Supplementary Table: Structure, Name, CAS and NSC number of the complete dataset

|  |  |  |  |
| --- | --- | --- | --- |
| STRUCTURE | NAME | CAS | NSC number |
|  |  |  |  |
|  | ASALEY | 42228-92-2 | 167780 |
|  | AZQ |  | 182986 |
|  | BCNU |  | 409962 |
|  | BUSULFEX (BUSULFAN) | 55-98-1 | 750 |
|  | CCNU | 13010-47-4 | 79037 |
|  | CHLORAMBUCIL | 305-03-3 | 3088 |
|  | CHLOROZOTOCIN | 54749-90-5 | 178248 |
|  | CLOMESONE | 88343-72-0 | 338947 |
|  | CYCLODISONE | 99591-73-8 | 348948 |
|  | DIANHYDROGALACTI-TOL | 23261-20-3 | 132313 |
|  | FLUORODOPAN | 834-91-3 | 73754 |
|  | HEPSULFAM | 96892-57-8 | 329680 |
|  | MELPHALAN | 3223-07-2 | 8806 |
|  | METHYL CCNU | 13909-09-6 | 95441 |
|  | MITOMYCIN C | 50-07-7 | 26980 |
|  | MITOZOLOMIDE | 85622-95-3 | 353451 |
|  | CARYOLYSINE (NITROGEN MUSTARD) | 55-86-7 | 762 |
|  | PCNU | 13909-02-9 | 349174 |
|  | PIPERAZINEDIONE | 41109-80-2 | 135758 |
|  | PIPOBROMAN | 54-91-1 | 25154 |
|  | PORFIROMYCIN | 801-52-5 | 56410 |
|  | TEROXIRONE | 2451-62-9 | 296934 |
|  | THIOTEPA | 52-24-4 | 6396 |
|  | TRIETHYLENEMELAMINE | 51-18-3 | 9706 |
|  | URACIL NITROGEN MUSTARD | 66-75-1 | 34462 |
|  | YOSHI 864 | 3458-22-8 | 102627 |
|  | AMONAFIDE | 69408-81-7 | 308847 |
|  | ANTHRAPYRAZOLE | 91440-30-1 | 355644 |
|  | BISANTRENE HYDROCHLORIDE | 71439684 | 337766 |
|  | DAUNORUBICIN | 23541-50-6 | 82151 |
|  | DEOXEODOXORUBIC-IN | 63950-06-1 | 267469 |
|  | DOXORUBICIN HYDROCHLORIDE | 25316-40-9 | 357704 |
|  | MAMSA(AMSACRINE) | 51264-14-3 | 249992 |
|  | MENOGARIL | 71628-96-1 | 269148 |
|  | MITOXANTRON | 70476-82-3 | 301739 |
|  | VP-16(ETOPOSIDE) | 33419-42-0 | 141540 |
|  | VM-26(TENIPOSIDE) | 29767-20-2 | 122819 |
|  | RUBIDAZONE | 36508-71-1 | 164011 |
|  | PYRAZOLOACRIDINE | 99009-21-9 | 366140 |
|  | OXANTHRAZOLE | 105118-12-5 | 349174 |
|  | N,N-DIBENZYLDAUNORUBICIN | 70878-51-2 | 268242 |
|  | VINCRISTINE SULFATE | 2068-78-2 | 67574 |
|  | VINBLASTINE SULFATE | 143-67-9 | 49842 |
|  | TRITYL LCYSTEINE | 2799-07-7 | 83265 |
|  | THIOCOLCHICINE | 87424-25-7 | 361792 |
|  |  PACLITAXEL (TAXOL) | 33069-62-4 | 125973 |
|  | RHIZOXIN | 90996-54-6 | 332598 |
|  | MAYTANSINE | 35846-53-8 | 153858 |
|  | DOLASTATIN 10 | 110417-88-4 | 376128 |
|  | COLCHICINE DERIVATIVE | 63989-75-3 | 33410 |
|  | ALLOCOLCHICINE | 641-28-1 | 406042 |
|  | THIOPURINE | 50-44-2 | 755 |
|  | THIOGUANINE | 154-42-7 | 752 |
|  | PYRAZOLOIMIDAZOLE | 6714-29-0 | 51143 |
|  | MACBECIN II | 73341-73-8 | 330500 |
|  | INOSINE DIALDEHYDE | 23590-99-0 | 118994 |
|  | HYDROXYLUREA | 127-07-1 | 32065 |
|  | GUANAZOLE | 1455-77-2 | 1895 |
|  | CYCLOCYTIDINE | 10212-25-6 | 145668 |
|  | B-TGDR | 789-61-7 | 71261 |
|  | ARA C | 69-74-9 | 63878 |
|  | APHIDICOLIN GLYCINATE | 92803-82-2 | 303812 |
|  | A-TGDR | 2133-81-5 | 71851 |
|  | 5 HP | 19494-89-4 | 107392 |
|  | 5-AZADEOXYCYTIDINE | 2353-33-5 | 127716 |
|  | 3-HP | 3814-79-7 | 95678 |
|  | 2'DEOXY5FLUOROURIDINE | 50-91-9 | 27640 |
|  | L-ALANOSINE | 59163-41-6 | 153353 |
|  | TRIMETREXATE | 82952-64-5 | 352122 |
|  | PYRAZOFURIN | 30868-30-5 | 143095 |
|  | METHOTREXATE | 59-05-2 | 740 |
|  | DIHYDROAZACYTIDINE | 62488-57-7 | 264880 |
|  | FTORAFUR | 37076-68-9 | 148958 |
|  | DUP 785 (BREQUINAR) | 96201-88-6 | 368390 |
|  | DICHLOROALLYL LAWSONE | 36417-16-0 | 126771 |
|  | PALA | 60342-56-5 | 224131 |
|  | ACIVICIN | 42228-92-2 | 163501 |
|  | 5-AZACYTIDINE | 320-67-2 | 102816 |
|  | BAKER'S ANTIFOL | 41191-04-2 | 139105 |
|  | 5-FLUOROURACIL | 51-21-8 | 19893 |
|  | 7-CHLOROCAMPTOTHECIN | 41646-05-3 |   249910 |
|  | 9-AMINO-20 (RS)-CAMPTOTHECIN | 130194-90-0 | 629971 |
|  | 11 FORMYL 20 (RS) CAMPTOTHECIN | 109466-93-5 | 606172 |
|  | 11-HYDROXYMETHYL20(RS)CAMPTOTHECIN |  | 606173 |
|  | MORPHOLINO-ADR | 89196-04-3 | 354646 |
|  | GLYCINATE |  | 364830 |
|  | 14CHLORO20(S) CAMPTOTHECIN HYDRATE |  | 643833 |
|  | CAMPTOTHECIN |  | 94600 |
|  | CAMPTOTHECIN ANALOGUE 1 |  | 295500 |
|  | CAMPTOTHECIN ANALOGUE 2 |  | 606985 |
|  | CAMPTOTHECIN ANALOGUE 3 |  | 295501 |
|  | CAMPTOTHECIN BUTYLGLYCINATE ESTER HYDROCHLORIDE |  | 606499 |
|  | CAMPTOTHECIN ETHYLGLYCINATE ESTER HYDROCHLORIDE |  | 606497 |
|  | CAMPTOTHECIN GLUTAMATE HCL |  | 610459 |
|  | CAMPTOTHECIN LYSINATE HCL |  | 610457 |
|  | CAMPTOTHECIN PHOSPHATE |  | 610458 |
|  | CAMPTOTHECIN,9-METHOXY |  | 176323 |
|  | CAMPTOTHECIN-20-O-(N,NDIMETHYL)GLYCINATE HCL |  | 618939 |
|  | CAMPTOTHECIN, ACETATE |  | 95382 |