Table S1. FDA approved 127 drugs

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **NSC** | **CAS** | **DRUG NAME (USAN)** | **MW** |
| 1 | 749226 |  154229-19-3 | Abiraterone | 349.51 |
| 2 | 750691 |  439081-18-2 | Afatinib | 485.94 |
| 3 | 764040 | 1256580-46-7 | Alectinib | 482.62 |
| 4 | 1390 |  315-30-0 | Allopurinol | 136.11 |
| 5 | 13875 |  645-05-6 | Altretamine | 210.28 |
| 6 | 296961 |  20537-88-6 | Amifostine | 214.22 |
| 7 | 18509 |  5451-09-2 | Aminolevulinic acid hydrochloride | 167.59 |
| 8 | 719344 |  120511-73-1 | Anastrozole  | 293.37 |
| 9 | 92859 |  1327-53-3 | Arsenic trioxide | 197.84 |
| 10 | 757441 |  319460-85-0 | Axitinib | 386.47 |
| 11 | 102816 |  320-67-2 | Azacitidine  | 244.21 |
| 12 | 758774 |  414864-00-9 | Belinostat | 318.35 |
| 13 | 138783 |  3543-75-7 | Bendamustine hydrochloride | 394.73 |
| 14 | 125066 |  9041-93-4 | Bleomycin sulfate | 1512.61 |
| 15 | 756655 |  179324-69-7 | Bortezomib | 384.24 |
| 16 | 765694 |  380843-75-4 | Bosutinib  | 530.45 |
| 17 | 750 |  55-98-1 | Busulfan | 246.30 |
| 18 | 761432 |  183133-96-2 | Cabazitaxel  | 835.94 |
| 19 | 761068 |  849217-68-1 | Cabozantinib  | 501.51 |
| 20 | 712807 |  154361-50-9 | Capecitabine  | 359.35 |
| 21 | 241240 |  41575-94-4 | Carboplatin  | 371.25 |
| 22 | 758252 |  868540-17-4 | Carfilzomib  | 719.92 |
| 23 | 409962 |  154-93-8 | Carmustine  | 214.05 |
| 24 | 719627 |  169590-42-5 | Celecoxib | 381.37 |
| 25 | 776422 | 1032900-25-6 | Ceritinib | 558.14 |
| 26 | 3088 |  305-03-3 | Chlorambucil  | 304.22 |
| 27 | 119875 |  15663-27-1 | Cisplatin | 300.06 |
| 28 | 105014 |  4291-63-8 | Cladribine | 285.69 |
| 29 | 606869 |  123318-82-1 | Clofarabine  | 303.68 |
| 30 | 768068 |  934660-93-2 | Cobimetinib | 531.32 |
| 31 | 756645 |  877399-52-5 | Crizotinib  | 450.34 |
| 32 | 26271 |  6055-19-2 | Cyclophosphamide  | 261.09 |
| 33 | 63878 |  69-74-9 | Cytarabine hydrochloride | 279.70 |
| 34 | 764134 | 1195768-06-9 | Dabrafenib mesylate | 615.65 |
| 35 | 45388 |  4342-03-4 | Dacarbazine  | 182.18 |
| 36 | 3053 |  50-76-0 | Dactinomycin | 1255.43 |
| 37 | 732517 |  863127-77-9 | Dasatinib  | 488.01 |
| 38 | 82151 |  23541-50-6 | Daunorubicin hydrochloride | 563.98 |
| 39 | 127716 |  2353-33-5 | Decitabine  | 228.21 |
| 40 | 169780 |  24584-09-6 | Dexrazoxane | 268.27 |
| 41 | 628503 |  114977-28-5 | Docetaxel  | 807.89 |
| 42 | 123127 |  25316-40-9 | Doxorubicin hydrochloride | 579.99 |
| 43 | 755605 |  915087-33-1 | Enzalutamide  | 464.42 |
| 44 | 256942 |  56390-09-1 | Epirubicin hydrochloride | 579.99 |
| 45 | 761385 |  956697-53-3 | Erismodegib | 485.49 |
| 46 | 718781 |  183319-69-9 | Erlotinib hydrochloride | 429.90 |
| 47 | 702294 |  52205-73-9 | Estramustine phosphate sodium | 564.35 |
| 48 | 141540 |  33419-42-0 | Etoposide  | 588.56 |
| 49 | 733504 |  159351-69-6 | Everolimus  | 958.24 |
| 50 | 713563 |  107868-30-4 | Exemestane  | 296.40 |
| 51 | 27640 |  50-91-9 | Floxuridine | 246.19 |
| 52 | 312887 |  75607-67-9 | Fludarabine phosphate  | 365.21 |
| 53 | 19893 |  51-21-8 | Fluorouracil | 130.08 |
| 54 | 719276 |  129453-61-8 | Fulvestrant | 606.75 |
| 55 | 715055 |  184475-35-2 | Gefitinib  | 446.90 |
| 56 | 613327 |  122111-03-9 | Gemcitabine hydrochloride | 299.65 |
| 57 | 32065 |  127-07-1 | Hydroxyurea | 76.05 |
| 58 | 761910 |  936563-96-1 | Ibrutinib | 440.50 |
| 59 | 256439 |  57852-57-0 | Idarubicin hydrochloride | 533.96 |
| 60 | 759224 |  870281-82-6 | Idelalisib | 415.42 |
| 61 | 109724 |  3778-73-2 | Ifosfamide  | 261.09 |
| 62 | 743414 |  152459-95-5 | Imatinib | 493.61 |
| 63 | 369100 |  99011-02-6 | Imiquimod  | 240.31 |
| 64 | 616348 |  100286-90-6 | Irinotecan hydrochloride | 623.15 |
| 65 | 747973 |  219989-84-1 | Ixabepilone  | 506.70 |
| 66 | 758254 | 1201902-80-8 | Ixazomib citrate | 517.13 |
| 67 | 745750 |  231277-92-2 | Lapatinib  | 581.06 |
| 68 | 747972 |  191732-72-6 | Lenalidomide  | 259.26 |
| 69 | 719345 |  112809-51-5 | Letrozole  | 285.30 |
| 70 | 79037 |  13010-47-4 | Lomustine | 233.70 |
| 71 | 762 |  55-86-7 | Mechlorethamine hydrochloride | 192.52 |
| 72 | 71423 |  595-33-5 | Megestrol acetate | 384.51 |
| 73 | 8806 |  3223-07-2 | Melphalan hydrochloride | 341.66 |
| 74 | 755 |  50-44-2 | Mercaptopurine | 152.18 |
| 75 | 740 |  59-05-2 | Methotrexate  | 454.44 |
| 76 | 45923 |  298-81-7 | Methoxsalen | 216.19 |
| 77 | 26980 |  50-07-7 | Mitomycin  | 334.33 |
| 78 | 38721 |  53-19-0 | Mitotane | 320.04 |
| 79 | 279836 |  65271-80-9 | Mitoxantrone | 444.49 |
| 80 | 755985 |  121032-29-9 | Nelarabine | 297.27 |
| 81 | 747599 |  641571-10-0 | Nilotinib  | 529.51 |
| 82 | 753686 |  763113-22-0 | Olaparib | 434.46 |
| 83 | 758253 |  26833-87-4 | Omacetaxine mepesuccinate | 545.63 |
| 84 | 779217 | 1421373-65-0 | Osimertinib | 499.61 |
| 85 | 266046 |  61825-94-3 | Oxaliplatin  | 397.29 |
| 86 | 125973 |  33069-62-4 | Paclitaxel  | 853.92 |
| 87 | 758247 |  571190-30-2 | Palbociclib | 447.54 |
| 88 | 761190 |  404950-80-7 | Panobinostat | 349.43 |
| 89 | 737754 |  635702-64-6 | Pazopanib hydrochloride | 473.98 |
| 90 | 755384 |  357166-30-4 | Pemetrexed, Disodium salt, Heptahydrate | 471.38 |
| 91 | 218321 |  53910-25-1 | Pentostatin | 268.27 |
| 92 | 25154 |  54-91-1 | Pipobroman | 356.06 |
| 93 | 761388 |  110078-46-1 | Plerixafor  | 502.79 |
| 94 | 24559 |  18378-89-7 | Plicamycin | 1085.16 |
| 95 | 775351 |  19171-19-8 | Pomalidomide | 273.25 |
| 96 | 758487 |  943319-70-8 | Ponatinib  | 532.55 |
| 97 | 754230 |  146464-95-1 | Pralatrexate  | 477.48 |
| 98 | 77213 |  366-70-1 | Procarbazine hydrochloride | 257.76 |
| 99 | 747974 |  84449-90-1 | Raloxifene | 473.59 |
| 100 | 763932 |  755037-03-7 | Regorafenib  | 482.80 |
| 101 | 754143 |  128517-07-7 | Romidepsin  | 540.69 |
| 102 | 226080 |  53123-88-9 | Sirolimus | 914.18 |
| 103 | 747971 |  284461-73-0 | Sorafenib | 464.82 |
| 104 | 85998 |  18883-66-4 | Streptozocin | 265.22 |
| 105 | 750690 |  557795-19-4 | Sunitinib  | 398.47 |
| 106 | 180973 |  54965-24-1 | Tamoxifen citrate | 563.65 |
| 107 | 362856 |  85622-93-1 | Temozolomide  | 194.15 |
| 108 | 683864 |  162635-04-3 | Temsirolimus  | 1030.29 |
| 109 | 122819 |  29767-20-2 | Teniposide | 656.66 |
| 110 | 66847 |  50-35-1 | Thalidomide  | 258.23 |
| 111 | 752 |  154-42-7 | Thioguanine | 167.19 |
| 112 | 6396 |  52-24-4 | Thiotepa | 189.22 |
| 113 | 609699 |  119413-54-6 | Topotecan hydrochloride | 457.91 |
| 114 | 758246 |  871700-17-3 | Trametinib  | 615.40 |
| 115 | 122758 |  302-79-4 | Tretinoin | 300.44 |
| 116 | 9706 |  51-18-3 | Triethylenemelamine | 204.23 |
| 117 | 75520 |  70-00-8 | Trifluridine | 296.20 |
| 118 | 34462 |  66-75-1 | Uracil mustard | 252.10 |
| 119 | 246131 |  56124-62-0 | Valrubicin | 723.64 |
| 120 | 760766 |  443913-73-3 | Vandetanib | 475.36 |
| 121 | 761431 | 1029872-54-5 | Vemurafenib  | 489.91 |
| 122 | 49842 |  143-67-9 | Vinblastine sulfate  | 909.06 |
| 123 | 67574 |  2068-78-2 | Vincristine sulfate  | 923.04 |
| 124 | 608210 |  125317-39-7 | Vinorelbine tartrate | 1079.00 |
| 125 | 755986 |  879085-55-9 | Vismodegib | 421.30 |
| 126 | 701852 |  149647-78-9 | Vorinostat  | 264.32 |
| 127 | 721517 |  118072-93-8 | Zoledronic acid | 272.09 |