K77998258 | ganglioside | SRC activator |
| 8514 | -99.72 | cp | BRD-K93176058 | AC-55649 | Retinoid receptor agonist |
| 8515 | -99.75 | cp | BRD-K65786282 | CGP-7930 | GABA receptor modulator |
| 8519 | -99.79 | cp | BRD-K17823458 | danoprevir | HCV inhibitor |
| 8521 | -99.82 | cp | BRD-K93258693 | GW-9662 | PPAR receptor antagonist |
| 8532 | -99.86 | cp | BRD-A01787639 | naftopidil | Adrenergic receptor antagonist |
| 8533 | -99.86 | cp | BRD-K14550461 | doxercalciferol | Vitamin D receptor agonist |
| 8534 | -99.86 | cp | BRD-A71009679 | KUC103420N | -666 |
| 8535 | -99.86 | cp | BRD-K32107296 | temozolomide | DNA alkylating agent |
| 8539 | -99.89 | cp | BRD-K68332390 | ponalrestat | Aldose reductase inhibitor |
| 8540 | -99.89 | cp | BRD-K64514229 | toltrazuril | Antiprotozoal |
| 8554 | -99.93 | cp | BRD-K81783531 | VX-222 | HCV inhibitor |
| 8555 | -99.93 | cp | BRD-K84639753 | safinamide | Dopamine uptake inhibitor |
| 8556 | -99.93 | cp | BRD-A07395371 | esmolol | Adrenergic receptor antagonist |