Table S1. FDA approved 127 drugs

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| **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 |