**Evolution of optimal descriptors: solved, unsolved, and unsoluble tasks**

**Supplementary materials 1**

Collection of data on drug-like compounds from from the “Galvez dataset”, available on the Internet: <http://www.uv.es/~galvez/tablevi.pdf>

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **CAS** | **SMILES** | **Structure** | **Rat LD50 oral, mg/kg** | **Boiling Point, ‘C** | **log P (octanol-water)** | **Water Solubilitymg/L** |
| 79-00-5 | ClCC(Cl)Cl |  | 836 | 113.8 | 1.89 | 4590 |
| 530-50-7 | NN(c1ccccc1)c2ccccc2 |  | - | - | 2.8 | 287 |
| 87-61-6 | Clc1cccc(Cl)c1Cl |  | 1830 | 218.5 | 4.05 | 18 |
| 150-61-8 | C(CNc1ccccc1)Nc2ccccc2 |  | - | - | 2.910 | - |
| 524-42-5 | O=C1c2ccccc2C=CC1=O |  | 250 | - | 2.110 | - |
| 108-70-3 | Clc1cc(Cl)cc(Cl)c1 |  | 800 | 208 | 4.19 | 6.01 |
| 106-99-0 | C=CC=C |  | 5480 | -4.40E+00 | 1.99 | 735 |
| 534-07-6 | ClCC(=O)CCl |  | 20 | 173.4 | 0.270 | 5.52E+04 |
| 102-06-7 | N=C(Nc1ccccc1)Nc2ccccc2 |  | 323 | - | 2.890 | 1000 |
| 130-15-4 | O=C2C=CC(=O)c1ccccc12 |  | 190 | - | 1.71 | 668 |
| 547-81-9 | Oc3cc4CC[C@H]2[C@H](CC[C@]1(C)[C@H]2C[C@H](O)[C@@H]1O)c4cc3 |  | - | - | 2.320 | - |
| 106-98-9 | C=CCC |  | - | -6.20E+00 | 2.4 | 221 |
| 112-53-8 | CCCCCCCCCCCCO |  | 12800 | 259 | 5.13 | 4 |
| 70-34-8 | Fc1ccc(cc1[N+](=O)[O-])[N+]([O-])=O |  | - | 296 | 1.830 | 400 |
| 288-88-0 | c1nncn1 |  | 1750 | - | -0.58 | 4.24E+05 |
| 86-55-5 | O=C(O)c2cccc1ccccc12 |  | - | 300 | 3.1 | 86 |
| 90-15-3 | Oc2cccc1ccccc12 |  | 1870 | 288 | 2.85 | 866 |
| 108-03-2 | [O-][N+](=O)CCC |  | 455 | 131.1 | 0.87 | 1.50E+04 |
| 131-91-9 | O=Nc1c2ccccc2ccc1O |  | - | - | 2.28 | 1000 |
| 109-67-1 | CCCC=C |  | - | 29.9 | 2.660 | 148 |
| 92-43-3 | O=C1CCN(N1)c2ccccc2 |  | 200 | - | 0.89 | 1.16E+04 |
| 118-79-6 | Brc1cc(Br)cc(Br)c1O |  | 2000 | 286 | 4.13 | 70 |
| 87-40-1 | COc1c(Cl)cc(Cl)cc1Cl |  | - | 241 | 4.11 | 10 |
| 88-06-2 | Clc1cc(Cl)cc(Cl)c1O |  | 820 | 246 | 3.69 | 800 |
| 118-96-7 | Cc1c(cc(cc1[N+](=O)[O-])[N+]([O-])=O)[N+]([O-])=O |  | 607 | - | 1.6 | 130 |
| 120-83-2 | Clc1cc(Cl)c(O)cc1 |  | 47 | 210 | 3.06 | 4500 |
| 367-25-9 | Fc1ccc(N)c(F)c1 |  | 820 | 170 | 1.54 | 4490 |
| 97-02-9 | O=[N+]([O-])c1cc(ccc1N)[N+]([O-])=O |  | 285 | 333.6 | 1.840 | 1440 |
| 51-28-5 | O=[N+]([O-])c1cc(ccc1O)[N+]([O-])=O |  | 30 | - | 1.67 | 2790 |
| 119-26-6 | NNc1ccc(cc1[N+]([O-])=O)[N+]([O-])=O |  | - | - | 1.47 | 2480 |
| 329-71-5 | O=[N+]([O-])c1ccc(cc1O)[N+]([O-])=O |  | - | - | 1.75 | 385 |
| 1904-98-9 | Nc1nc(N)nc2ncnc12 |  | - | - | -0.790 | 2380 |
| 87-65-0 | Clc1cccc(Cl)c1O |  | - | 220 | 2.75 | 1900 |
| 573-56-8 | O=[N+]([O-])c1cccc([N+]([O-])=O)c1O |  | - | - | 1.37 | 5190 |
| 108-48-5 | Cc1cccc(C)n1 |  | 400 | 144.1 | 1.68 | 3.00E+05 |
| 695-34-1 | Cc1ccnc(N)c1 |  | 200 | - | 0.56 | - |
| 136-95-8 | Nc1nc2ccccc2s1 |  | - | - | 2.000 | 310 |
| 96-50-4 | Nc1nccs1 |  | 480 | - | 0.38 | 5.53E+04 |
| 110-43-0 | CC(=O)CCCCC |  | 1670 | 151 | 1.98 | 4300 |
| 149-30-4 | Sc1nc2ccccc2s1 |  | 100 | - | 2.42 | 120 |
| 137-32-6 | C[C@@H](CC)CO |  | - | 128 | 1.29 | 2.97E+04 |
| 115-19-5 | C#CC(C)(C)O |  | 1950 | 104 | 0.28 | 1.00E+06 |
| 84-54-8 | Cc2ccc3C(=O)c1ccccc1C(=O)c3c2 |  | - | - | 3.890 | - |
| 91-60-1 | Sc1ccc2ccccc2c1 |  | - | 288 | 3.860 | - |
| 135-19-3 | Oc1ccc2ccccc2c1 |  | 1960 | 285 | 2.7 | 755 |
| 79-46-9 | CC(C)[N+]([O-])=O |  | 720 | 120.2 | 0.93 | 1.70E+04 |
| 123-96-6 | CC(O)CCCCCC |  | - | 178.5 | 2.9 | 1120 |
| 6032-29-7 | C[C@@H](O)CCC |  | - | 119.3 | 1.19 | 4.46E+04 |
| 109-68-2 | C\C=C\CC |  | - | 37 | 2.580 | 203 |
| 122-99-6 | OCCOc1ccccc1 |  | 1260 | 245 | 1.16 | 2.67E+04 |
| 141-90-2 | O=C1C=CNC(=S)N1 |  | - | - | 0.900 | 709 |
| 54-96-6 | Nc1ccncc1N |  | - | - | -1.030 | - |
| 95-76-1 | Nc1cc(Cl)c(Cl)cc1 |  | 545 | 272 | 2.69 | 92 |
| 300-38-9 | Brc1cc(cc(Br)c1O)C[C@H](N)C(=O)O |  | - | - | 0.020 | 4000 |
| 90-59-5 | Oc1c(C=O)cc(Br)cc1Br |  | - | - | 3.790 | - |
| 13466-78-9 | CC2(C)[C@H]1CC=C(C)C[C@@H]12 |  | 4800 | 170 | 4.38 | 2.910 |
| 536-78-7 | CCc1cccnc1 |  | - | 165 | 1.66 | 3.70E+05 |
| 598-75-4 | CC(C)[C@@H](C)O |  | - | 112 | 1.28 | 5.60E+04 |
| 56-49-5 | Cc2ccc3cc1c5ccccc5ccc1c4CCc2c34 |  | - | - | 6.42 | 0.0029 |
| 584-02-1 | CCC(O)CC |  | 1870 | 116.2 | 1.21 | 5.15E+04 |
| 536-75-4 | CCc1ccncc1 |  | - | 168.3 | 1.65 | 1.07E+05 |
| 104-91-6 | O=Nc1ccc(O)cc1 |  | - | - | 1.29 | 2.94E+04 |
| 537-47-3 | O=C(Nc1ccccc1)NN |  | - | - | 0.16 | 700 |
| 51-20-7 | BrC1=CNC(=O)NC1=O |  | - | - | -0.21 | 815 |
| 2435-76-9 | N#N=C1/C=NC(=O)NC1=O |  | - | - | -1.950 | - |
| 608-07-1 | COc1cc2c(cc1)ncc2CCN |  | - | - | 1.350 | - |
| 480-68-2 | O=C1NC(=O)NC(=O)C1[N+]([O-])=O |  | - | - | -1.190 | 900 |
| 54-25-1 | O=C1NC(=O)C=NN1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O |  | - | - | -2.14E+00 | 8.28E+04 |
| 134-58-7 | O=C1NC(N)=Nc2nnnc12 |  | - | - | -0.71 | 1.47E+04 |
| 523-27-3 | Brc2c1ccccc1c(Br)c3ccccc23 |  | - | - | 6.130 | - |
| 37517-30-9 | CC(C)NCC(O)COc1ccc(cc1C(C)=O)NC(=O)CCC |  | - | - | 1.71 | 259 |
| 32795-44-1 | O=C(C)Nc1ccc(cc1)C(=O)NCCN(CC)CC |  | - | - | 0.990 | - |
| 89796-99-6 | Clc2cccc(Cl)c2Nc1ccccc1CC(=O)OCC(=O)O |  | 130 | - | - | - |
| 77-46-3 | O=S(=O)(c1ccc(NC(C)=O)cc1)c2ccc(NC(C)=O)cc2 |  | - | - | 0.820 | - |
| 80-03-5 | O=S(=O)(c1ccc(N)cc1)c2ccc(NCC(=O)O)cc2 |  | - | - | 0.570 | - |
| 642-83-1 | O=C1O[C@@H]2[C@H](OC(C)=O)C(=O)O[C@@H]2[C@H]1OC(C)=O |  | 10000 | - | - | - |
| 2490-97-3 | O=C(C)N[C@H](CCC(N)=O)C(=O)O |  | - | - | -2.110 | - |
| 83-32-9 | c1cc2cccc3CCc(c1)c23 |  | - | 279 | 3.92 | 3.9 |
| 152-72-7 | [O-][N+](=O)c1ccc(cc1)[C@@H](CC(C)=O)C2=C(O)c3ccccc3OC2=O |  | 513 | - | 1.98 | 49.1 |
| 807-31-8 | Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)(CNC(C)=O)c3ccccc3 |  | - | - | 3.980 | - |
| 33665-90-6 | CC1=CC(=O)NS(=O)(=O)O1 |  | - | - | -1.330 | - |
| 75-07-0 | CC=O |  | 661 | 20.1 | -0.34 | 1.00E+06 |
| 107-29-9 | C\C=N\O |  | - | 115 | -0.13 | 1.77E+05 |
| 60-35-5 | CC(N)=O |  | 7000 | 222 | -1.26E+00 | 2.25E+06 |
| 103-84-4 | O=C(C)Nc1ccccc1 |  | 800 | 304 | 1.16 | 6390 |
| 59-66-5 | O=S(N)(=O)c1nnc(NC(C)=O)s1 |  | - | - | -0.26 | 980 |
| 299-89-8 | Nc1nc(C)ncc1CN(C=O)C(\C)=C(/CCOC(C)=O)SC(C)=O |  | - | - | - | - |
| 968-81-0 | O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(cc2)C(C)=O |  | 2000 | - | 2.44 | 3430 |
| 75-05-8 | CC#N |  | 2460 | 81.6 | -0.34 | 1.00E+06 |
| 2751-68-0 | CC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2 |  | - | - | 2.62 | 11.9 |
| 98-86-2 | CC(=O)c1ccccc1 |  | 815 | 202 | 1.58 | 6130 |
| 616-91-1 | CC(=O)N[C@@H](CS)C(O)=O |  | 5050 | - | -0.660 | - |
| 74-86-2 | C#C |  | - | -8.47E+01 | 0.37 | 1200 |
| 72420-38-3 | C[C@]1(OC(=CC1=O)C(=O)O)c2ccccc2 |  | 3000 | - | - | - |
| 51037-30-0 | [O-][n+]1cc(ncc1C)C(O)=O |  | - | - | -0.520 | - |
| 55079-83-9 | Cc1c(C)c(/C=CC(\C)=C\C=C\C(\C)=C\C(=O)O)c(C)cc1OC |  | 4000 | - | 6.4 | 0.073 |
| 87848-99-5 | O=C(O)/C=C/c1cccc(n1)/C(=C\CN2CCCC2)c3ccc(C)cc3 |  | - | - | 2.830 | - |
| 79-06-1 | C=CC(N)=O |  | 124 | 192.6 | -0.67 | 6.40E+05 |
| 15301-40-3 | O=S(=O)(O)c1ccc(OCC)c2ncccc12 |  | - | - | -0.440 | - |
| 59277-89-3 | NC2=Nc1c(ncn1COCCO)C(=O)N2 |  | 20000 | - | -1.56E+00 | 1620 |
| 281-23-2 | C1C3CC2CC1CC(C2)C3 |  | 10000 | - | 4.24 | 6.030 |
| 73-24-5 | NC=1NC=NC2=NC=NC=12 |  | 227 | - | -0.09 | 1030 |
| 63547-13-7 | O=S(CC(=O)NO)C(c1ccccc1)c2ccccc2 |  | - | - | - | - |
| 56287-74-2 | Cc1ccccc1N3C(=Nc2ccc(N)cc2C3=O)CF |  | 249 | - | - | - |
| 522-27-0 | O\N=C(/C(=N/O)c1ccco1)c2ccco2 |  | - | - | 2.250 | - |
| 3011-89-0 | O=C(N)c1ccc(cc1Cl)[N+]([O-])=O |  | - | - | 0.470 | - |
| 74258-86-9 | O=C(N[C@@H](Cc1ccccc1)C(=O)O)[C@@H]2CCCN2C(=O)[C@H](C)CSC(C)=O |  | 5000 | - | - | - |
| 546-43-0 | C[C@H]2CCC[C@]1(C)C[C@@H]3OC(=O)C(=C)[C@H]3C=C12 |  | - | 275 | 3.38 | 38.4 |
| 54965-21-8 | O=C(OC)Nc1nc2ccc(cc2n1)SCCC |  | 2400 | - | 3.140 | - |
| 18559-94-9 | OCc1cc(ccc1O)[C@@H](O)CNC(C)(C)C |  | 660 | - | 0.640 | 1.43E+04 |
| 830-89-7 | S=C1N[C@H](CC(C)C)C(=O)N1CC=C |  | - | - | - | - |
| 22131-79-9 | Clc1cc(ccc1OCC=C)CC(=O)O |  | 1050 | - | 2.48 | 600 |
| 67452-97-5 | OCC(=O)[C@]4(O)[C@H](C)C[C@@H]1[C@@]4(C)C[C@H](O)[C@H]3[C@H]1[C@H](Cl)CC2=CC(=O)C=C[C@]23C |  | - | - | - | - |
| 116-06-3 | CC(C)(\C=N\OC(=O)NC)SC |  | 5 | - | 1.13 | 6030 |
| 52-39-1 | OCC(=O)[C@H]4CC[C@@H]2[C@@]4(C=O)C[C@H](O)[C@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 |  | - | - | 1.08 | 51.2 |
| 309-00-2 | ClC3=C(Cl)[C@@]4(Cl)[C@@H]2[C@@H]([C@@H]1C[C@H]2C=C1)[C@]3(Cl)C4(Cl)Cl |  | 39 | - | 6.5 | 0.017 |
| 22573-93-9 | CCCC[C@@H](CC)CNC(=N)NC(=N)NCCCCCCNC(=N)NC(=N)NC[C@H](CC)CCCC |  | - | - | 3.580 | - |
| 74176-31-1 | O[C@H]2C[C@H](O)[C@H](C#C[C@@H](O)CCC1CCCCC1)[C@H]2C\C=C/CCCC(=O)OC |  | - | - | - | - |
| 595-77-7 | CC(=O)[C@]2(O)[C@@]3(C)CC[C@@H]1[C@@]4(C)CCC(=O)C=C4CC[C@H]1[C@@H]3C[C@H]2O |  | - | - | 3.150 | - |
| 33178-86-8 | C=CCN(C1=NCCN1)c2c(Cl)cccc2Cl |  | 500 | - | - | - |
| 59338-93-1 | C=CCN3CCC[C@@H]3CNC(=O)c1cc2nnnc2cc1OC |  | - | - | 1.79 | 295 |
| 97-59-6 | O=C1NC(=O)NC1NC(=O)N |  | - | - | -3.140 | 5260 |
| 5486-77-1 | O=C(NCCN(CC)CC)c1ccc(Cl)cc1OCC=C |  | 3000 | - | 3.450 | - |
| 107-11-9 | C=CCN |  | 102 | 53.3 | 0.03 | 1.00E+06 |
| 432-60-0 | C[C@]32CC[C@H]1[C@H]4CCCC=C4CC[C@@H]1[C@@H]3CC[C@@]2(O)CC=C |  | - | - | 5.880 | - |
| 39718-89-3 | O=C(O)[C@H](C)c1ccc(NCC(=C)C)cc1 |  | 550 | - | 2.870 | - |
| 1415-73-2 | O[C@H]1[C@H](O)[C@@H](O)[C@@H](O[C@@H]1CO)[C@@H]4c2cccc(O)c2C(=O)c3c(O)cc(CO)cc34 |  | - | - | 0.550 | 8300 |
| 77-20-3 | C[C@@H]2CN(C)CC[C@]2(OC(=O)CC)c1ccccc1 |  | - | - | 2.83 | 797 |
| 82626-01-5 | CCCN(CCC)C(=O)Cc1c(nc2ccc(Cl)cn12)c3ccc(Cl)cc3 |  | - | - | - | - |
| 850-52-2 | O=C3C=C4CC[C@@H]2C(C=C[C@@]1(C)[C@H]2CC[C@@]1(O)CC=C)=C4CC3 |  | - | - | 3.710 | - |
| 150-59-4 | CCN(CCCc1ccccc1)CCCc2ccccc2 |  | - | - | 5.910 | - |
| 537-17-7 | Nc2ncnc(Nc1ccccc1)n2 |  | - | - | 1.890 | - |
| 768-94-5 | NC12CC3CC(C1)CC(C2)C3 |  | 900 | - | 2.44 | 6290 |
| 539-21-9 | N=C(N)N\N=C1\C=C/C(=N\NC(N)=S)C=C1 |  | 750 | - | 1.23 | 2470 |
| 519-88-0 | COc1ccc(cc1)[C@H](C(N)=O)N(CCCC)CCCC |  | - | - | 3.860 | - |
| 3754-19-6 | O=S(N)(=O)c1cc(c(cc1Cl)\N=C\C=C(/C)O)S(=O)(=O)NCC=C |  | - | - | 1.600 | - |
| 51022-69-6 | CC(=O)OCC(=O)[C@]56OC1(CCCC1)O[C@@H]6C[C@H]4C3CCC2=CC(=O)C=C[C@]2(C)[C@@]3(F)[C@@H](O)C[C@@]45C |  | 2000 | - | 3.780 | - |
| 32887-01-7 | OC(=O)[C@@H]2N3C(=O)[C@@H](/N=C/N1CCCCCC1)[C@H]3SC2(C)C |  | 10000 | - | 3.090 | - |
| 834-12-8 | CSc1nc(NCC)nc(NC(C)C)n1 |  | 508 | 345 | 2.98 | 209 |
| 51579-82-9 | Nc1c(cccc1CC(=O)O)C(=O)c2ccccc2 |  | - | - | - | - |
| 37517-28-5 | NCC[C@H](O)C(=O)N[C@@H]3C[C@H](N)[C@@H](O[C@H]1O[C@H](CN)[C@@H](O)[C@H](O)[C@H]1O)[C@H](O)[C@H]3O[C@H]2O[C@H](CO)[C@@H](O)[C@H](N)[C@H]2O |  | - | - | -8.780 | 1.85E+05 |
| 125-84-8 | CC[C@@]1(CCC(=O)NC1=O)c2ccc(N)cc2 |  | - | - | 0.820 | - |
| 79-17-4 | N=C(N)NN |  | - | - | - | - |
| 642-44-4 | O=C1N(CC=C)C(N)=CC(=O)N1CC |  | 2300 | - | 0.080 | - |
| 60-46-8 | NC(=O)C(CC(C)N(C)C)(c1ccccc1)c2ccccc2 |  | - | - | 2.750 | - |
| 58-37-7 | CN(C)CC(CN1c3ccccc3Sc2ccccc12)N(C)C |  | - | - | 4.76 | - |
| 54-62-6 | O=C(O)[C@H](CCC(=O)O)NC(=O)c1ccc(cc1)NCc2nc3c(nc2)nc(N)nc3N |  | - | - | -1.820 | - |
| 58-15-1 | CN(C)C=2C(=O)N(c1ccccc1)N(C)C=2C |  | 285 | - | 1 | 5.44E+04 |
| 3811-56-1 | Nc1cc(C)nc2ccc(cc12)NC(=O)Nc3ccc4nc(C)cc(N)c4c3 |  | - | - | - | - |
| 2207-50-3 | NC1=NC[C@@H](O1)c2ccccc2 |  | - | - | 1.150 | - |
| 1951-25-3 | CCN(CC)CCOc1c(I)cc(cc1I)C(=O)c2c3ccccc3oc2CCCC |  | - | - | 7.57 | 2.83E-04 |
| 50-48-6 | CN(C)CC\C=C1\c3ccccc3CCc2ccccc12 |  | 320 | - | 4.92 | 9.71 |
| 24622-72-8 | CC(C)CCO[C@@H](CN1CCCC1)c2ccccc2 |  | - | - | - | - |
| 68302-57-8 | CC(C)c1cc2C(=O)c3cc(c(N)nc3Oc2cc1)C(=O)O |  | 10000 | - | - | - |
| 88150-42-9 | O=C(OC)C1=C(C)NC(COCCN)=C(C(=O)OCC)[C@@H]1c2ccccc2Cl |  | - | - | 3 | 75.3 |
| 22661-76-3 | COc1cc(cc(OC)c1OC)C(=O)O[C@@H](CN2CCOCC2)COCCC(C)C |  | - | - | - | - |
| 78613-35-1 | C[C@H]2CN(C[C@H](C)Cc1ccc(cc1)C(C)(C)CC)C[C@@H](C)O2 |  | - | - | - | - |
| 26328-53-0 | [O-][N+](=O)c1ccc(cc1)Nc2ccc(cc2)/N=C=S |  | - | - | - | - |
| 5585-64-8 | COc1ccc(cc1)C(\CN(C)C)=C(\c2ccc(OC)cc2)c3ccc(OC)cc3 |  | - | - | - | - |
| 14028-44-5 | Clc1ccc2Oc4ccccc4N=C(c2c1)N3CCNCC3 |  | 313 | - | 3.380 | - |
| 75558-90-6 | Fc1ccc(cc1)C(CCCN2CCN(CC2)C(=O)NCC)c3ccc(F)cc3 |  | - | - | - | - |
| 5581-35-1 | ClC(Cl)(Cl)/C=N/[C@H](C)Cc1ccccc1 |  | - | - | - | - |
| 134-37-2 | Nc1cc(ccc1)N2C=CC=CC2=O |  | 2300 | - | 0.450 | - |
| 300-62-9 | NC(C)Cc1ccccc1 |  | 30 | 203 | 1.76 | 2.80E+04 |
| 1673-06-9 | Nc1ccc(cc1)OCCCCCN3C(=O)c2ccccc2C3=O |  | - | - | 3.800 | - |
| 69-53-4 | OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)[C@H](N)c1ccccc1)[C@H]3SC2(C)C |  | - | - | 1.35 | 1.01E+04 |
| 99464-64-9 | O=C(OCC)O[C@@H](C)OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 |  | 747 | - | - | - |
| 51264-14-3 | CS(=O)(=O)Nc4ccc(Nc1c3ccccc3nc2ccccc12)c(OC)c4 |  | - | - | 3.890 | - |
| 29883-15-6 | O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]3OC[C@H]2O[C@@H](O[C@H](C#N)c1ccccc1)[C@H](O)[C@@H](O)[C@@H]2O |  | 405 | - | -4.340 | - |
| 538-68-1 | CCCCCc1ccccc1 |  | - | 205.4 | 4.9 | 3.37 |
| 2740-52-5 | CC(=O)[C@@]3(O)CC[C@@H]2[C@@H]4C[C@H](C)C1=CCCC[C@]1(C)[C@H]4CC[C@@]23C |  | - | - | - | - |
| 68475-42-3 | Clc1c2CN3CC(=O)NC3=Nc2ccc1Cl |  | - | - | - | - |
| 31698-14-3 | N=C1N=C2O[C@H]3[C@H](O)[C@@H](CO)O[C@H]3N2C=C1 |  | 7000 | - | -2.37E+00 | 1.00E+06 |
| 53-41-8 | O=C4CC[C@@H]3[C@]4(C)CC[C@H]1[C@H]3CC[C@H]2C[C@H](O)CC[C@]12C |  | - | - | 3.69 | 12 |
| 62-53-3 | Nc1ccccc1 |  | 250 | 184.1 | 0.9 | 3.60E+04 |
| 72432-10-1 | O=C2CCCN2C(=O)c1ccc(OC)cc1 |  | 4500 | - | - | - |
| 117-37-3 | COc1ccc(cc1)C3C(=O)c2ccccc2C3=O |  | - | - | 2.88 | 79.8 |
| 100-66-3 | COc1ccccc1 |  | 3700 | 153.7 | 2.11 | 1040 |
| 91-75-8 | C(c1ccccc1)N(CC2=NCCN2)c3ccccc3 |  | - | - | 3.380 | 663 |
| 120-12-7 | c1ccc2cc3ccccc3cc2c1 |  | - | 339.9 | 4.45 | 0.0434 |
| 1143-38-0 | Oc2cccc1Cc3cccc(O)c3C(=O)c12 |  | - | - | 4.400 | - |
| 60-80-0 | O=C2C=C(C)N(C)N2c1ccccc1 |  | 1705 | 319 | 0.38 | 5.19E+04 |
| 55300-29-3 | FC(F)(F)c1ccc5c(c1)nccc5Nc2ccccc2C(=O)OCCN3CCN(CC3)c4cc(ccc4)C(F)(F)F |  | - | - | - | - |
| 63469-19-2 | OC(=O)[C@@H]4N5C(=O)[C@H](NC(=O)[C@H](NC(=O)c1cnc2cccnc2c1O)c3ccccc3)[C@H]5SC4(C)C |  | - | - | - | - |
| 2835-06-5 | N[C@H](C(=O)O)c1ccccc1 |  | - | - | -2.07E+00 | 1.15E+05 |
| 52-46-0 | C1CN1p2(np(np(n2)(N3CC3)N4CC4)(N5CC5)N6CC6)N7CC7 |  | 98 | - | 2.190 | - |
| 520-36-5 | Oc1ccc(cc1)C3=CC(=O)c2c(cc(O)cc2O)O3 |  | - | - | 3.02 | 183 |
| 58-00-4 | Oc3ccc2C[C@@H]1c4c(CCN1C)cccc4c2c3O |  | - | - | 2.3 | 1.66E+04 |
| 37321-09-8 | O[C@@H]4[C@@H](O)[C@H](N)[C@@H](CO)O[C@@H]4O[C@H]2O[C@@H]3C[C@@H](N)[C@@H](O[C@@H]1[C@@H](N)C[C@@H](N)[C@H](O)[C@H]1O)O[C@@H]3[C@H](O)[C@@H]2NC |  | - | - | -8.120 | - |
| 147-81-9 | O[C@H](C=O)[C@H](O)[C@H](O)CO |  | - | - | -3.02E+00 | 5.00E+05 |
| 51025-85-5 | NCC[C@H](O)C(=O)N[C@@H]3C[C@H](N)[C@@H](O[C@H]1O[C@H](CN)CC[C@H]1N)[C@H](O)[C@H]3O[C@H]2O[C@H](CO)[C@@H](O)[C@H](N)[C@H]2O |  | - | - | - | - |
| 499-04-7 | OC(=O)C=1CN(C)CCC=1 |  | - | - | -1.210 | - |
| 74-79-3 | N[C@@H](CCCNC(=N)N)C(=O)O |  | - | - | -4.20E+00 | 1.82E+05 |
| 68377-92-4 | O[C@H](CSc1nc(cs1)c2ccc(s2)C(N)=O)CNC(C)(C)C |  | - | - | - | - |
| 63968-64-9 | O=C4O[C@H]2O[C@@]1(C)CC[C@@H]3[C@]2(OO1)[C@@H](CC[C@H]3C)[C@H]4C |  | 5576 | - | 2.9 | 51.9 |
| 22839-47-0 | O=C(O)C[C@@H](N)C(=O)N[C@H](Cc1ccccc1)C(=O)OC |  | 10000 | - | 0.070 | - |
| 466-49-9 | CC(=O)N2c1c(cccc1OC)[C@]35CCN4CCC[C@@](CC[C@@H]23)(CC)[C@@H]45 |  | - | - | 3.680 | 1.67E+04 |
| 63358-49-6 | OC(=O)[C@@H]2N3C(=O)[C@H](NC(=O)[C@H](NC(=O)[C@H](N)CC(=O)NC)c1ccc(O)cc1)[C@H]3SC2(C)C |  | - | - | - | - |
| 68844-77-9 | Fc1ccc(cc1)Cn4c5ccccc5nc4NC3CCN(CCc2ccc(OC)cc2)CC3 |  | 2560 | - | 6.430 | - |
| 29122-68-7 | CC(C)NCC(O)COc1ccc(cc1)CC(N)=O |  | 2000 | - | 0.16 | 1.33E+04 |
| 479-20-9 | O=Cc2c(O)cc(C)c(C(=O)Oc1cc(C)c(C(=O)OC)c(O)c1C)c2O |  | - | - | 6.860 | - |
| 51-55-8 | CN3C1CCC3CC(C1)OC(=O)C(CO)c2ccccc2 |  | 500 | - | 1.83 | 2200 |
| 320-67-2 | NC1=NC(=O)N(C=N1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O |  | - | - | -3.830 | 8.90E+04 |
| 313-05-3 | CN(C)CCCN(C)[C@H]4CC[C@H]3[C@]4(C)CC[C@H]2[C@@H]3CC=C1C[C@@H](O)CC[C@@]12C |  | - | - | - | - |
| 115-46-8 | OC(c1ccccc1)(C2CCNCC2)c3ccccc3 |  | - | - | 3.450 | - |
| 62973-76-6 | Cn2c(cnc2/C=C/c1ccnc(N)n1)[N+]([O-])=O |  | 7600 | - | 0.85 | 1900 |
| 1649-18-9 | Fc1ccc(cc1)C(=O)CCCN2CCN(CC2)c3ccccn3 |  | 245 | - | 3.3 | 131 |
| 3964-81-6 | CN1CC\C(CC1)=C2\c4ncccc4CCc3ccccc23 |  | - | - | 3.59 | - |
| 58581-89-8 | Clc1ccc(cc1)CC3=NN(C(=O)c2ccccc23)[C@@H]4CCCN(C)CC4 |  | 310 | - | - | - |
| 17243-38-8 | OC(=O)[C@H]2N3C(=O)[C@H](NC(=O)[C@@H](\N=N#N)c1ccccc1)[C@H]3SC2(C)C |  | - | - | 2.650 | - |
| 1830-32-6 | CCN(CC)C(=O)CSc1ccc(Cl)nn1 |  | 1550 | - | 1.310 | 5000 |
| 37091-66-0 | OC(=O)[C@@H]3N4C(=O)[C@H](NC(=O)[C@H](NC(=O)N1CCNC1=O)c2ccccc2)[C@H]4SC3(C)C |  | - | - | 1.710 | - |
| 103-33-3 | N(=N/c1ccccc1)\c2ccccc2 |  | 1000 | 293 | 3.82 | 6.4 |
| 527-73-1 | [O-][N+](=O)c1nccn1 |  | - | - | 0.15 | 3.22E+04 |
| 27589-33-9 | NS(=O)(=O)c2cc(c(NCc1cccs1)cc2Cl)c3nnnn3 |  | 2545 | - | 0.060 | - |
| 78110-38-0 | [NH3+]c1nc(cs1)\C(=N\OC(C)(C)C(=O)O)C(=O)N[C@@H]2C(=O)N(S([O-])(=O)=O)[C@H]2C |  | 10000 | - | - | - |
| 275-51-4 | c1cccc2cccc2c1 |  | 4000 | - | 3.2 | 50.2 |
| 531-55-5 | [Cl-].CN(C)c1cc2[s+]c3cc(NC)ccc3nc2cc1 |  | - | - | 3.480 | - |
| 531-57-7 | [Cl-].Nc1ccc2nc3ccc(cc3[s+]c2c1)NC |  | - | - | 2.380 | - |
| 50972-17-3 | N[C@H](c1ccccc1)C(=O)N[C@@H]3C(=O)N2[C@@H](C(=O)O[C@@H](C)OC(=O)OCC)C(C)(C)S[C@@H]23 |  | - | - | - | - |
| 1134-47-0 | Clc1ccc(cc1)C(CN)CC(=O)O |  | 145 | - | -0.96 | 2090 |
| 81732-65-2 | O=C(Oc1cc(cc(c1)OC(=O)N(C)C)[C@H](O)CNC(C)(C)C)N(C)C |  | - | - | - | - |
| 3703-79-5 | O[C@H](CNCCCC)c1ccc(O)cc1 |  | - | - | 1.260 | - |
| 2016-63-9 | CCN(CCO)CCn2c3C(=O)N(C)C(=O)N(C)c3nc2Cc1ccccc1 |  | - | - | 1.630 | - |
| 4945-47-5 | CN1CCC(CC1)N(Cc2ccccc2)c3ccccc3 |  | - | - | 4.070 | - |
| 101-27-9 | Clc1cc(NC(=O)OCC#CCCl)ccc1 |  | 527 | 224 dec | 3.410 | 11 |
| 39552-01-7 | CC(C)NC[C@@H](O)COc1cccc2cc(oc12)C(C)=O |  | - | - | 2.02 | 2640 |
| 64-65-3 | CCC1(C)CC(=O)NC(=O)C1 |  | - | - | 0.520 | - |
| 22487-42-9 | OC(C(=O)OCCN(CC)CCC)(c1ccccc1)c2ccccc2 |  | - | - | - | - |
| 2179-37-5 | CN(C)CCCOC1(CCCCCC1)Cc2ccccc2 |  | - | - | 5.180 | - |
| 20187-55-7 | O=C(O)COc3nn(Cc1ccccc1)c2ccccc23 |  | 1200 | - | 3.280 | - |
| 22781-23-3 | CNC(=O)Oc1cccc2OC(C)(C)Oc12 |  | 40 | - | 1.7 | 260 |
| 73-48-3 | FC(F)(F)c1cc2N[C@H](NS(=O)(=O)c2cc1S(N)(=O)=O)Cc3ccccc3 |  | - | - | 1.89 | 108 |
| 23602-78-0 | FC(F)(F)c2cccc(C[C@H](C)NCCOC(=O)c1ccccc1)c2 |  | - | - | 4.670 | - |
| 17804-35-2 | O=C(OC)Nc2nc1ccccc1n2C(=O)NCCCC |  | 10000 | - | 2.12 | 3.8 |
| 51234-28-7 | O=C(O)[C@@H](C)c1cc2nc(oc2cc1)c3ccc(Cl)cc3 |  | 118 | - | 3.23 | 52 |
| 2062-84-2 | Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)N3c4ccccc4NC3=O |  | - | - | 3.91 | 1.830 |
| 322-35-0 | Oc1ccc(CNNC(=O)[C@H](N)CO)c(O)c1O |  | - | - | - | - |
| 100-52-7 | O=Cc1ccccc1 |  | 1300 | 179 | 1.48 | 6570 |
| 55-21-0 | NC(=O)c1ccccc1 |  | - | 290 | 0.64 | 1.35E+04 |
| 93-98-1 | O=C(Nc1ccccc1)c2ccccc2 |  | - | - | 2.62 | 262 |
| 3562-84-3 | Brc1cc(cc(Br)c1O)C(=O)c2c3ccccc3oc2CC |  | 248 | - | 6.030 | - |
| 71-43-2 | c1ccccc1 |  | 930 | 80 | 2.13 | 1790 |
| 85-95-0 | Oc1ccc(cc1)[C@H](CC)[C@H](CC)[C@H](C)c2ccc(O)cc2 |  | - | - | - | - |
| 14051-33-3 | O=C4NC(=O)CCC4(C2CCN(Cc1ccccc1)CC2)c3ccccc3 |  | - | - | - | - |
| 134-81-6 | O=C(C(=O)c1ccccc1)c2ccccc2 |  | - | 347 | 3.38 | 50.3 |
| 51-17-2 | c1cccc2ncnc12 |  | - | 360 | 1.32 | 2010 |
| 22994-85-0 | O=C(Cn1ccnc1[N+]([O-])=O)NCc2ccccc2 |  | - | - | 0.91 | 400 |
| 17243-39-9 | CNCC24CCC(c1ccccc12)c3ccccc34 |  | 600 | - | 3.540 | - |
| 1980-45-6 | O=P(NC(=O)OCc1ccccc1)(N2CC2)N3CC3 |  | - | - | - | - |
| 271-89-6 | c1cccc2occc12 |  | - | 174 | 2.67 | 678 |
| 65-85-0 | O=C(O)c1ccccc1 |  | 1700 | 249.2 | 1.87 | 3400 |
| 104-31-4 | O=C(OCCOCCOCCOCCOCCOCCOCCOCCOCCOC)c1ccc(NCCCC)cc1 |  | - | - | 2.45 | 1.230 |
| 100-47-0 | N#Cc1ccccc1 |  | - | 191.1 | 1.56 | 2000 |
| 119-61-9 | O=C(c1ccccc1)c2ccccc2 |  | 10000 | 305.4 | 3.18 | 137 |
| 95-16-9 | c1cccc2scnc12 |  | 380 | 231 | 2.01 | 4300 |
| 86-75-9 | O=C(Oc1cccc2cccnc12)c3ccccc3 |  | - | - | 3.190 | - |
| 98-88-4 | ClC(=O)c1ccccc1 |  | 1900 | 197.2 | 1.440 | 4940 |
| 519-09-5 | CN1[C@@H]2CC[C@@H]1[C@@H](C(=O)O)[C@H](C2)OC(=O)c3ccccc3 |  | - | - | -1.320 | - |
| 13898-58-3 | OC(=O)c1ccc(cc1O)NC(=O)c2ccccc2 |  | - | - | - | - |
| 156-08-1 | CN(Cc1ccccc1)[C@@H](C)Cc2ccccc2 |  | 160 | - | 4.140 | - |
| 53-89-4 | CN1CCC(CC1)N3NC(=C(Cc2ccccc2)C3=O)c4ccccc4 |  | 2700 | - | 2.930 | - |
| 100-51-6 | OCc1ccccc1 |  | 1230 | 205.3 | 1.1 | 4.29E+04 |
| 103-41-3 | O=C(OCc1ccccc1)/C=C/c2ccccc2 |  | 5530 | 350 | 4.060 | 9.270 |
| 103-50-4 | C(OCc1ccccc1)c2ccccc2 |  | 2500 | 298 | 3.31 | 40 |
| 100-46-9 | NCc1ccccc1 |  | - | 185 | 1.09 | 1.00E+06 |
| 483-49-8 | C2c4ccccc4CN3CCc1ccccc1[C@H]23 |  | - | - | 4.030 | - |
| 5638-76-6 | CNCCc1ccccn1 |  | 6110 | - | 0.68 | 1.00E+06 |
| 378-44-9 | OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@@H]3C |  | - | - | 1.94 | 66.5 |
| 83-46-5 | C[C@@H](C)[C@@H](CC)CC[C@@H](C)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C |  | - | - | 9.650 | - |
| 105-20-4 | NCCc1ccnn1 |  | - | - | -0.730 | - |
| 55-73-2 | C\N=C(\NCc1ccccc1)NC |  | - | - | 1.560 | - |
| 59170-23-9 | COc1cc(ccc1OC)CCNC[C@H](O)COc2cc(C)ccc2 |  | - | - | 3 | 184 |
| 41859-67-0 | O=C(NCCc1ccc(OC(C)(C)C(=O)O)cc1)c2ccc(Cl)cc2 |  | 1082 | - | 4.250 | - |
| 15301-48-1 | CCC(=O)N5c1ccccc1N(C4CCN(CCC(C#N)(c2ccccc2)c3ccccc3)CC4)C5=O |  | 141 | - | 4.8 | 0.092 |
| 493-75-4 | Oc1c(cc(cc1CN(CC)CC)c2cc(CC=C)c(O)c(CN(CC)CC)c2)CC=C |  | - | - | 7.050 | - |
| 103-29-7 | C(Cc1ccccc1)c2ccccc2 |  | 4518 | 284 | 4.79 | 4.3 |
| 485-49-4 | CN2CCc1cc6OCOc6cc1[C@H]2[C@@H]5OC(=O)c4c5ccc3OCOc34 |  | - | - | - | - |
| 42576-02-3 | Clc2cc(Cl)ccc2Oc1cc(C(=O)OC)c(cc1)[N+]([O-])=O |  | 6400 | - | 4.48 | 0.398 |
| 34633-34-6 | Fc1cc(ccc1O)[C@H](CC)[C@H](C)c2ccc(O)c(F)c2 |  | - | - | - | - |
| 60628-96-8 | c1cc(ccc1c2ccccc2)[C@H](c3ccccc3)n4ccnc4 |  | 1463 | - | 4.77 | 0.110 |
| 60662-16-0 | CN(C)CCN(C)n2cc(c1ccccc12)c3ccccc3 |  | 1160 | - | - | - |
| 69047-39-8 | Clc1ccc(cc1)OC(C)(C)C(=O)OC(COC(=O)c2cccnc2)COC(=O)c3cccnc3 |  | 4000 | - | - | - |
| 28434-01-7 | C/C(C)=C/[C@@H]3C(C(=C)CCC=2C=C(Cc1ccccc1)CC=2)C3(C)C |  | 1244 | - | 7.110 | 0.3 |
| 58-85-5 | O=C1N[C@H]2[C@@H](CCCCC(=O)O)SC[C@@H]2N1 |  | - | - | 0.390 | 220 |
| 514-65-8 | OC(CCN1CCCCC1)(c2ccccc2)C4CC3C=CC4C3 |  | 750 | - | 4.25 | 25.1 |
| 3572-52-9 | Oc1c(cccc1C(=O)OCCN(CC)CC)c2ccccc2 |  | - | - | 5.050 | - |
| 66722-44-9 | CC(C)NC[C@H](O)COc1ccc(cc1)COCCOC(C)C |  | - | - | 1.87 | 2240 |
| 30392-40-6 | O=C(Oc2cc(ccc2OC(=O)c1ccc(C)cc1)[C@@H](O)CNC(C)(C)C)c3ccc(C)cc3 |  | - | - | - | - |
| 4044-65-9 | S=C=N\c1ccc(cc1)\N=C=S |  | - | - | 4.670 | - |
| 1605-89-6 | C[C@@H]4CC1=CC(=O)CC[C@]1(C)[C@H]3CC[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@@H]34 |  | - | - | 4.140 | - |
| 846-48-0 | O=C3C=C4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)C=C3 |  | - | - | 3.050 | - |
| 62658-63-3 | CC(C)(C)NCC(OC(=O)c1ccccc1)COc3cccc2nc(C)cc23 |  | - | - | - | - |
| 56518-41-3 | Nc2nc(N)ncc2Cc1cc(OC)c(Br)c(OC)c1 |  | 2514 | - | 2.01 | 138 |
| 314-40-9 | CC[C@@H](C)N1C(=O)C(Br)=C(C)NC1=O |  | 641 | - | 2.11 | 815 |
| 1812-30-2 | Brc1ccc2NC(=O)CN=C(c2c1)c3ccccn3 |  | 1950 | - | 2.05 | 175 |
| 91714-94-2 | O=C(c1ccc(Br)cc1)c2cccc(CC(=O)O)c2N |  | - | - | - |  |
| 1146-98-1 | Brc1ccc(cc1)C3C(=O)c2ccccc2C3=O |  | - | - | 3.76 | 7.440 |
| 496-67-3 | CC(C)[C@@H](Br)C(=O)NC(N)=O |  | 1000 | - | 1.14 | 3520 |
| 108-86-1 | Brc1ccccc1 |  | 2383 | 156 | 2.99 | 446 |
| 118-23-0 | Brc1ccc(cc1)[C@@H](OCCN(C)C)c2ccccc2 |  | - | - | - | - |
| 75-25-2 | BrC(Br)Br |  | 933 | 149.1 | 2.4 | 3100 |
| 2104-96-3 | Clc1cc(OP(=S)(OC)OC)c(Cl)cc1Br |  | 1600 | - | 5.21 | 0.3 |
| 4093-35-0 | Nc1cc(OC)c(cc1Br)C(=O)NCCN(CC)CC |  | 545 | - | 2.83 | 25.7 |
| 10457-90-6 | Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Br)cc3 |  | 359 | - | 4.450 | 90 |
| 521-74-4 | Oc1c(Br)cc(Br)c2cccnc12 |  | - | - | 3.440 | 19.4 |
| 357-57-3 | COc1cc2c(cc1OC)N3C(=O)C[C@@H]7OCC=C6CN4CC[C@@]25C3[C@H]7[C@H]6C[C@H]45 |  | - | - | 0.98 | 3200 |
| 65002-17-7 | O=C(N[C@H](CS)C(=O)O)C(C)(C)S |  | 3900 | - | - | - |
| 362-74-3 | CCCC(=O)Nc4ncnc1c4ncn1[C@@H]3O[C@H]2COP(=O)(O)O[C@H]2[C@H]3OC(=O)CCC |  | - | - | 0.450 | - |
| 82-95-1 | CC(C)(C)c1ccc(cc1)CN2CCN(CC2)[C@@H](c3ccc(Cl)cc3)c4ccccc4 |  | - | - | - | - |
| 841-73-6 | O=C2N(C1CCCCC1)C(=O)NC(=O)[C@H]2CCCC |  | 1115 | - | 3.120 | - |
| 58409-59-9 | CC(C)(C)NC[C@@H](O)COc1ccc(C)c2C=CC(=O)Oc12 |  | - | - | - | - |
| 51333-22-3 | OCC(=O)[C@@]45O[C@@H](O[C@H]5C[C@@H]3[C@@H]2CCC1=CC(=O)C=C[C@]1(C)[C@H]2[C@@H](O)C[C@@]34C)CCC |  | 3200 | - | 2.180 | - |
| 57982-78-2 | CC(C)(C)N1CCC(CC1)(c2ccccc2)c3ccccc3 |  | 165 | - | 5.100 | - |
| 36798-79-5 | C\C(C)=CC(\C)=N\N=C1/NN=Cc2ccccc12 |  | 620 | - | - | - |
| 22103-14-6 | Ic1cc(cc(I)c1O)[C@@H](O)[C@@H](C)N[C@H](C)CCc2ccccc2 |  | - | - | 5.640 | - |
| 53684-49-4 | CC(C)(C)NC[C@@H](O)COc2ccccc2OC[C@@H]1CCCO1 |  | - | - | - | - |
| 54340-62-4 | CC(C)(C)NC[C@@H](O)c1cc2cccc(CC)c2o1 |  | - | - | 3.5 | 214 |
| 3748-77-4 | CCCCN(CCCC)C(=N)c1ccc(OCCCCCC)c2ccccc12 |  | - | - | - | - |
| 41483-43-6 | CCNc1nc(C)c(CCCC)c(OS(=O)(=O)N(C)C)n1 |  | 4000 | - | 2.7 | 22 |
| 38396-39-3 | Cc2cccc(C)c2NC(=O)[C@H]1CCCCN1CCCC |  | - | - | - | - |
| 14556-46-8 | Clc1ccc(C)cc1OC[C@H](O)CNC(C)(C)C |  | - | - | 2.97 | 739 |
| 52485-79-7 | CC(C)(C)[C@@](C)(O)[C@H]1C[C@]74CC[C@]1(OC)[C@@H]5Oc3c(O)ccc2C[C@H]7N(CC[C@@]45c23)CC6CC6 |  | - | - | 4.98 | 0.636 |
| 4663-83-6 | O=C(NCc1ccccc1)OCCO |  | - | - | - | - |
| 36505-84-7 | O=C4CC1(CCCC1)CC(=O)N4CCCCN2CCN(CC2)c3ncccn3 |  | - | - | 2.63 | 21.4 |
| 149-16-6 | Nc1ccc(cc1)C(=O)OCCCN(CCCC)CCCC |  | - | - | 4.440 | - |
| 23184-66-9 | ClCC(=O)N(COCCCC)c1c(cccc1CC)CC |  | 1740 | - | 4.5 | 23 |
| 22131-35-7 | CCCCN(CCCC)CCNc1nc(no1)c2ccccc2 |  | - | - | 4.380 | - |
| 54400-59-8 | CC(C)C(=O)Nc1cccc(c1)[C@H]2N=C3SCCN3C2 |  | - | - | - | - |
| 3785-21-5 | Clc1cccc(C)c1NC(=O)CNCCCC |  | - | - | 2.040 | - |
| 653-03-2 | CCCC(=O)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 |  | 413 | - | 4.810 | 0.165 |
| 55837-14-4 | O=C(C[C@H](c1ccccc1)N2CCCCC2)OCCCC |  | - | - | - | - |
| 2090-89-3 | Nc1ccc(cc1)C(=O)OCCNCC(C)C |  | - | - | 2.190 | - |
| 2043-38-1 | NS(=O)(=O)c2cc1c(N[C@H](NS1(=O)=O)CC(C)C)cc2Cl |  | - | - | 1.200 | - |
| 55837-18-8 | CC[C@H](C(=O)O)c1ccc(cc1)CC(C)C |  | 1600 | - | 4.280 | - |
| 64872-76-0 | Clc1ccc(cc1)CC[C@@H](Sc2c(Cl)cccc2Cl)Cn3ccnc3 |  | - | - | - | - |
| 58930-32-8 | CC(C)(C)NC[C@@H](O)COc1ccc(F)cc1C(=O)CCC |  | - | - | - | - |
| 42408-82-2 | Oc3ccc4C[C@H]1N(CC[C@@]2(CCCC[C@]12O)c4c3)CC5CCC5 |  | - | - | 3.680 | - |
| 33629-47-9 | [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N[C@H](C)CC)C(C)(C)C |  | 2500 | - | 4.93 | 1 |
| 35941-65-2 | CN(C)CC(C)CC2c3ccccc3CCc1ccccc12 |  | - | - | - | - |
| 123-72-8 | CCCC=O |  | 2490 | 74.8 | 0.88 | 7.10E+04 |
| 109-74-0 | CCCC#N |  | 50 | 117.6 | 0.53 | 3.30E+04 |
| 64241-34-5 | O=C(OCC)NNc1ccc(nn1)N(C[C@@H](C)O)CC |  | 2060 | - | - | - |
| 58-08-2 | O=C2c1n(C)cnc1N(C)C(=O)N2C |  | 192 | - | -0.07 | 2.16E+04 |
| 63283-36-3 | O.C=C3CC[C@H](O)C/C3=C\C=C1/CCC[C@]2(C)[C@H](CC[C@@H]12)[C@H](C)CCCC(C)(C)O |  | - | - | - | - |
| 32222-06-3 | C=C1C(\C[C@@H](O)CC1O)=C\C=C3\CCC[C@@]2(C)C3CC[C@@H]2C(C)CCCC(C)(C)O |  | 0.62 | - | 7.600 | - |
| 36104-80-0 | CN(C)C(=O)OC2N=C(c1cc(Cl)ccc1N(C)C2=O)c3ccccc3 |  | 4000 | - | 2.660 | - |
| 26097-80-3 | CC(C)OC(=O)Nc1ccc2nc(nc2c1)c3cscn3 |  | - | - | 2.670 | - |
| 59721-28-7 | O=C(Oc1ccc(cc1)CC(=O)OCC(=O)N(C)C)c2ccc(NC(=N)N)cc2 |  | - | - | - | - |
| 76-22-2 | CC2(C)[C@@H]1CC(=O)[C@]2(C)CC1 |  | - | 204 | 2.38 | 1600 |
| 7689-03-4 | CC[C@]1(O)C=2C=C3c4nc5ccccc5cc4CN3C(=O)C=2COC1=O |  | 153 | - | 1.74 | 207 |
| 5579-13-5 | NC(=O)NC(=O)[C@H](CC)[C@H](C)CC |  | - | - | - | - |
| 298-46-4 | NC(=O)N2c3ccccc3C=Cc1ccccc12 |  | 1957 | - | 2.45 | 17.7 |
| 86-74-8 | c1cccc2nc3ccccc3c12 |  | - | 354.7 | 3.72 | 1.8 |
| 10605-21-7 | O=C(OC)Nc1nc2ccccc2n1 |  | 6400 | - | 1.52 | 29 |
| 77-23-6 | CCN(CC)CCOCCOC(=O)C1(CCCC1)c2ccccc2 |  | 150 | - | 4.150 | - |
| 486-16-8 | Clc1ccc(cc1)[C@@H](OCCN(C)C)c2ccccn2 |  | - | - | 2.560 | - |
| 15687-16-8 | CN(CCc1ccccc1)CCN(C)C(=O)C(OCC)(c2ccccc2)c3ccccc3 |  | - | - | 4.710 | - |
| 541-79-7 | O[C@@H](NC(=O)OCC)C(Cl)(Cl)Cl |  | - | - | 1.84 | 753 |
| 638-23-3 | OC(=O)[C@@H](N)CSCC(O)=O |  | 15000 | - | -4.240 | - |
| 1563-66-2 | CNC(=O)Oc1cccc2CC(C)(C)Oc12 |  | 5 | - | 2.32 | 320 |
| 35700-23-3 | O[C@H]1C[C@@H](O)[C@H](/C=C/[C@@](C)(O)CCCCC)[C@H]1C\C=C/CCCC(=O)O |  | - | - | - | - |
| 24279-91-2 | NC(=O)OC[C@@H](OC)C=1C(=O)C(=C(C)C(=O)C=1N2CC2)N3CC3 |  | 27.3 | - | -0.15 | 6160 |
| 960-05-4 | O=C1NC(=O)NC(=O)C1(CCOC(N)=O)CCCC |  | - | - | - | - |
| 339-43-5 | Nc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC |  | 4400 | - | 1.01 | 535 |
| 34866-47-2 | Oc1ccc(cc1NC(N)=O)[C@H](O)CNC(C)(C)C |  | - | - | - | - |
| 1260-17-9 | O[C@H]1[C@H](O)[C@@H](O)[C@H](O[C@@H]1CO)c4c(O)c3C(=O)c2c(C)c(C(=O)O)c(O)cc2C(=O)c3c(O)c4O |  | - | - | 0.970 | 1300 |
| 61422-45-5 | O=C1NC(=O)C(F)=CN1C(=O)NCCCCCC |  | 268 | - | 2.63 | 122 |
| 23465-76-1 | COc1ccc(cc1)CC3=Nc2ccccc2N(CCN(CC)CC)C3=O |  | - | - | - | - |
| 2622-30-2 | CCC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2 |  | - | - | 3.340 | - |
| 5942-95-0 | NC(=O)C4(CCN(CCCN2c3ccccc3CCc1ccccc12)CC4)N5CCCCC5 |  | 1025 | - | 5.230 | - |
| 53716-49-7 | O=C(O)C(C)c1ccc2c3cc(Cl)ccc3nc2c1 |  | 74 | - | 3.790 | - |
| 2037-95-8 | O=C2NC(=O)Oc1ccccc12 |  | 750 | - | - | - |
| 72956-09-3 | COc4ccccc4OCCNC[C@@H](O)COc2cccc3nc1ccccc1c23 |  | - | - | 4.19 | 0.583 |
| 138-41-0 | O=S(N)(=O)c1ccc(cc1)C(=O)O |  | - | - | 0.5 | 1.61E+04 |
| 79831-76-8 | O[C@H]2CCN1C[C@H](O)[C@H](O)[C@H](O)[C@H]12 |  | - | - | - | - |
| 5265-18-9 | O=C(c1ccccc1)[C@H](C)N |  | - | - | - | - |
| 53994-73-3 | ClC=3CS[C@H]2N(C(=O)[C@@H]2NC(=O)[C@H](N)c1ccccc1)C=3C(=O)O |  | 20000 | - | 0.350 | 1.00E+04 |
| 34444-01-4 | O[C@H](c1ccccc1)C(=O)N[C@H]4C(=O)N3C(=C(CSc2nnnn2C)CS[C@@H]34)C(=O)O |  | - | - | 0.5 | 465 |
| 51627-14-6 | Oc1ccc(cc1)[C@@H](N)C(=O)N[C@H]4C(=O)N3C(=C(CSc2cnnn2)CS[C@@H]34)C(=O)O |  | - | - | -1.210 | - |
| 56187-47-4 | ClC1=CN(C=C(Cl)C1=O)CC(=O)N[C@@H]4C(=O)N3C(=C(CSc2nnc(C)s2)CS[C@@H]34)C(=O)O |  | - | - | - | - |
| 25953-19-9 | O=C(O)C=3N4C(=O)[C@@H](NC(=O)Cn1cnnn1)[C@H]4SCC=3CSc2nnc(C)s2 |  | - | - | -0.58 | 214 |
| 79350-37-1 | Nc1scc(n1)/C(=N\OCC(=O)O)C(=O)N[C@@H]3C(=O)N2C(=C(C=C)CS[C@@H]23)C(=O)O |  | 10000 | - | 0.120 | - |
| 75481-73-1 | O=C(O)[C@H](N)CSCC(=O)N[C@]3(OC)C(=O)N2C(=C(CSc1nnnn1C)CS[C@@H]23)C(=O)O |  | - | - | - | - |
| 63527-52-6 | Nc1scc(n1)\C(=N\OC)C(=O)N[C@@H]3C(=O)N2C(=C(COC(C)=O)CS[C@H]23)C(=O)O |  | - | - | 0.640 | - |
| 35607-66-0 | O=C(O)C=2N3C(=O)[C@](NC(=O)Cc1cccs1)(OC)[C@H]3SCC=2COC(N)=O |  | 10000 | 149.5 dec | -0.02 | 105 |
| 70797-11-4 | Oc1cc(C)ncc1C(=O)N[C@H](c2ccc(O)cc2)C(=O)N[C@@H]5C(=O)N4C(=C(CSc3nnnn3C)CS[C@@H]45)C(=O)O |  | - | - | - | - |
| 51762-05-1 | N[C@H](C1C=CCC=C1)C(=O)N[C@@H]3C(=O)N2C(=C(OC)CS[C@@H]23)C(=O)O |  | 22500 | - | -0.980 | - |
| 82547-58-8 | Nc1scc(n1)\C(=N\OC)C(=O)N[C@H]4C(=O)N3C(=C(Cn2nc(C)nn2)CS[C@@H]34)C(=O)O |  | - | - | - | - |
| 68401-81-0 | Nc1scc(n1)\C(=N\OC)C(=O)N[C@H]3C(=O)N2C(=CCS[C@@H]23)C(=O)O |  | - | - | - | - |
| 73384-59-5 | Nc1scc(n1)\C(=N\OC)C(=O)N[C@@H]4C(=O)N3C(=C(CSC2=NC(=O)C(O)=NN2C)CS[C@@H]34)C(=O)O |  | - | - | - | - |
| 55268-75-2 | CO\N=C(\c1ccco1)C(=O)N[C@H]3C(=O)N2C(=C(COC(N)=O)CS[C@@H]23)C(=O)O |  | 10000 | - | -0.16 | 145 |
| 153-61-7 | O=C(O)C=2N3C(=O)[C@@H](NC(=O)Cc1cccs1)[C@H]3SCC=2COC(C)=O |  | - | - | 0.0 | 158 |
| 38821-53-3 | CC=3CS[C@H]2N(C(=O)[C@@H]2NC(=O)[C@H](N)C1=CCC=CC1)C=3C(=O)O |  | 12000 | - | 0.410 | 2.13E+04 |
| 14176-10-4 | O=C(OCCN1CCCCCC1)[C@@H](C2CCCCC2)c3ccsc3 |  | - | - | 6.140 | - |
| 83881-51-0 | O=C(O)COCCN1CCN(CC1)[C@@H](c2ccc(Cl)cc2)c3ccccc3 |  | - | - | -0.610 | - |
| 34675-84-8 | NC[C@@H]1CC[C@H](CC1)C(=O)Oc2ccc(CCC(=O)O)cc2 |  | - | - | - | - |
| 103-47-9 | O=S(=O)(O)CCNC1CCCCC1 |  | - | - | -0.630 | - |
| 791-35-5 | O[C@](CCN(C)C)(c1ccccc1Cl)c2ccccc2 |  | - | - | 3.500 | - |
| 133-90-4 | Clc1cc(C(=O)O)c(Cl)c(N)c1 |  | 3500 | 312 | 1.900 | 700 |
| 305-03-3 | O=C(O)CCCc1ccc(cc1)N(CCCl)CCCl |  | 76 | - | 1.7 | 1.24E+04 |
| 56-75-7 | O=[N+]([O-])c1ccc(cc1)[C@@H](O)[C@@H](CO)NC(=O)C(Cl)Cl |  | 2500 | - | 1.14 | 2500 |
| 522-18-9 | Cc4ccccc4CN3CCN(CCO[C@@H](c1ccccc1)c2ccccc2Cl)CC3 |  | - | - | - | - |
| 97-27-8 | Clc1cc(Cl)ccc1CN(CCO)C(=O)C(Cl)Cl |  | - | - | - | - |
| 82-93-9 | Clc1ccc(cc1)[C@H](c2ccccc2)N3CCN(C)CC3 |  | - | - | - | - |
| 5588-20-5 | O=C1N[C@@H](C(=O)N1SC(Cl)(Cl)Cl)[C@H](CC)CCCC |  | 1165 | - | 3.690 | - |
| 58-25-3 | Clc1ccc2N=C(C[N+]([O-])=C(c2c1)c3ccccc3)NC |  | 392 | - | 2.44 | 2000 |
| 6164-98-3 | Clc1cc(C)c(/N=C/N(C)C)cc1 |  | 160 | - | 2.89 | 270 |
| 85-34-7 | Clc1c(CC(=O)O)c(Cl)ccc1Cl |  | 1780 | - | 3.2 | 200 |
| 3563-58-4 | ClC(Cl)(Cl)[C@H](O)O[C@H](C)CC(O)(C)C |  | - | - | 1.590 | - |
| 145-94-8 | Oc1ccc(Cl)c2CCCc12 |  | - | - | 3.630 | - |
| 80-77-3 | O=C1CCS(=O)(=O)C(N1C)c2ccc(Cl)cc2 |  | 605 | - | -0.260 | 2500 |
| 3689-76-7 | Clc1ccc(cc1)Cn2c3ccccc3nc2C |  | - | - | 4.680 | - |
| 78-95-5 | CC(=O)CCl |  | 100 | 119 | 0.020 | 9.00E+04 |
| 502-98-7 | Cl\N=C(\N)/N=NC(\N)=N\Cl |  | - | - | -0.470 | - |
| 108-90-7 | Clc1ccccc1 |  | 1110 | 131.7 | 2.84 | 498 |
| 510-15-6 | OC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)C(=O)OCC |  | 700 | - | 4.74 | 13 |
| 57-15-8 | ClC(Cl)(Cl)C(C)(C)O |  | - | 167 | 2.03 | 8000 |
| 67-66-3 | ClC(Cl)Cl |  | 695 | 61.1 | 1.97 | 7950 |
| 76-06-2 | ClC(Cl)(Cl)[N+]([O-])=O |  | 250 | 112 | 2.09 | 1620 |
| 59-32-5 | Clc1ccc(cc1)CN(CCN(C)C)c2ccccn2 |  | 920 | - | 3.370 | - |
| 148-65-2 | Clc2ccc(CN(CCN(C)C)c1ccccn1)s2 |  | - | - | 3.190 | 2010 |
| 58-94-6 | NS(=O)(=O)c2cc1c(N=CNS1(=O)=O)cc2Cl |  | 10000 | - | -0.24 | 266 |
| 54749-90-5 | O[C@H]1O[C@H](CO)[C@@H](O)[C@@H](O)[C@H]1NC(=O)N(CCCl)N=O |  | - | - | -1.02E+00 | 1830 |
| 104-29-0 | Clc1ccc(OCC(O)CO)cc1 |  | - | - | 1.500 | 1.00E+04 |
| 77-38-3 | Clc1ccc(cc1)[C@](C)(OCCN(C)C)c2ccccc2 |  | - | - | 4.200 | - |
| 461-78-9 | Clc1ccc(CC(C)(C)N)cc1 |  | 250 | - | 2.6 | 3240 |
| 50-53-3 | CN(C)CCCN1c3ccccc3Sc2ccc(Cl)cc12 |  | 142 | - | 5.41 | 2.55 |
| 113-59-7 | CN(C)CC\C=C1\c3ccccc3Sc2ccc(Cl)cc12 |  | 200 | - | 5.18 | 0.295 |
| 72-80-0 | Oc1c(Cl)cc(Cl)c2ccc(C)nc12 |  | 660 | - | 3.500 | - |
| 57-62-5 | NC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@@]2(O)C1=O)C(=O)c3c(O)ccc(Cl)c3[C@@]4(C)O |  | - | - | -0.62 | 630 |
| 57-88-5 | CC(C)CCC[C@@H](C)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C |  | - | 360 | 8.740 | 0.095 |
| 218-01-9 | c1cc4ccccc4c2ccc3ccccc3c12 |  | - | 448 | 5.81 | 0.002 |
| 481-74-3 | Oc3cccc2C(=O)c1cc(C)cc(O)c1C(=O)c23 |  | - | - | 4.490 | - |
| 53449-58-4 | C[C@@H]2C[C@H](OC(=O)c1cccnc1)CC(C)(C)C2 |  | - | - | 4.200 | - |
| 82009-34-5 | O=C(N/C(=C\CCCCSC[C@H](N)C(=O)O)C(=O)O)[C@H]1CC1(C)C |  | - | - | - | - |
| 92077-78-6 | O.O=C(OCC)[C@H](CCc1ccccc1)N[C@H]2CCCN3CCC[C@H](N3C2=O)C(=O)O |  | 5000 | - | - | - |
| 73963-72-1 | O=C1CCc2cc(ccc2N1)OCCCCc4nnnn4C3CCCCC3 |  | 5000 | - | 4.040 | - |
| 54239-37-1 | N#Cc1cc(ccc1N)[C@@H](O)CNC(C)C |  | - | - | - | - |
| 51481-61-9 | N#C\N=C(/NC)NCCSCc1ncnc1C |  | 5000 | - | 0.4 | 9380 |
| 118-10-5 | O[C@H](C2CC1CCN2C[C@@H]1C=C)c4ccnc3ccccc34 |  | - | - | 2.68 | 240 |
| 132-60-5 | O=C(O)c1cc(nc2ccccc12)c3ccccc3 |  | - | - | 3.790 | 160 |
| 66564-14-5 | [O-][N+](=O)c1cc(c(OCC)cc1N)C(=O)NC3CCN(C[C@@H]2CCC=CC2)CC3 |  | - | - | - | - |
| 90-86-8 | O[C@@H](c1ccccc1)[C@H](C)N(C)C/C=C/c2ccccc2 |  | - | - | 3.370 | - |
| 104-54-1 | OC\C=C\c1ccccc1 |  | 2000 | 250 | 1.95 | 6190 |
| 298-57-7 | c1ccccc1C(c2ccccc2)N3CCN(CC3)C/C=C/c4ccccc4 |  | 6500 | - | 5.77 | 750 |
| 253-66-7 | c1cnnc2ccccc12 |  | - | - | 0.93 | 1.48E+04 |
| 28657-80-9 | O=C(O)C2=NN(CC)c1cc3OCOc3cc1C2=O |  | 3610 | - | 1.590 | - |
| 104-28-9 | COc1ccc(/C=C/C(=O)OCCOCC)cc1 |  | - | - | 2.650 | 500 |
| 58473-74-8 | Brc1cc(/C=C/C(=O)NCC)ccc1 |  | 4437 | - | - | - |
| 52214-84-3 | ClC2(Cl)C[C@@H]2c1ccc(OC(C)(C)C(=O)O)cc1 |  | - | - | 3.940 | - |
| 85721-33-1 | O=C(O)C2=CN(c1cc(c(F)cc1C2=O)N3CCNCC3)C4CC4 |  | 2000 | - | 0.28 | 3.00E+04 |
| 81098-60-4 | Clc1cc(c(OC)cc1N)C(=O)N[C@H]3CCN(CCCOc2ccc(F)cc2)C[C@H]3OC |  | 4166 | - | 3.090 | 2.710 |
| 1195-16-0 | O=C1SCC[C@H]1NC(=O)C |  | - | - | -0.35 | 1.37E+05 |
| 372-75-8 | N[C@@H](CCCNC(N)=O)C(=O)O |  | - | - | -3.19E+00 | 1.28E+04 |
| 30544-61-7 | O=C(c1ccc(Cl)cc1)N(CCCC(=O)O)c2ccc(OC)cc2 |  | 2000 | - | 2.7 | 31.6 |
| 55905-53-8 | Clc1cc(c(OC)cc1N)C(=O)NC3CCN(Cc2ccccc2)CC3 |  | - | - | 3.58 | 3.890 |
| 15686-51-8 | CN3CCC[C@@H]3CCO[C@](C)(c1ccccc1)c2ccc(Cl)cc2 |  | - | - | - | - |
| 442-52-4 | Clc1ccc(cc1)Cn3c4ccccc4nc3CN2CCCC2 |  | - | - | 4.400 | - |
| 37148-27-9 | Clc1cc(cc(Cl)c1N)C(O)CNC(C)(C)C |  | - | - | 2.000 | - |
| 18323-44-9 | O[C@@H]1[C@@H](O)[C@@H](O)[C@H](O[C@@H]1SC)C(NC(=O)[C@@H]2C[C@@H](CCC)CN2C)[C@H](C)Cl |  | - | - | 2.16 | 30.6 |
| 30299-08-2 | O=C(O)[C@@](C)(CC)Oc1ccc(cc1)C2(CCCCC2)c3ccc(O[C@@](C)(CC)C(=O)O)cc3 |  | 4000 | - | - | - |
| 14437-41-3 | Clc2ccc(NC(=O)c1cc(I)cc(I)c1OC(C)=O)cc2 |  | 5000 | - | 5.280 | - |
| 1159-93-9 | CN(C)CCN2c3ccc(Cl)cc3Nc1ccccc1C2=O |  | - | - | 3.73 | 0.502 |
| 13364-32-4 | Clc2ccccc2CN[C@H](C)Cc1ccccc1 |  | - | - | 4.570 | - |
| 5627-46-3 | CN4[C@H]1CC[C@H]4CC(C1)O[C@H](c2ccccc2)c3ccc(Cl)cc3 |  | - | - | - | - |
| 25122-41-2 | ClCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@@H]3C |  | - | - | 2.48 | 20 |
| 54063-32-0 | ClCC(=O)[C@]2(O)[C@@]3(C)CC(=O)[C@]1(F)[C@]4(C)C=CC(=O)C=C4CC[C@H]1[C@@H]3C[C@@H]2C |  | - | - | 2.61 | 51.5 |
| 22494-47-9 | Clc1ccc(cc1)c2ccc(COC(C)(C)C(=O)O)cc2 |  | - | - | 4.310 | - |
| 298-55-5 | Clc1ccc(cc1)[C@@H](c2ccccc2)N3CCN(CC3)C/C=C/c4ccccc4 |  | - | - | - | - |
| 4828-27-7 | OCC(=O)[C@@H]3[C@@]4(C)C[C@H](O)[C@@]2(Cl)C(C[C@H](F)C1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C |  | - | - | 2.270 | - |
| 2030-63-9 | Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5 |  | 8400 | - | 7.66 | 0.225 |
| 671-95-4 | O=S(N)(=O)c1cc(ccc1Cl)S(N)(=O)=O |  | 340 | - | 0.410 | - |
| 369-77-7 | FC(F)(F)c1cc(ccc1Cl)NC(=O)Nc2ccc(Cl)cc2 |  | - | - | 5.220 | - |
| 37693-01-9 | Clc2cc(Cl)ccc2Cc1cc(ccc1O)C(C)(C)CC(C)(C)C |  | 4000 | - | 8.590 | - |
| 14261-75-7 | Clc1ccc(CC(C)(C)NC(=O)OCC)cc1 |  | - | - | 4.160 | - |
| 5310-55-4 | CN(C)CCC[C@@H]2c3ccccc3Nc1ccc(Cl)cc12 |  | 379 | - | - | - |
| 25803-14-9 | Clc1ccc(cc1)C(=O)c3c2ccc(cc2n(CC(=O)O)c3C)OC |  | - | - | 3.530 | - |
| 533-45-9 | ClCCc1scnc1C |  | - | - | 2.12 | 1040 |
| 1926-49-4 | OC(=O)[C@H]2N3C(=O)[C@@H](NC(=O)[C@H](OC)c1ccc(Cl)c(Cl)c1)[C@H]3SC2(C)C |  | - | - | 2.860 | - |
| 911-45-5 | CCN(CCOc1ccc(cc1)/C(c2ccccc2)=C(/Cl)c3ccccc3)CC |  | 5750 | - | 6.740 | - |
| 1181-54-0 | OCNC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@@]2(O)C1=O)C(=O)c3c(O)ccc(Cl)c3[C@]4(C)O |  | - | - | -1.540 | - |
| 1622-61-3 | [O-][N+](=O)c1ccc2NC(=O)CN=C(c2c1)c3ccccc3Cl |  | 15000 | - | 2.41 | 100 |
| 4205-90-7 | Clc2cccc(Cl)c2NC1=NCCN1 |  | 67.3 | - | 1.59 | 1.36E+04 |
| 3861-76-5 | [O-][N+](=O)c2cc3nc(Cc1ccc(Cl)cc1)n(CCN(CC)CC)c3cc2 |  | - | - | 5.180 | - |
| 636-54-4 | O=C(NN1[C@@H](C)CCC[C@H]1C)c2ccc(Cl)c(c2)S(N)(=O)=O |  | - | - | 1.870 | - |
| 3703-76-2 | Clc1ccc(cc1)[C@H](OCCN2CCCCC2)c3ccccc3 |  | - | - | 5.110 | - |
| 113665-84-2 | Clc1ccccc1[C@H](N2CCc3sccc3C2)C(=O)OC |  | - | - | - | - |
| 2971-90-6 | Oc1c(Cl)c(C)nc(C)c1Cl |  | 18000 | - | 2.710 | 10 |
| 5251-34-3 | OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3C=C(Cl)C1=CC(=O)C=C[C@@]12C |  | - | - | 1.680 | - |
| 40665-92-7 | O[C@H]2C[C@@H](O)[C@H](/C=C/[C@@H](O)COc1cccc(Cl)c1)[C@H]2C\C=C/CCCC(=O)O |  | - | - | 3.950 | - |
| 68206-94-0 | O=C(OCC)COc2ccc1c(OC(=O)C(CCN(CC)CC)=C1C)c2Cl |  | 1250 | - | - | - |
| 120-32-1 | Oc2ccc(Cl)cc2Cc1ccccc1 |  | 1700 | - | 4.180 | 149 |
| 3811-25-4 | O[C@H](CNC(C)C)c1ccccc1Cl |  | - | - | 1.820 | - |
| 10389-73-8 | Clc1ccccc1CC(C)(C)N |  | - | - | 2.850 | - |
| 57808-65-8 | Clc2cc(NC(=O)c1cc(I)cc(I)c1O)c(C)cc2[C@H](C#N)c3ccc(Cl)cc3 |  | 262 | - | 8.110 | - |
| 1093-58-9 | ClC=4C(=O)CC[C@]3(C)C=4CC[C@@H]2[C@H]3CC[C@]1(C)[C@H]2CC[C@@H]1O |  | - | - | 3.760 | - |
| 2058-52-8 | CN1CCN(CC1)C3=Nc4ccccc4Sc2ccc(Cl)cc23 |  | 280 | - | 3.840 | - |
| 33671-46-4 | Clc3ccccc3C1=NCC(=O)N(C)c2sc(cc12)CC |  | 1461 | - | 3.18 | 18.3 |
| 23593-75-1 | Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4 |  | 708 | - | 6.260 | - |
| 61-72-3 | OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1ccccc1Cl)[C@H]4SC3(C)C |  | - | - | 2.48 | 13.9 |
| 24166-13-0 | Clc1ccccc1C34OCCN4CC(=O)Nc2ccc(Cl)cc23 |  | 1780 | - | 3.910 | - |
| 53608-96-1 | ClC(Cl)(Cl)[C@@H](O)O[C@H]3CC[C@@H]2[C@@H]4CCC1=CC(=O)CC[C@]1(C)[C@H]4CC[C@]23C |  | - | - | - | - |
| 5786-21-0 | CN1CCN(CC1)C2=Nc4cc(Cl)ccc4Nc3ccccc23 |  | 251 | - | 3.23 | 11.8 |
| 76-57-3 | COc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 |  | 427 | - | 1.19 | 9000 |
| 477-27-0 | CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(O)C(=O)C=C12 |  | - | - | 1.2 | 6000 |
| 64-86-8 | CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12 |  | - | - | 1.3 | 4.50E+04 |
| 66575-29-9 | CC(=O)O[C@H]2[C@@H](O)[C@@H]1[C@](C)([C@@H](O)CCC1(C)C)[C@@]3(O)C(=O)C[C@](C)(C=C)O[C@]23C |  | 2550 | - | - | - |
| 546-06-5 | CN(C)[C@H]4CC5=CC[C@@H]1[C@@H](CC[C@@]23CN(C)[C@H](C)[C@@H]3CC[C@H]12)[C@]5(C)CC4 |  | - | - | 5.140 | - |
| 458-35-5 | Oc1ccc(cc1OC)/C=C\CO |  | - | - | 1.190 | 1.65E+04 |
| 50-22-6 | OCC(=O)[C@H]4CC[C@@H]2[C@]4(C)C[C@H](O)[C@@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 |  | - | - | 1.94 | 199 |
| 1110-40-3 | CC(=O)OCC(=O)[C@@]3(O)[C@H](C)C[C@H]2[C@@H]4C=C(C)C1=Cc6c(C[C@]1(C)[C@H]4[C@@H](O)C[C@@]23C)cnn6c5ccccc5 |  | - | - | 5.480 | - |
| 483-10-3 | O=C(OC)[C@@H]2[C@@H](O)CC[C@@H]3CN4CCc1c5ccccc5nc1[C@H]4C[C@H]23 |  | - | - | 2.110 | - |
| 486-56-6 | CN2C(=O)CC[C@H]2c1cnccc1 |  | - | - | 0.07 | 9.99E+05 |
| 56-72-4 | CCOP(=S)(OCC)Oc1ccc2c(c1)OC(=O)C(Cl)=C2C |  | 13 | - | 4.13 | 1.5 |
| 91-64-5 | O=C1C=Cc2ccccc2O1 |  | 293 | 301.7 | 1.39 | 1900 |
| 4366-18-1 | OC=1c4ccccc4OC(=O)C=1C(COC)C2=C(O)c3ccccc3OC2=O |  | - | - | 1.38 | 268 |
| 60-27-5 | N=C1NC(=O)CN1C |  | - | - | -1.76E+00 | 8.01E+04 |
| 483-63-6 | CCN(C(=O)\C=C\C)c1ccccc1C |  | 1500 | - | 2.730 | - |
| 458-37-7 | Oc1ccc(cc1OC)/C=C/C(=O)CC(=O)/C=C/c2ccc(O)c(OC)c2 |  | - | - | 3.290 | - |
| 21725-46-2 | Clc1nc(NCC)nc(NC(C)(C)C#N)n1 |  | 149 | - | 2.22 | 170 |
| 460-19-5 | N#CC#N |  | - | -2.11E+01 | 0.07 | 1.51E+05 |
| 456-59-7 | O=C(O[C@H]1C[C@@H](C)CC(C)(C)C1)[C@H](O)c2ccccc2 |  | 5000 | - | 4.100 | - |
| 3572-80-3 | Oc1ccc2C[C@@H]3N(CC[C@](C)(c2c1)[C@@H]3C)CC4CC4 |  | - | - | 4.510 | - |
| 15301-52-7 | O=C3CCCC3(CCN1CCOCC1)C2=CCCC2 |  | - | - | - | - |
| 82-92-8 | CN1CCN(CC1)C(c2ccccc2)c3ccccc3 |  | - | - | 2.970 | 1000 |
| 52-31-3 | O=C1NC(=O)NC(=O)C1(CC)C2=CCCCC2 |  | - | - | 1.77 | 1600 |
| 31431-43-3 | O=C(OC)Nc1nc2cc(ccc2n1)C(=O)C3CC3 |  | - | - | 2.030 | - |
| 303-53-7 | CN(C)CC\C=C2/c3ccccc3C=Cc1ccccc12 |  | - | - | 4.790 | - |
| 512-16-3 | OC1(CCCCC1)[C@H](CC)C(=O)O |  | 4820 | - | 2.250 | - |
| 516-21-2 | Clc1ccc(cc1)N2C(N)=NC(N)=NC2(C)C |  | - | - | 0.960 | - |
| 108-93-0 | OC1CCCCC1 |  | 1400 | 160.8 | 1.23 | 4.20E+04 |
| 108-94-1 | O=C1CCCCC1 |  | 1.62mL/kg | 155.4 | 0.81 | 2.50E+04 |
| 110-83-8 | C1C=CCCC1 |  | 2.4mL/kg | 82.9 | 2.86 | 213 |
| 139-62-8 | C[C@@H]3CCCCN3CCCOC(=O)c2ccc(OC1CCCCC1)cc2 |  | - | - | 6.150 | - |
| 120-92-3 | O=C1CCCC1 |  | - | 130.5 | 0.630 | 9180 |
| 512-15-2 | OC1(CCCC1)[C@H](C(=O)OCCN(C)C)c2ccccc2 |  | - | - | 2.470 | - |
| 75-19-4 | C1CC1 |  | - | -3.28E+01 | 1.72 | 381 |
| 68-41-7 | N[C@@H]1CONC1=O |  | 5000 | - | -1.720 | - |
| 2259-96-3 | NS(=O)(=O)c4cc1c(N[C@H](NS1(=O)=O)[C@@H]3C[C@H]2C=C[C@H]3C2)cc4Cl |  | 5000 | - | 1.95 | 2.510 |
| 579-23-7 | Oc1ccc(cc1OC)/C=C3\CCC\C(=C\c2cc(OC)c(O)cc2)C3=O |  | - | - | 4.180 | - |
| 7199-29-3 | NC(=O)C2c3ccccc3CCc1ccccc12 |  | 2400 | - | 3.160 | - |
| 4406-22-8 | CC(C)(O)[C@@H]1C[C@]74C=C[C@@]1(OC)[C@H]5Oc3c(O)ccc2C[C@@H]7N(CC[C@]45c23)CC6CC6 |  | - | - | - | - |
| 52-90-4 | O=C(O)[C@@H](N)CS |  | 1890 | - | -2.49E+00 | 2.77E+05 |
| 485-35-8 | O=C3C=CC=C2N3C[C@H]1C[C@H]2CNC1 |  | - | - | 0.600 | 4.39E+05 |
| 71-30-7 | NC=1C=CNC(=O)N=1 |  | - | - | -1.73E+00 | 8000 |
| 486-66-8 | Oc1ccc(cc1)C3=COc2cc(O)ccc2C3=O |  | - | - | 2.550 | - |
| 75-99-0 | CC(Cl)(Cl)C(=O)O |  | - | 187.5 | 0.78 | 5.02E+05 |
| 79094-20-5 | O=S(=O)(NCCc1ccc(CC(=O)O)cc1)c2ccc(Cl)cc2 |  | - | - | - | - |
| 17230-88-5 | C#C[C@]3(O)CC[C@H]2[C@@H]4CCC1=Cc5oncc5C[C@]1(C)[C@H]4CC[C@]23C |  | 17000 | - | 4.210 | - |
| 605-65-2 | CN(C)c2cccc1c2cccc1S(Cl)(=O)=O |  | - | - | 4.290 | - |
| 72822-12-9 | Cc4ccccc4N3CCN(CCc1nnc2CCCCn12)CC3 |  | - | - | - | - |
| 50-29-3 | Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl |  | 87 | - | 6.91 | 0.0055 |
| 1131-64-2 | N=C(N)N1Cc2ccccc2CC1 |  | - | - | 0.75 | 1.33E+04 |
| 14817-09-5 | NC(=O)c1cc(OC)c(OCCCCCCCCCC)c(c1)OC |  | 1650 | - | 4.670 | - |
| 18507-89-6 | O=C(OCC)c1cnc2cc(OCC)c(cc2c1O)OCCCCCCCCCC |  | - | - | 7.800 | - |
| 14484-47-0 | CC(=O)OCC(=O)[C@]45N=C(C)O[C@@H]5C[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3CCC1=CC(=O)C=C[C@@]12C |  | - | - | 1.310 | - |
| 4914-30-1 | COc4cc5CCN[C@H](CC=1C[C@H]2c3cc(OC)c(OC)cc3CCN2CC=1CC)c5cc4OC |  | - | - | 5.240 | - |
| 83435-66-9 | O=C(OCC)[C@H](CCc1ccccc1)N[C@@H](C)C(=O)N(CC(=O)O)C2Cc3ccccc3C2 |  | - | - | - | - |
| 477-30-5 | COc2c3C1=CC=C(OC)C(=O)C=C1[C@@H](CCc3cc(OC)c2OC)NC |  | - | - | 1.37 | 3160 |
| 24701-51-7 | CNCCO\N=C2/c3ccccc3C=Cc1ccccc12 |  | - | - | - | - |
| 83-44-3 | O=C(O)CC[C@@H](C)[C@H]2CC[C@H]1[C@@H]3CC[C@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@@]12C |  | 1000 | - | 3.5 | 43.6 |
| 64-85-7 | OCC(=O)[C@H]3CC[C@H]2[C@@H]4CCC1=CC(=O)CC[C@]1(C)[C@H]4CC[C@]23C |  | - | - | 2.88 | 59.5 |
| 131-01-1 | COc1cc(cc(OC)c1OC)C(=O)O[C@@H]3C[C@@H]4CN5CCc2c6ccccc6nc2[C@H]5C[C@H]4[C@H](C(=O)OC)[C@H]3OC |  | - | - | 3.240 | - |
| 50-47-5 | CNCCCN2c3ccccc3CCc1ccccc12 |  | 375 | - | 4.9 | 58.6 |
| 382-67-2 | OCC(=O)[C@@H]3[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C |  | - | - | 2.35 | 42.1 |
| 76631-46-4 | Cc2cccc(Cc1cncn1)c2C |  | - | - | - | - |
| 50-02-2 | OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C |  | 3000 | - | 1.83 | 89 |
| 53648-55-8 | Oc1ccc2C[C@@H]3CCCCC[C@](C)(c2c1)[C@H]3N |  | - | - | - | - |
| 475-26-3 | Fc1ccc(cc1)C(c2ccc(F)cc2)C(Cl)(Cl)Cl |  | - | - | 5.910 | 0.083 |
| 13739-02-1 | CC(=O)Oc3cccc2C(=O)c1cc(cc(OC(C)=O)c1C(=O)c23)C(=O)O |  | - | - | 2.420 | - |
| 83-63-6 | O=C(C)N(C(C)=O)c1ccc(cc1C)/N=N/c2ccccc2C |  | - | - | 2.670 | - |
| 509-71-7 | CC(=O)Oc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@H](CC[C@@H]23)OC(C)=O |  | - | - | - | - |
| 124-02-7 | C=CCNCC=C |  | 578 | 111 | 1.11 | 8.60E+04 |
| 36141-82-9 | CC(=O)Nc1ccc(cc1)OCCOCCOc2ccc(cc2)NC(C)=O |  | - | - | 1.750 | - |
| 552-25-0 | CCC(=O)N(C[C@H](C)N(C)CCc1ccccc1)c2ccccc2 |  | - | - | 3.510 | - |
| 5964-62-5 | O=S(=O)(c2ccc(/N=N/c1cc(C(C)C)c(O)cc1C)cc2)c4ccc(/N=N/c3cc(C(C)C)c(O)cc3C)cc4 |  | - | - | - | - |
| 333-41-5 | Cc1cc(OP(=S)(OCC)OCC)nc(n1)C(C)C |  | 66 | - | 3.81 | 40 |
| 57998-68-2 | O=C(OCC)NC=1C(=O)C(=C(NC(=O)OCC)C(=O)C=1N2CC2)N3CC3 |  | - | - | -0.02 | 2630 |
| 364-98-7 | Clc1ccc2N=C(C)NS(=O)(=O)c2c1 |  | 980 | - | 1.2 | 2850 |
| 120-46-7 | O=C(CC(=O)c1ccccc1)c2ccccc2 |  | - | - | 2.510 | - |
| 103-49-1 | C(NCc1ccccc1)c2ccccc2 |  | - | - | 2.67 | 782 |
| 1918-00-9 | COc1c(c(Cl)ccc1Cl)C(=O)O |  | 1039 | - | 2.21 | 8310 |
| 2463-84-5 | Clc1cc(ccc1OP(=S)(OC)OC)[N+]([O-])=O |  | 284 | - | 3.58 | 14.7 |
| 97-17-6 | Clc1cc(Cl)ccc1OP(=S)(OCC)OCC |  | 172 | - | 5.14 | 0.245 |
| 7008-26-6 | OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](Cl)[C@@]2(Cl)[C@H]3CCC1=CC(=O)C=C[C@@]12C |  | - | - | 3.340 | - |
| 75-71-8 | ClC(Cl)(F)F |  | - | -2.98E+01 | 2.16 | 280 |
| 133-53-9 | Cc1cc(O)c(Cl)c(C)c1Cl |  | - | - | 3.900 | 200 |
| 120-97-8 | Clc1c(cc(cc1Cl)S(N)(=O)=O)S(N)(=O)=O |  | 10070 | - | 1.060 | - |
| 101831-37-2 | Clc1ccc(cc1)C(C#N)c2c(Cl)cc(cc2Cl)N3N=CC(=O)NC3=O |  | - | - | - | - |
| 2164-09-2 | Clc1ccc(NC(=O)C(=C)C)cc1Cl |  | 1800 | - | 3.290 | 8.5 |
| 66-76-2 | OC=3c4ccccc4OC(=O)C=3CC1=C(O)c2ccccc2OC1=O |  | 250 | - | 2.07 | 128 |
| 84-17-3 | Oc1ccc(cc1)C(=C\C)\C(=C\C)c2ccc(O)cc2 |  | - | - | 5.320 | 3 |
| 702-54-5 | CCC1(CC)COC(=O)NC1=O |  | 71 | - | 1.170 | - |
| 111-42-2 | OCCNCCO |  | - | 268.8 | -1.43E+00 | 1.00E+06 |
| 60-91-3 | CCN(CC)CCN1c3ccccc3Sc2ccccc12 |  | - | - | 5.94 | 0.053 |
| 109-89-7 | CCNCC |  | 540 | 55.5 | 0.58 | 1.00E+06 |
| 90-89-1 | O=C(N1CCN(C)CC1)N(CC)CC |  | - | - | 0.370 | - |
| 56-53-1 | Oc1ccc(cc1)C(\CC)=C(\CC)c2ccc(O)cc2 |  | 3000 | - | 5.07 | 12 |
| 3477-97-2 | OC(C(=O)OCC(C)(C)N(C)C)(c1ccccc1)c2ccccc2 |  | - | - | - | - |
| 20170-20-1 | CN(C)[C@H](C)C(=O)Nc2cc(nn2c1ccccc1)c3ccccc3 |  | 815 | - | - | - |
| 28782-42-5 | O=C(O)C3(CCN(CCC(C#N)(c1ccccc1)c2ccccc2)CC3)c4ccccc4 |  | 149 | - | 1.990 | - |
| 2557-49-5 | OCC(=O)[C@@]3(O)[C@]4(C)C[C@H](O)[C@@]2(F)[C@@H](C[C@H](F)C1=CC(=O)C=C[C@]12C)[C@@H]4C[C@@H]3C |  | - | - | 1.590 | - |
| 35367-38-5 | Clc2ccc(NC(=O)NC(=O)c1c(F)cccc1F)cc2 |  | 4640 | - | 3.88 | 0.08 |
| 22494-42-4 | OC(=O)c1cc(ccc1O)c2ccc(F)cc2F |  | 392 | - | 4.44 | 14.5 |
| 484-23-1 | NNc2nnc(NN)c1ccccc12 |  | - | - | -0.750 | - |
| 125-28-0 | COc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)CC[C@@H]23 |  | - | - | 1.490 | - |
| 67-96-9 | C[C@@H]3CC[C@H](O)C\C3=C\C=C1/CCC[C@@]2(C)[C@H](CC[C@H]12)[C@H](C)/C=C/[C@H](C)C(C)C |  | - | - | 10.45 | - |
| 5966-41-6 | CC(C)N(CCC(c1ccccc1)c2ccccc2)C(C)C |  | - | - | 5.660 | - |
| 579-38-4 | CN(c1ccc(O)cc1)C(=O)C(Cl)Cl |  | - | - | 1.78 | 873 |
| 42399-41-7 | CN(C)CCN2c3ccccc3S[C@@H](c1ccc(OC)cc1)[C@@H](OC(C)=O)C2=O |  | - | - | 2.790 | 465 |
| 545-90-4 | OC(CC)C(CC(C)N(C)C)(c1ccccc1)c2ccccc2 |  | - | - | 4.160 | - |
| 59-52-9 | OC[C@H](S)CS |  | - | - | 0.160 | 8.70E+04 |
| 519-30-2 | CN(C)CCn2cnc1c2C(=O)N(C)C(=O)N1C |  | - | - | -0.150 | - |
| 5221-53-4 | Cc1nc(nc(O)c1CCCC)N(C)C |  | 2350 | - | - | 1200 |
| 41354-30-7 | O.C[C@H]4C[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#CC)[C@@]3(C)CCC(=O)C=C34 |  | - | - | - | - |
| 60-51-5 | COP(=S)(OC)SCC(=O)NC |  | 60 | - | 0.78 | 2.50E+04 |
| 477-93-0 | CN(C)CCOCCOC(=O)N1c3ccccc3Sc2ccccc12 |  | - | - | 4.120 | - |
| 131-11-3 | COC(=O)c1ccccc1C(=O)OC |  | 6800 | 283.7 | 1.6 | 4000 |
| 124-40-3 | CNC |  | 698 | 6.8 | -0.38 | 1.63E+06 |
| 22950-29-4 | COc1cc(cc(OC)c1O)[C@H](O)CNC |  | - | - | -0.560 | - |
| 551-92-8 | O=[N+]([O-])c1cnc(C)n1C |  | - | - | 0.31 | 1.83E+04 |
| 148-01-6 | Cc1c(cc(cc1[N+](=O)[O-])[N+]([O-])=O)C(N)=O |  | 600 | - | 0.190 | 1000 |
| 88-85-7 | O=[N+]([O-])c1cc(cc(c1O)[C@H](C)CC)[N+]([O-])=O |  | 25 | 332 | 3.56 | 52 |
| 96-62-8 | O=S(=O)(NCCNS(=O)(=O)c1cc(ccc1)[N+]([O-])=O)c2cc(ccc2)[N+]([O-])=O |  | - | - | - | - |
| 520-27-4 | COc1ccc(cc1O)C2=CC(=O)c3c(O)cc(cc3O2)O[C@@H]5O[C@H](CO[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O)[C@@H](O)[C@H](O)[C@H]5O |  | - | - | 0.14 | 408 |
| 47255-57-2 | c1ccc(cc1)C2(OC[C@H](O2)[C@@H]3CCCCN3)c4ccccc4 |  | - | - | - | - |
| 537-12-2 | Cl.O=C(Nc1ccccc1)OC[C@H](OC(=O)Nc2ccccc2)CN3CCCCC3 |  | - | - | 2.630 | 1.00E+04 |
| 82-66-6 | O=C2c1ccccc1C(=O)C2C(=O)C(c3ccccc3)c4ccccc4 |  | 1.5 | - | 4.850 | 0.3 |
| 58-73-1 | CN(C)CCOC(c1ccccc1)c2ccccc2 |  | 390 | - | 3.27 | 3060 |
| 972-02-1 | OC(CCCN1CCCCC1)(c2ccccc2)c3ccccc3 |  | 815 | - | 4.710 | - |
| 915-30-0 | O=C(OCC)C3(CCN(CCC(C#N)(c1ccccc1)c2ccccc2)CC3)c4ccccc4 |  | 221 | - | 6.340 | 800 |
| 117-34-0 | OC(=O)C(c1ccccc1)c2ccccc2 |  | 5540 | - | 3.09 | 127 |
| 122-39-4 | c1ccccc1Nc2ccccc2 |  | 1120 | 302 | 3.5 | 53 |
| 538-62-5 | O=C(NNc1ccccc1)/N=N/c2ccccc2 |  | - | - | 0.980 | - |
| 101-81-5 | c1ccccc1Cc2ccccc2 |  | 2250 | 265 | 4.14 | 14.1 |
| 52365-63-6 | O=C(Oc1cc(ccc1OC(=O)C(C)(C)C)[C@H](O)CNC)C(C)(C)C |  | - | - | - | - |
| 14357-78-9 | CC(C)(O)[C@H]1C[C@]74CC[C@]1(OC)[C@@H]5Oc3c(O)ccc2C[C@H]7N(CC[C@@]45c23)CC6CC6 |  | - | - | - | - |
| 4147-51-7 | CCSc1nc(nc(NC(C)C)n1)NC(C)C |  | 3900 | - | 3.81 | 16 |
| 58-32-2 | OCCN(CCO)c2nc1c(nc(nc1c(n2)N3CCCCC3)N(CCO)CCO)N4CCCCC4 |  | 8400 | - | 2.740 | - |
| 68-89-3 | [Na+].[O-]S(=O)(=O)CN(C)C=2C(=O)N(c1ccccc1)N(C)C=2C |  | 3000 | - | - | - |
| 65717-97-7 | O=C(Nc1c(cccc1C(C)C)C(C)C)CN(CC(=O)O)CC(=O)O |  | - | - | - | - |
| 3737-09-5 | CC(C)N(CC[C@](c1ccccn1)(c2ccccc2)C(N)=O)C(C)C |  | 333 | - | 2.58 | 44.9 |
| 330-54-1 | Clc1ccc(NC(=O)N(C)C)cc1Cl |  | 1017 | - | 2.68 | 42 |
| 502-55-6 | CCOC(=S)SSC(=S)OCC |  | 480 | - | 2.060 | 2.76 |
| 34368-04-2 | Oc2ccc(CCN[C@H](C)CCc1ccc(O)cc1)cc2O |  | - | - | - | - |
| 74639-40-0 | CC(=O)N[C@@H](CCSC)C(=O)NCCc1cc(OC(=O)OCC)c(cc1)OC(=O)OCC |  | 2000 | - | - | - |
| 1593-77-7 | C[C@H]1CN(C[C@@H](C)O1)C2CCCCCCCCCCC2 |  | 2645 | - | - | - |
| 61869-07-6 | OC[C@@H]1CO[C@H](CI)O1 |  | - | - | - | - |
| 57808-66-9 | Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4 |  | 5243 | - | 3.9 | 0.986 |
| 51-61-6 | Oc1ccc(CCN)cc1O |  | - | - | -0.98 | 1.00E+06 |
| 86197-47-9 | Oc2ccc(CCNCCCCCCNCCc1ccccc1)cc2O |  | - | - | 4.270 | - |
| 309-29-5 | O=C4N(CC)C[C@@H](CCN1CCOCC1)C4(c2ccccc2)c3ccccc3 |  | - | - | 3.420 | - |
| 74191-85-8 | COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)[C@H]4COc5ccccc5O4 |  | - | - | 2.090 | - |
| 3254-93-1 | O=C2NCNC2(c1ccccc1)c3ccccc3 |  | - | - | 1.400 | - |
| 1668-19-5 | CN(C)CC\C=C1/c3ccccc3OCc2ccccc12 |  | 147 | - | 4.29 | 31.6 |
| 3094-09-5 | FC1=CN(C(=O)NC1=O)[C@@H]2O[C@H](C)[C@@H](O)[C@H]2O |  | 3390 | - | -1.400 | - |
| 69975-86-6 | O=C2c1n(cnc1N(C)C(=O)N2C)CC3OCCO3 |  | 965 | - | - | - |
| 564-25-0 | NC(=O)C=4C(=O)[C@@]3(O)C(O)=C2C(=O)c1c(O)cccc1[C@H](C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C |  | 2000 | - | -0.02 | 630 |
| 1679-76-1 | CCN(CC)CCOC(=O)[C@@H](c1ccccc1)C2CCCCC2 |  | - | - | - | - |
| 82413-20-5 | Oc1cccc(c1)C(/c2ccc(OCCN(C)C)cc2)=C(/CC)c3ccccc3 |  | 4500 | - | - | - |
| 58-19-5 | O=C3C[C@H]4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)C[C@H]3C |  | - | - | 3.99 | 14.6 |
| 548-73-2 | Fc1ccc(cc1)C(=O)CCCN2CC=C(CC2)N3c4ccccc4NC3=O |  | 750 | - | 3.5 | 4.210 |
| 17692-31-8 | O[C@@H](CN1CCN(CC1)c2ccccc2)CO |  | 750 | - | 0.140 | - |
| 3176-03-2 | O[C@@H]3CC[C@]4(O)[C@H]2Cc1ccc(OC)c(OC)c1[C@@]4(CCN2C)C3 |  | 339 | - | - | - |
| 90101-16-9 | O=C3OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)N3c4ccccn4 |  | 1434 | - | - | - |
| 23651-95-8 | Oc1ccc(cc1O)[C@@H](O)[C@H](N)C(=O)O |  | 10000 | - | - | - |
| 527-18-4 | Cc1c(O)c(C)c(C)c(O)c1C |  | - | - | 3.220 | - |
| 527-17-3 | CC=1C(=O)C(C)=C(C)C(=O)C=1C |  | - | - | 2.23 | 443 |
| 586-60-7 | CCCCOc1ccc(cc1)C(=O)CCN2CCCCC2 |  | - | - | - | - |
| 124-28-7 | CN(C)CCCCCCCCCCCCCCCCCC |  | - | - | 8.390 | - |
| 479-18-5 | OC[C@@H](O)Cn2cnc1c2C(=O)N(C)C(=O)N1C |  | - | - | -1.460 | 3.33E+05 |
| 90729-43-4 | CC(C)(C)c1ccc(cc1)C(=O)CCCN2CCC(CC2)OC(c3ccccc3)c4ccccc4 |  | 4000 | - | - | - |
| 27220-47-9 | Clc3ccc(C(OCc1ccc(Cl)cc1)Cn2ccnc2)c(Cl)c3 |  | - | - | - | - |
| 95-04-5 | CC\C(=C\C)C(=O)NC(N)=O |  | 2500 | - | 0.800 | - |
| 70052-12-9 | FC(F)[C@@](N)(CCCN)C(=O)O |  | - | - | - | - |
| 98224-03-4 | c1cc(c2OCCOc2c1)N3CCNCC3 |  | - | - | - | - |
| 483-18-1 | COc4cc5CCN[C@H](C[C@H]1C[C@H]2c3cc(OC)c(OC)cc3CCN2C[C@@H]1CC)c5cc4OC |  | - | - | 5.200 | 984 |
| 518-82-1 | Cc3cc2C(=O)c1cc(O)cc(O)c1C(=O)c2c(O)c3 |  | - | - | 4.010 | - |
| 75847-73-3 | OC(=O)[C@@H]2CCCN2C(=O)[C@H](C)N[C@H](CCc1ccccc1)C(=O)OCC |  | - | - | 2.450 | 1.64E+04 |
| 66778-36-7 | CN3CCCC[C@@H]3CCc2ccccc2NC(=O)c1ccc(OC)cc1 |  | - | - | 4.240 | - |
| 68576-86-3 | O[C@@H](CN1CCN(CC1)c2ccccc2OC)COc3cc(OC)c(OC)c(OC)c3 |  | - | - | - | - |
| 39715-02-1 | N\N=C1\C=C2CN(CCC2=NN1)C(=O)c3ccccc3 |  | - | - | - | - |
| 72-20-8 | ClC1=C(Cl)[C@]2(Cl)C(Cl)(Cl)[C@]1(Cl)[C@@H]3[C@@H]2[C@H]4C[C@@H]3[C@H]5O[C@H]45 |  | 3 | - | 5.2 | 0.25 |
| 55726-47-1 | CCCCCCCCCCCCCCCCCCCCCC(=O)NC1=NC(=O)N(C=C1)[C@@H]2O[C@H](CO)[C@@H](O)[C@@H]2O |  | 1000 | - | - | - |
| 74011-58-8 | O=C(O)C2=CN(CC)c1nc(c(F)cc1C2=O)N3CCNCC3 |  | 5000 | - | -0.2 | 3.43E+04 |
| 77671-31-9 | O=C(C=1NC(=O)NC=1C)c2ccc(SC)cc2 |  | - | - | 1.860 | - |
| 73121-56-9 | O[C@H]2CC(=O)[C@@H](C/C=C=C\CCC(=O)OC)[C@@H]2\C=C/[C@@H](O)COc1ccccc1 |  | 1.6 | - | - | - |
| 72301-79-2 | CC(C)S(=O)(=O)n1c2cc(ccc2nc1N)\C(=N\O)c3ccccc3 |  | - | - | 3.1 | 12.4 |
| 82159-09-9 | OC(=O)CN2C(=O)C(=CC(\C)=C\c1ccccc1)\SC2=S |  | 5.3 | - | - | - |
| 86880-51-5 | Oc1ccc(cc1)CC(=O)NCCNC[C@H](O)COc2ccccc2C#N |  | - | - | 0.92 | 1600 |
| 299-42-3 | O[C@H](c1ccccc1)[C@H](C)NC |  | 600 | 255 | 1.13 | 6.36E+04 |
| 481-29-8 | O=C4CC[C@@H]3[C@]4(C)CC[C@H]1[C@H]3CC[C@H]2C[C@@H](O)CC[C@]12C |  | - | - | 3.070 | 20.2 |
| 26774-90-3 | OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)[C@H](N)C1=CCC=CC1)[C@H]3SC2(C)C |  | - | - | - | - |
| 7004-98-0 | COc3cc4CC[C@@H]2[C@H](CC[C@]1(C)[C@@H]2C[C@H](O)[C@H]1O)c4cc3 |  | - | - | 3.370 | - |
| 1764-85-8 | NS(=O)(=O)c2cc1c(N[C@H](NS1(=O)=O)CSCC(F)(F)F)cc2Cl |  | - | - | 0.790 | - |
| 2363-58-8 | O[C@H]2CC[C@H]1[C@@H]3CC[C@H]4C[C@@H]5S[C@@H]5C[C@]4(C)[C@H]3CC[C@@]12C |  | - | - | 4.450 | 1.2 |
| 10402-90-1 | O=C(c1ccccc1)[C@@H](C)CN3CCN(C[C@@H](OCC)c2ccccc2)CC3 |  | - | - | 3.220 | - |
| 32665-36-4 | O[C@@H](CCN2CCN(C[C@H](OC)c1ccccc1)CC2)c3ccccc3 |  | 640 |  | 2.140 |  |
| 98123-83-2 | O=C1CN(C[C@H]2c3ccccc3CCCN12)C(=O)C4CCCCC4 |  | - | - | - | - |
| 72522-13-5 | Oc2ccc3C[C@H]1C[C@](C)(CCN(C)C1)c3c2 |  | - | - | - | - |
| 474-86-2 | Oc3cc4CC=C1[C@H](CC[C@@]2(C)C(=O)CC[C@H]12)c4cc3 |  | - | - | 3.350 | 1.41 |
| 84611-23-4 | O=C1SCC[C@H]1NC(=O)CSCC(=O)O |  | 10000 | - | - | - |
| 57-87-4 | CC(C)[C@@H](C)/C=C/[C@@H](C)[C@H]2CC[C@@H]3C4=CC=C1C[C@@H](O)CC[C@]1(C)[C@H]4CC[C@]23C |  | - | - | 8.860 | - |
| 149-32-6 | OC[C@H](O)[C@H](O)CO |  | - | 330.5 | -2.29E+00 | 6.10E+05 |
| 64204-55-3 | O=C(CN1CCNCC1)NC2CCCCC2 |  | 3900 | - | - | - |
| 305-01-1 | Oc1cc2C=CC(=O)Oc2cc1O |  | - | - | 0.550 | - |
| 25573-43-7 | CNC(=O)Oc1ccc2c(c1)[C@@]3(C)CCN(C)O[C@@H]3N2C |  | - | - | 2.120 | - |
| 81147-92-4 | CC(C)NCC(O)COc1ccc(cc1)CCC(=O)OC |  | - | - | - | - |
| 50-28-2 | Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@H]1O)c4cc3 |  | - | - | 4.01 | 3.6 |
| 2998-57-4 | ClCCN(CCCl)C(=O)Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@H]1O)c4cc3 |  | - | - | 5.500 | - |
| 50-27-1 | Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2C[C@@H](O)[C@@H]1O)c4cc3 |  | 2000 | - | 2.45 | 441 |
| 53-16-7 | Oc3cc4CC[C@@H]1[C@H](CC[C@]2(C)C(=O)CC[C@@H]12)c4cc3 |  | - | 154 | 3.13 | 30 |
| 90-54-0 | CCC(=O)c1cccc(c1)c2ccccc2OCCN(CC)CC |  | - | - | 4.690 | - |
| 314-35-2 | CCN(CC)CCn2cnc1c2C(=O)N(C)C(=O)N1C |  | - | - | 0.840 | - |
| 7432-25-9 | CCc1ccccc1N3C(C)=Nc2ccccc2C3=O |  | - | - | 4.820 | - |
| 55283-68-6 | [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CC(=C)C)CC)C(F)(F)F |  | 10000 | 256 dec | 5.11 | 0.3 |
| 304-84-7 | Oc1ccc(cc1OC)C(=O)N(CC)CC |  | 154 | - | 1.060 | - |
| 75-08-1 | CCS |  | 682 | 35.1 | 1.270 | 1.56E+04 |
| 141-43-5 | NCCO |  | 1720 | 171 | -1.31E+00 | 1.00E+06 |
| 486-47-5 | CCOc1ccc(cc1OCC)Cc3nccc2cc(OCC)c(cc23)OCC |  | - | - | 5.650 | - |
| 563-12-2 | S=P(SCSP(=S)(OCC)OCC)(OCC)OCC |  | 13 | - | 5.07 | 2 |
| 23947-60-6 | CCNC1=NC(=O)C(CCCC)=C(C)N1 |  | 4000 | - | 2.22 | 150 |
| 434-03-7 | O=C4CC[C@@]3(C)C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)=C4 |  | - | - | 3.11 | 0.687 |
| 26225-79-6 | CS(=O)(=O)Oc1cc2c(cc1)O[C@H](OCC)C2(C)C |  | 1130 | - | 2.7 | 50 |
| 77-15-6 | CN1CCC[C@@](CC1)(C(=O)OCC)c2ccccc2 |  | 355 | - | 3.520 | - |
| 77-67-8 | C[C@@]1(CC)CC(=O)NC1=O |  | 1820 | - | 0.38 | 3.92E+04 |
| 86-35-1 | O=C2N[C@H](c1ccccc1)C(=O)N2CC |  | 1500 | - | 1.05 | 5280 |
| 524-83-4 | CCN4[C@H]1CC[C@@H]4CC(C1)OC(c2ccccc2)c3ccccc3 |  | - | - | 4.770 | - |
| 93-89-0 | O=C(OCC)c1ccccc1 |  | 2100 | 212 | 2.64 | 720 |
| 101-97-3 | O=C(OCC)Cc1ccccc1 |  | 3300 | 227 | 2.28 | 739 |
| 118-61-6 | Oc1ccccc1C(=O)OCC |  | 1320 | 232.5 | 2.95 | 737 |
| 75-04-7 | CCN |  | 400 | 16.5 | -0.13 | 1.00E+06 |
| 100-41-4 | CCc1ccccc1 |  | 3500 | 136.1 | 3.15 | 169 |
| 107-15-3 | NCCN |  | 1200 | 117 | -2.04E+00 | 1.00E+06 |
| 965-90-2 | C[C@]32CC[C@@H]1[C@H]4CCCC=C4CC[C@H]1[C@@H]3CC[C@@]2(O)CC |  | - | - | 5.520 | - |
| 76-58-4 | CCOc5ccc1C[C@H]2N(C)CC[C@]34c1c5O[C@@H]4[C@@H](O)C=C[C@@H]23 |  | 810 | - | 1.770 | 2610 |
| 21715-46-8 | Clc1ccc2N=C(NCC)O[C@@](C)(c2c1)c3ccccc3 |  | 1500 | - | - | - |
| 17365-01-4 | O=C(OCC)[C@](C)(N)Cc2cc(I)c(Oc1cc(I)c(O)c(I)c1)c(I)c2 |  | - | - | - | - |
| 40054-69-1 | Clc1ccccc1C4=NCc2nnc(C)n2c3sc(cc34)CC |  | 3509 | - | - | - |
| 41340-25-4 | O=C(O)C[C@]3(CC)OCCc2c3nc1c(cccc12)CC |  | 94 | - | 3.930 | - |
| 30544-47-9 | FC(F)(F)c1cc(ccc1)Nc2ccccc2C(=O)OCCOCCO |  | 292 | - | 4.200 | 1.6 |
| 1954-28-5 | C(OCCOC[C@H]1CO1)COCCOC[C@@H]2CO2 |  | - | - | -1.680 | - |
| 33125-97-2 | CC(c1ccccc1)n2cncc2C(=O)OCC |  | - | - | 3.05 | 63.2 |
| 52942-31-1 | Clc1cccc(c1)N3CCN(CCCN2N=C(CC)N(CC)C2=O)CC3 |  | - | - | - | - |
| 38260-54-7 | CCc1nc(OCC)cc(OP(=S)(OC)OC)n1 |  | 1800 | - | 2.940 | 40 |
| 2235-90-7 | CC[C@@H](N)Cc2cnc1ccccc12 |  | - | - | 2.170 | 510 |
| 470-82-6 | CC2(C)OC1(C)CCC2CC1 |  | 2480 | 176.4 | 2.74 | 3500 |
| 100-91-4 | C[C@@H]2C[C@@H](OC(=O)[C@H](O)c1ccccc1)CC(C)(C)N2C |  | - | - | 1.870 | - |
| 97-53-0 | Oc1ccc(cc1OC)CC=C |  | 1930 | 253.2 | 2.27 | 2460 |
| 1301-42-4 | CC(C)CCOc1cc2c(cc1)nccc2[C@H](O)[C@H]4C[C@H]3CCN4C[C@H]3CC |  | - | - | 5.320 | - |
| 53370-90-4 | NC(=O)c1ccccc1OCCCCCC |  | 5000 | - | 2.740 | - |
| 52479-85-3 | Oc2ccc(C(=O)c1cc(O)c(O)c(O)c1)c(O)c2O |  | 1425 | - | 1.890 | - |
| 26281-69-6 | O=C(O)c1ccccc1OC[C@H](O)COCCCCCC |  | - | - | - | - |
| 76824-35-6 | N/C(N)=N/c1nc(CSCCC(\N)=N/S(N)(=O)=O)cs1 |  | 4049 | - | -0.64 | 1000 |
| 52-85-7 | O=S(=O)(N(C)C)c1ccc(OP(=S)(OC)OC)cc1 |  | 28 | - | 2.23 | 109 |
| 3102-00-9 | CCCCOC[C@@H](O)COc1ccccc1 |  | 2370 | - | 2.230 | - |
| 3590-16-7 | CCN(CC)CC(CN(CC)CC)[C@@H](c1ccccc1)C2CCCCC2 |  | - | - | - | - |
| 25451-15-4 | NC(=O)OCC(COC(N)=O)c1ccccc1 |  | 5000 | - | 0.760 | - |
| 5728-52-9 | OC(=O)Cc1ccc(cc1)c2ccccc2 |  | 164 | - | 3.190 | - |
| 1008-65-7 | Oc1ccccc1c2nnco2 |  | - | - | 0.220 | - |
| 34616-39-2 | CC[C@H](O)c2ccc(OCCN[C@H](C)Cc1ccccc1)cc2 |  | - | - | - | - |
| 22224-92-6 | Cc1cc(ccc1SC)OP(=O)(NC(C)C)OCC |  | 8 | - | 3.23 | 329 |
| 61019-78-1 | N#C[C@@](CCCC)(Cn1ccnc1)c2ccccc2 |  | 1590 | - | 2.94 | 38 |
| 60168-88-9 | O[C@@](c1ccccc1Cl)(c2cncnc2)c3ccc(Cl)cc3 |  | 2500 | - | 3.6 | 14 |
| 1926-48-3 | OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)[C@@H](Oc1ccccc1)c2ccccc2)[C@H]4SC3(C)C |  | - | - | - | - |
| 36330-85-5 | O=C(CCC(=O)O)c1ccc(cc1)c2ccccc2 |  | 200 | - | 3.2 | 2.21 |
| 4378-36-3 | CC[C@H](c1ccccc1)C(=O)OCCN3CCO[C@H](c2ccccc2)[C@@H]3C |  | - | - | 4.350 | - |
| 5977-10-6 | OC1(CCC(CC1)c2ccccc2)[C@H](CC)C(=O)O |  | - | - | 3.890 | - |
| 458-24-2 | FC(F)(F)c1cccc(C[C@H](C)NCC)c1 |  | 130 | - | 3.36 | 412 |
| 49562-28-9 | O=C(c1ccc(Cl)cc1)c2ccc(OC(C)(C)C(=O)OC(C)C)cc2 |  | 2000 | - | 5.190 | - |
| 67227-56-9 | Oc1ccc(cc1)[C@H]3CNCCc2c3cc(O)c(O)c2Cl |  | - | - | 2.39 | 4000 |
| 31879-05-7 | O=C(O)[C@@H](C)c2cc(Oc1ccccc1)ccc2 |  | - | - | 3.900 | - |
| 13392-18-2 | Oc1cc(cc(O)c1)[C@H](O)CN[C@H](C)Cc2ccc(O)cc2 |  | - | - | 1.220 | - |
| 37561-27-6 | O=C(CN3CCN(Cc1ccc2OCOc2c1)CC3)N4c6ccccc6Sc5ccccc45 |  | - | - | 3.370 | - |
| 4846-91-7 | CC(C)c2ccccc2OCC1=NCCN1 |  | - | - | 3.330 | - |
| 54063-40-0 | CCOc2ccc(cc2N(CCN(CC)CC)C(=O)COc1ccc(OCCCC)cc1)OCC |  | - | - | - | - |
| 15302-16-6 | CCNC1=NC(=O)[C@H](O1)c2ccccc2 |  | - | - | 0.050 | - |
| 69381-94-8 | O[C@H]2C[C@@H](O)[C@H](/C=C/[C@@H](O)COc1ccccc1)[C@H]2C/C=C=C/CCC(=O)OC |  | - | - | - | - |
| 65646-68-6 | CC=2CCCC(C)(C)C=2/C=CC(\C)=C\C=C\C(\C)=C\C(=O)Nc1ccc(O)cc1 |  | - | - | - | - |
| 437-38-7 | CCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3 |  | 18 | - | 4.05 | 200 |
| 55-38-9 | Cc1cc(ccc1SC)OP(=S)(OC)OC |  | 180 | - | 4.09 | 7.5 |
| 18046-21-4 | O=C(O)Cc1sc(nc1c2ccc(Cl)cc2)c3ccccc3 |  | 409 | - | 5.19 | 3.58 |
| 97-24-5 | Oc2ccc(Cl)cc2Sc1cc(Cl)ccc1O |  | - | - | 4.620 | - |
| 51630-58-1 | Clc1ccc(cc1)C(C(C)C)C(=O)OC(C#N)c3cccc(Oc2ccccc2)c3 |  | 70.2 | - | 6.2 | 0.024 |
| 528-48-3 | Oc1ccc(cc1O)C=3Oc2cc(O)ccc2C(=O)C=3O |  | - | - | 1.180 | - |
| 525-82-6 | O=C2C=C(Oc1ccccc12)c3ccccc3 |  | - | - | 3.56 | 30.5 |
| 15301-69-6 | O=C(OCCN1CCCCC1)c4cccc2c4OC(=C(C)C2=O)c3ccccc3 |  | - | - | 4.950 | 10 |
| 54143-55-4 | FC(F)(F)COc2cc(C(=O)NC[C@@H]1CCCCN1)c(OCC(F)(F)F)cc2 |  | - | - | 3.78 | 1.480 |
| 79660-72-3 | CN1CCN(CC1)c2c(F)c3c(cc2F)C(=O)C(=CN3CCF)C(=O)O |  | 4000 | - | 0.24 | 7320 |
| 99665-00-6 | O=C2N1C(=C(CO[C@@H]1[C@@]2(OC)NC(=O)CSC(F)F)CSc3nnnn3CCO)C(=O)O |  | - | - | - | - |
| 73231-34-2 | O=S(C)(=O)c1ccc(cc1)[C@@H](O)[C@@H](CF)NC(=O)C(Cl)Cl |  | - | - | - | - |
| 76568-02-0 | Fc1ccc2c(c1)N(C)C=C(SOC)C2=O |  | - | - | - | - |
| 5250-39-5 | OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1c(F)cccc1Cl)[C@H]4SC3(C)C |  | - | - | 2.58 | 8.820 |
| 1480-19-9 | Fc1ccc(cc1)C(=O)CCCN2CCN(CC2)c3ccccc3OC |  | - | - | 3.6 | - |
| 31430-15-6 | Fc1ccc(cc1)C(=O)c2cc3nc(NC(=O)OC)nc3cc2 |  | 2560 | - | 2.910 | - |
| 33245-39-5 | [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCCl)CCC)C(F)(F)F |  | 2940 | - | 5.070 | 0.9 |
| 3693-39-8 | OCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@H]3[C@]4(C)C[C@@H](Cl)[C@@]2(Cl)[C@@H]3C[C@H](F)C1=CC(=O)C=C[C@@]12C |  | - | - | 4.180 | - |
| 86386-73-4 | OC(Cn1cncn1)(Cn2cncn2)c3ccc(F)cc3F |  | 1271 | - | - | - |
| 21679-14-1 | Nc3nc(F)nc1c3ncn1[C@H]2O[C@H](CO)[C@@H](O)[C@@H]2O |  | - | - | -1.180 | 3530 |
| 78755-81-4 | O=C(OCC)c3ncn2c3CN(C)C(=O)c1cc(F)ccc12 |  | 4200 | - | 1 | 128 |
| 56430-99-0 | FC(F)(F)c1cccc(c1)[C@](O)(CC)c2ccccc2 |  | 2235 | - | 4.620 | - |
| 52468-60-7 | Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4 |  | - | - | 5.78 | 0.339 |
| 3385-03-3 | OCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3C[C@H](F)C1=CC(=O)C=C[C@]12C |  | - | - | 2.660 | - |
| 2321-07-5 | Oc4cc5Oc1cc(O)ccc1C3(OC(=O)c2ccccc23)c5cc4 |  | - | - | 3.350 | - |
| 462-06-6 | Fc1ccccc1 |  | 4399 | 84.7 | 2.27 | 1540 |
| 426-13-1 | CC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3C[C@H](C)C1=CC(=O)C=C[C@@]12C |  | - | - | 2 | 30 |
| 54910-89-3 | FC(F)(F)c2ccc(O[C@@H](CCNC)c1ccccc1)cc2 |  | 825 | - | 4.05 | 60.3 |
| 76-43-7 | C[C@]4(O)CC[C@@H]2[C@]4(C)C[C@H](O)[C@]1(F)[C@@]3(C)CCC(=O)C=C3CC[C@H]12 |  | - | - | 2.38 | 67.5 |
| 2709-56-0 | FC(F)(F)c2cc3C(=C\CCN1CCN(CCO)CC1)/c4ccccc4Sc3cc2 |  | - | - | 4.51 | 0.346 |
| 69-23-8 | FC(F)(F)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2 |  | - | - | 4.36 | 31.1 |
| 56995-20-1 | Nc1nc(ccc1NC(=O)OCC)NCc2ccc(F)cc2 |  | - | - | 2.660 | - |
| 53-34-9 | OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3C[C@H](F)C1=CC(=O)C=C[C@@]12C |  | - | - | 1.270 | - |
| 40507-23-1 | Fc1ccc(cc1)C3=NC(=O)N(c2cc(C)ccc23)C(C)C |  | 3000 | - | - | - |
| 40666-16-8 | O[C@@H]2C[C@H](O)[C@@H](/C=C/[C@H](O)COc1cc(ccc1)C(F)(F)F)[C@@H]2C\C=C/CCCC(=O)O |  | - | - | 4.300 | - |
| 17617-23-1 | Fc3ccccc3C2=NCC(=O)N(CCN(CC)CC)c1ccc(Cl)cc12 |  | 980 | - | 3.020 | - |
| 5104-49-4 | Fc2cc(ccc2c1ccccc1)[C@H](C)C(=O)O |  | 117 | - | 4.16 | 8 |
| 1841-19-6 | Fc1ccc(cc1)C(CCCN2CCC4(CC2)C(=O)NCN4c3ccccc3)c5ccc(F)cc5 |  | - | - | 5.86 | 10 |
| 27060-91-9 | Fc1ccccc1[C@@]34OCCN4CC(=O)N(CCO)c2ccc(Cl)cc23 |  | 6000 | - | - | - |
| 69409-94-5 | Clc3cc(ccc3NC(C(=O)OC(C#N)c2cccc(Oc1ccccc1)c2)C(C)C)C(F)(F)F |  | 261 | - | 6.810 | 0.005 |
| 15687-22-6 | Oc2cc3OC(=O)C=C(CN1CCOCC1)c3cc2O |  | - | - | -0.080 | - |
| 17692-39-6 | C(CCN1CCOCC1)c3ccc(COc2ccccc2)cc3 |  | - | - | 4.130 | - |
| 2454-11-7 | O=C2C=C3CC[C@H]1[C@@H]4CC[C@](C)(O)[C@@]4(C)C[C@@H](O)[C@@H]1[C@@]3(C)C=C2C=O |  | - | - | 1.430 | - |
| 2825-60-7 | CC(=O)OCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@H]3[C@]4(C)C[C@@H](O)[C@@]2(F)[C@@H]3CC(C=O)=C1C=C(OCCCl)CC[C@@]12C |  | - | - | 3.760 | - |
| 13425-53-1 | OP(=O)(O)Oc1ccc(cc1)C(/CC)=C(/CC)c2ccc(OP(=O)(O)O)cc2 |  | - | - | - | - |
| 23155-02-4 | O=P(O)(O)[C@H]1O[C@@H]1C |  | - | - | -1.230 | - |
| 6064-83-1 | OP(=O)(O)Oc1ccccc1C(=O)O |  | 1104 | - | 0.590 | - |
| 5598-52-7 | Clc1cc(Cl)c(Cl)nc1OP(=O)(OC)OC |  | 869 | - | 1.910 | - |
| 21548-32-3 | CCOP(=O)(/N=C1\SCS1)OCC |  | 4.7 | - | 0.680 | 5.00E+04 |
| 92118-27-9 | O=P(OCC)(OCC)C(C)NC(=O)N(CCCl)N=O |  | - | - | - | - |
| 23110-15-8 | C[C@@]1(O[C@@H]1C\C=C(\C)C)[C@H]3[C@@]2(CO2)CC[C@@H](OC(=O)\C=C\C=C\C=C\C=C\C(=O)O)[C@H]3OC |  | - | - | 4.790 | - |
| 110-00-9 | c1ccco1 |  | - | 31.5 | 1.34 | 1.00E+04 |
| 67-45-8 | [O-][N+](=O)c2oc(/C=N/N1CCOC1=O)cc2 |  | 2336 | - | -0.04 | 40 |
| 98-01-1 | O=Cc1ccco1 |  | 65 | 161.7 | 0.41 | 7.70E+04 |
| 54-31-9 | NS(=O)(=O)c2cc(c(NCc1ccco1)cc2Cl)C(=O)O |  | 2600 | - | 2.03 | 73.1 |
| 60142-96-3 | NCC1(CC(=O)O)CCCCC1 |  | - | - | -1.10E+00 | 4490 |
| 39492-01-8 | O=C(Oc1ccc(cc1)C(=O)OCC)CCCCCNC(=N)N |  | - | - | - | - |
| 299-61-6 | CCN(CC)C[C@@H](C)[C@@H](C)OC(=O)c1ccc(OCC(C)C)cc1 |  | - | - | - | - |
| 64318-79-2 | O[C@H]1CC(=O)[C@@H](CCCC/C=C/C(=O)OC)[C@@H]1/C=C/[C@@H](O)C(C)(C)CCCC |  | 56.5 | - | - | - |
| 1075-61-2 | Oc1cc(C[C@H](C)N)ccc1 |  | - | - | - | - |
| 106-24-1 | C\C(C)=C\CCC(/C)=C\CO |  | 3600 | 230 | 3.56 | 100 |
| 60282-87-3 | O=C4CC[C@@]3(C)C(CC[C@@H]2[C@@H]3CC[C@@]1(CC)[C@H]2C=C[C@@]1(O)C#C)=C4 |  | - | - | 3.260 | - |
| 545-26-6 | O[C@H]5CC[C@@]3(C)[C@H](CC[C@@H]2[C@@]4(O)C[C@H](O)[C@H](C1=CC(=O)OC1)[C@]4(C)CC[C@@H]23)C5 |  | - | - | 1.6 | 151 |
| 3820-67-5 | OC[C@@H](O)COC(=O)c3ccccc3Nc1ccnc2cc(Cl)ccc12 |  | 2300 | - | 3.660 | 4.00E+04 |
| 26944-48-9 | O[C@H]3[C@]1(C)CC[C@H](C1(C)C)[C@@H]3NC(=O)NS(=O)(=O)c2ccc(C)cc2 |  | 18000 | - | - | - |
| 21187-98-4 | Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2C[C@H]3CCC[C@@H]3C2 |  | 3000 | - | 2.120 | - |
| 29094-61-9 | Cc1cnc(cn1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3 |  | - | - | 1.91 | 37.2 |
| 33342-05-1 | O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(cc2)CCN4C(=O)c3cc(ccc3C(C)(C)C4=O)OC |  | - | - | 4.650 | - |
| 52443-21-7 | OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](C=O)NC(=O)Cc2c1cc(ccc1n(c2C)C(=O)c3ccc(Cl)cc3)OC |  | - | - | 2.250 | - |
| 50-99-7 | O[C@H]([C@@H](O)C=O)[C@H](O)[C@H](O)CO |  | 25800 | - | -3.24E+00 | 1.20E+06 |
| 77-21-4 | CC[C@@]1(CCC(=O)NC1=O)c2ccccc2 |  | 600 | - | 1.9 | 999 |
| 10238-21-8 | O=C(NC1CCCCC1)NS(=O)(=O)c3ccc(CCNC(=O)c2cc(Cl)ccc2OC)cc3 |  | 20000 | - | 4.790 | 4 |
| 56-81-5 | OCC(O)CO |  | 12600 | 290 | -1.76E+00 | 1.00E+06 |
| 56-40-6 | NCC(=O)O |  | 7930 | - | -3.21E+00 | 2.49E+05 |
| 451-71-8 | O=C(NC1CCCCC1)NS(=O)(=O)c2cc3CCCc3cc2 |  | - | - | - | - |
| 339-44-6 | O=S(=O)(Nc1ncc(cn1)OCCOC)c2ccccc2 |  | 3100 | - | 0.390 | - |
| 87-52-5 | CN(C)Cc2cnc1ccccc12 |  | - | - | 1.450 | - |
| 109889-09-0 | CN4[C@@H]1CCC[C@@H]4CC(C1)NC(=O)c3nn(C)c2ccccc23 |  | - | - | - | - |
| 126-07-8 | O=C2c3c(O[C@@]21C(=CC(=O)C[C@H]1C)OC)c(Cl)c(OC)cc3OC |  | 10000 | - | 2.18 | 8.64 |
| 90-05-1 | Oc1ccccc1OC |  | 520 | 205 | 1.32 | 1.87E+04 |
| 93-14-1 | OCC(O)COc1ccccc1OC |  | 1510 | - | 1.39 | 5.00E+04 |
| 1463-28-1 | N=C(N)NCCN1CC=C(C)CC1 |  | - | - | - | - |
| 40580-59-4 | N=C(N)NCC2COC1(CCCCC1)O2 |  | - | - | - | - |
| 55-65-2 | N=C(N)NCCN1CCCCCCC1 |  | 1050 | - | 0.880 | - |
| 113-00-8 | N=C(N)N |  | - | - | -1.630 | 1840 |
| 73-40-5 | NC2=Nc1ncnc1C(=O)N2 |  | - | - | -0.91 | 2080 |
| 118-00-3 | NC3=Nc1c(ncn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N3 |  | - | - | -1.90E+00 | 700 |
| 24047-25-4 | Clc1cccc(Cl)c1/C=N/NC(=N)NO |  | - | - | - | - |
| 2165-19-7 | N=C(N)NC[C@H]1COc2ccccc2O1 |  | - | - | - | - |
| 23092-17-3 | FC(F)(F)CN2c1ccc(Cl)cc1C(=NCC2=O)c3ccccc3 |  | - | - | 3.97 | 2.410 |
| 80-13-7 | O=S(=O)(N(Cl)Cl)c1ccc(cc1)C(=O)O |  | - | - | -0.170 | - |
| 3093-35-4 | ClCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3CCC1=CC(=O)CC[C@@]12C |  | 5000 | - | 2.930 | - |
| 15599-36-7 | CCN(CC)CCOc1ccc(cc1)c2nc3cc(Cl)ccc3s2 |  | - | - | - | - |
| 69756-53-2 | CCCCN(CCCC)CCC(O)c2cc1c(Cl)cc(Cl)cc1c3cc(ccc23)C(F)(F)F |  | - | - | - | - |
| 55837-20-2 | O[C@@H]3CCCN[C@H]3CC(=O)CN2C=Nc1cc(Br)c(Cl)cc1C2=O |  | - | - | - | - |
| 52-86-8 | Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3 |  | 128 | - | 4.3 | 14 |
| 777-11-7 | Clc1cc(OCC#CI)c(Cl)cc1Cl |  | 5600 | - | 5.030 | - |
| 59128-97-1 | Fc1ccccc1[C@@]34OCCN4CC(=O)Nc2ccc(Br)cc23 |  | 2858 | - | - | - |
| 442-51-3 | COc1ccc3c(c1)nc2c3ccnc2C |  | - | - | 3.56 | 2.680 |
| 7237-81-2 | CCCCCCC(COC(=O)c1cccnc1)(COC(=O)c2cccnc2)COC(=O)c3cccnc3 |  | 5000 | - | - | - |
| 509-86-4 | O=C1NC(=O)NC(=O)C1(CC)C2=CCCCCC2 |  | 5000 | - | 2.03 | 250 |
| 76-44-8 | ClC2=C(Cl)[C@]3(Cl)[C@@H]1C=C[C@H](Cl)[C@@H]1[C@@]2(Cl)C3(Cl)Cl |  | 40 | 310 | 6.1 | 0.18 |
| 372-66-7 | CC(C)(O)CCC[C@H](N)C |  | - | - | 1.150 | - |
| 23560-59-0 | ClC1=C(OP(=O)(OC)OC)C2CC=CC12 |  | 96 | - | 2.32 | 2500 |
| 3511-16-8 | OC(=O)[C@@H]3N4C(=O)[C@H](N1C(=O)[C@H](NC1(C)C)c2ccccc2)[C@H]4SC3(C)C |  | - | - | 2.350 | - |
| 118-74-1 | Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl |  | 10000 | 325 | 5.73 | 0.0062 |
| 67-72-1 | ClC(Cl)(Cl)C(Cl)(Cl)Cl |  | 4460 | - | 4.14 | 50 |
| 70-30-4 | Clc2c(Cc1c(O)c(Cl)cc(Cl)c1Cl)c(O)c(Cl)cc2Cl |  | 56 | 479 | 7.54 | 140 |
| 3811-75-4 | N=C(N)c1ccc(cc1)OCCCCCCOc2ccc(cc2)C(=N)N |  | - | - | - | - |
| 51235-04-2 | CN(C)C2=NC(=O)N(C1CCCCC1)C(=O)N2C |  | 1690 | - | 1.85 | 3.30E+04 |
| 5980-31-4 | CC[C@H](CCCC)CN1CN2CN(C[C@H](CC)CCCC)CC2(C)C1 |  | - | - | - | - |
| 84-16-2 | Oc1ccc(cc1)[C@@H](CC)[C@@H](CC)c2ccc(O)cc2 |  | 2000 | - | 5.600 | 12 |
| 141-94-6 | CCC(CCCC)CN1CC(C)(N)CN(CC(CCCC)CC)C1 |  | - | - | 5.260 | - |
| 56-29-1 | C[C@@]1(C(=O)N=C(O)N(C)C1=O)C2=CCCCC2 |  | - | - | 1.98 | 435 |
| 54-03-5 | COc1c(cc(cc1OC)C(=O)OCCCN(C)CCN(C)CCCOC(=O)c2cc(OC)c(OC)c(OC)c2)OC |  | - | - | 2.710 | - |
| 495-69-2 | O=C(NCC(=O)O)c1ccccc1 |  | - | - | 0.31 | 3750 |
| 51-45-6 | NCCc1cncn1 |  | - | - | -0.7 | 1.00E+06 |
| 493-80-1 | C(N(CCN1CCCC1)c2ccccc2)c3ccccc3 |  | - | - | 4.150 | - |
| 71-00-1 | N[C@@H](Cc1cncn1)C(=O)O |  | 15000 | - | -3.32E+00 | 4.56E+04 |
| 87-00-3 | CN3[C@@H]1CC[C@@H]3C[C@H](C1)OC(=O)C(O)c2ccccc2 |  | - | - | 1.420 | 1.00E+04 |
| 848-53-3 | Clc1ccc(cc1)[C@H](c2ccccc2)N3CCCN(C)CC3 |  | 490 | - | 4.100 | - |
| 3833-99-6 | FC(F)(F)c2cc3N(CCCN1CCCN(CCO)CC1)c4ccccc4Sc3cc2 |  | - | - | 4.630 | - |
| 118-56-9 | O=C(O[C@H]1C[C@@H](C)CC(C)(C)C1)c2ccccc2O |  | - | - | 6.160 | - |
| 3105-97-3 | CCN(CC)CCNc1ccc(CO)c2Sc3ccccc3C(=O)c12 |  | 980 | - | 4.580 | - |
| 461-72-3 | O=C1NC(=O)CN1 |  | - | - | -1.69E+00 | 3.97E+04 |
| 3614-47-9 | O=C(N)C=1C=C/C(=N\N)NN=1 |  | - | - | -1.010 | - |
| 86-54-4 | N\N=C1/NN=Cc2ccccc12 |  | 90 | - | 1 | 9560 |
| 118-08-1 | CN2CCc1cc5OCOc5cc1[C@@H]2[C@H]4OC(=O)c3c(OC)c(ccc34)OC |  | - | - | 1.890 | 30 |
| 6592-85-4 | CN2CCc1cc3OCOc3cc1[C@H]2O |  | - | - | 1.890 | - |
| 5103-42-4 | O=C2c1ccccc1C(=O)C2(O)C4(O)C(=O)c3ccccc3C4=O |  | - | - | -0.390 | - |
| 58-93-5 | NS(=O)(=O)c2cc1c(NCNS1(=O)=O)cc2Cl |  | 2750 | - | -0.07 | 722 |
| 76-47-1 | CCN(CC)CC(=O)OCC(=O)[C@@]4(O)CC[C@@H]2[C@]4(C)C[C@H](O)[C@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 |  | - | - | 2.540 | - |
| 50-23-7 | OCC(=O)[C@@]4(O)CC[C@@H]2[C@]4(C)C[C@H](O)[C@@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 |  | - | - | 1.61 | 320 |
| 123-31-9 | Oc1ccc(O)cc1 |  | 302 | 287 | 0.59 | 7.20E+04 |
| 118-42-3 | CCN(CCO)CCC[C@@H](C)Nc1ccnc2cc(Cl)ccc12 |  | - | - | 3.030 | - |
| 50-19-1 | O[C@](COC(N)=O)(CC)c1ccccc1 |  | 607 | - | 1.090 | 2.50E+04 |
| 495-99-8 | Oc2cc(ccc2/C=C/c1ccc(cc1)C(=N)N)C(=N)N |  | - | - | 1.560 | - |
| 490-98-2 | Oc1cc(ccc1C(=O)OCCN(C)C)NCCCC |  | - | - | - | - |
| 127-07-1 | NC(=O)NO |  | 5760 | - | -1.80E+00 | 1.00E+06 |
| 68-88-2 | Clc1ccc(cc1)[C@@H](c2ccccc2)N3CCN(CC3)CCOCCO |  | 840 | - | 2.360 | - |
| 68-94-0 | O=C2NC=Nc1ncnc12 |  | - | - | -1.11E+00 | 700 |
| 50847-11-5 | CC(C)C(=O)c1c2ccccn2nc1C(C)C |  | 1340 | - | - | - |
| 53648-05-8 | C[C@@H](C(=O)NO)c1ccc(CC(C)C)cc1 |  | - | - | 2.790 | 200 |
| 78919-13-8 | O[C@@H]2C[C@@H]1C\C(C[C@@H]1[C@H]2/C=C/[C@@H](O)[C@H](C)CC#CC)=C\CCCC(=O)O |  | 100 | - | - | - |
| 288-32-4 | c1cncn1 |  | 220 | 257 | -0.08 | 1.59E+05 |
| 27885-92-3 | O=C(Nc1cc(ccc1)C2=NCCN2)Nc3cccc(c3)C4=NCCN4 |  | - | - | 3.880 | - |
| 318-23-0 | CCN(CC)CCN2C(=N)ON=C2c1ccccc1 |  | - | - | 3.570 | - |
| 496-11-7 | c1cccc2CCCc12 |  | - | 177.9 | 3.18 | 109 |
| 26807-65-8 | NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C |  | 3000 | - | 2.660 | - |
| 74517-78-5 | NC(=O)C3(CCCNC(C)C)c1ccccc1c2ccccc23 |  | - | - | 3.11 | 1.880 |
| 95-13-6 | c1cccc2CC=Cc12 |  | - | 182 | 2.92 | 332 |
| 60607-68-3 | CC(C)NC[C@@H](O)COc2cccc1CC=Cc12 |  | - | - | 2.680 | - |
| 60607-68-3 | CC(C)NC[C@@H](O)COc2cccc1CC=Cc12 |  | - | - | 2.680 | - |
| 482-89-3 | O=C3c4ccccc4N\C3=C2/Nc1ccccc1C2=O |  | - | - | 3.72 | 13.4 |
| 120-72-9 | c1cccc2nccc12 |  | 1000 | 254 | 2.14 | 3560 |
| 53-86-1 | Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC |  | 2.42 | - | 4.27 | 0.937 |
| 26844-12-2 | O=C(NC3CCN(CCc1cnc2ccccc12)CC3)c4ccccc4 |  | 1800 | - | 3.600 | - |
| 87-89-8 | O[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O)[C@H]1O |  | - | - | -2.080 | 1.43E+05 |
| 440-58-4 | O=C(C)Nc1c(I)c(c(I)c(CNC(C)=O)c1I)C(=O)O |  | 7000 | - | 1.280 | 3000 |
| 606-17-7 | O=C(Nc1c(I)c(c(I)cc1I)C(=O)O)CCCCC(=O)Nc2c(I)c(C(=O)O)c(I)cc2I |  | - | - | 5.160 | 460 |
| 18181-70-9 | Clc1cc(I)c(Cl)cc1OP(=S)(OC)OC |  | 2330 | - | 5.51 | 0.1 |
| 66108-95-0 | OC[C@@H](O)CNC(=O)c1c(I)c(N(C[C@H](O)CO)C(C)=O)c(I)c(c1I)C(=O)NC[C@H](O)CO |  | 20000 | - | -3.05E+00 | 107 |
| 60166-93-0 | O=C(Nc1c(I)c(c(I)c(c1I)C(=O)NC(CO)CO)C(=O)NC(CO)CO)[C@H](C)O |  | - | - | -2.42E+00 | 1.40E+05 |
| 89797-00-2 | OC[C@@H](O)CNC(=O)c1c(I)c(N(C[C@H](O)COC)C(C)=O)c(I)c(c1I)C(=O)NC[C@H](O)CO |  | - | - | - | - |
| 73334-07-3 | O=C(Nc1c(I)c(c(I)c(c1I)C(=O)N(C)C[C@H](O)CO)C(=O)NC[C@H](O)CO)COC |  | - | - | -2.05E+00 | 23.8 |
| 5579-92-0 | O[C@@H](CN1C=C(I)C(=O)C(I)=C1)CO |  | - | - | 0.010 | - |
| 5560-72-5 | CN(C)CCCn3c1CCCCCCc1c2ccccc23 |  | 775 | - | 5.740 | - |
| 36734-19-7 | O=C2CN(C(=O)NC(C)C)C(=O)N2c1cc(Cl)cc(Cl)c1 |  | 3500 | - | 3 | 13.9 |
| 54-92-2 | O=C(NNC(C)C)c1ccncc1 |  | 365 | - | 0.37 | 2.68E+04 |
| 95847-70-4 | O=C4c1ccccc1S(=O)(=O)N4CCCCN2CCN(CC2)c3ncccn3 |  | - | - | - | - |
| 91-56-5 | O=C1c2ccccc2NC1=O |  | - | - | 0.83 | 1.53E+04 |
| 89667-40-3 | O=C(O)CCCC\C=C(\c1cccnc1)c2ccccc2 |  | 2000 | - | - | - |
| 58152-03-7 | NC[C@@H](O)C(=O)N[C@@H]3C[C@@H](N)[C@H](O[C@H]1O[C@@H](CN)[C@@H](O)[C@@H](O)[C@H]1O)[C@H](O)[C@@H]3O[C@H]2OC[C@@](C)(O)[C@@H](NC)[C@H]2O |  | - | - | -7.170 | - |
| 124-76-5 | C[C@@]21CC[C@@H](C[C@H]1O)C2(C)C |  | 5200 | - | 3.24 | 1190 |
| 538-93-2 | CC(C)Cc1ccccc1 |  | - | 172.7 | 4.68 | 10.1 |
| 59-63-2 | Cc1cc(no1)C(=O)NNCc2ccccc2 |  | 280 | - | 1.49 | 1600 |
| 530-08-5 | Oc1ccc(cc1O)[C@H](O)[C@H](CC)NC(C)C |  | - | - | 1.420 | - |
| 97-54-1 | Oc1ccc(cc1OC)\C=C\C |  | 1560 | 266 | 3.04 | 356 |
| 25311-71-1 | S=P(Oc1ccccc1C(=O)OC(C)C)(NC(C)C)OCC |  | 21.1 | - | 4.12 | 22.1 |
| 50270-33-2 | O=C(O)Cc2c(c(nn2c1ccccc1)c3ccccc3)c4ccccc4 |  | - | - | 4.790 | - |
| 338-95-4 | OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3CCC1=CC(=O)C=C[C@@]12C |  | - | - | 1.51 | 214 |
| 26675-46-7 | FC(F)(F)[C@H](Cl)OC(F)F |  | 4.77mL/kg | 48.5 | 2.06 | 4470 |
| 466-40-0 | CCC(=O)C(C(C)CN(C)C)(c1ccccc1)c2ccccc2 |  | - | - | 4.170 | - |
| 503-01-5 | C[C@H](CC\C=C(\C)C)NC |  | - | 177 | 3.030 | - |
| 54-85-3 | O=C(NN)c1ccncc1 |  | 1250 | - | -0.7 | 1.40E+05 |
| 55-22-1 | O=C(O)c1ccncc1 |  | 5000 | - | 0.32 | 5200 |
| 498-94-2 | O=C(O)C1CCNCC1 |  | - | - | -3.05E+00 | 3.17E+05 |
| 57021-61-1 | O=C(Nc1c(C)cccc1C)C2=CC=CNC2=O |  | 6000 | - | 1.010 | - |
| 78-59-1 | O=C1C=C(C)CC(C)(C)C1 |  | 1870 | 215.2 | 1.7 | 1.20E+04 |
| 121-91-5 | OC(=O)c1cccc(c1)C(=O)O |  | 10400 | - | 1.66 | 130 |
| 33820-53-0 | [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)C(C)C |  | 5000 | - | 5.800 | 0.11 |
| 119-65-3 | c1cccc2ccncc12 |  | 360 | 243.2 | 2.08 | 4520 |
| 482-15-5 | CN(C)[C@@H](C)CN1c3ccccc3Sc2cccnc12 |  | - | - | 3.940 | - |
| 55453-87-7 | O=C(O)Cc1ccc2OCc3ccccc3C(=O)c2c1 |  | 143 | - | - | - |
| 395-28-8 | Oc1ccc(cc1)[C@H](O)[C@H](C)N[C@H](C)COc2ccccc2 |  | - | - | 2.350 | - |
| 520-18-3 | Oc1ccc(cc1)C=3Oc2cc(O)cc(O)c2C(=O)C=3O |  | - | - | 1.960 | - |
| 59-01-8 | O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CN)O[C@@H]3O[C@H]2[C@H](O)[C@@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](N)[C@H]1O)[C@H](N)C[C@@H]2N |  | 10000 | - | -6.700 | 1.00E+06 |
| 853-34-9 | CC(=O)CCC2C(=O)N(c1ccccc1)N(C2=O)c3ccccc3 |  | 720 | - | 1.470 | 174 |
| 27762-78-3 | OC(O)C(=O)[C@H](C)OCC |  | - | 145 | 0.600 | 1.00E+05 |
| 469-79-4 | O=C(CC)C1(CCN(C)CC1)c2cccc(O)c2 |  | - | - | 1.940 | - |
| 22071-15-4 | C[C@H](C(=O)O)c1cccc(c1)C(=O)c2ccccc2 |  | 62.4 | - | 3.12 | 51 |
| 74103-06-3 | O=C(O)[C@H]2CCn1c(ccc12)C(=O)c3ccccc3 |  | - | - | 2.320 | - |
| 34580-13-7 | CN1CC/C(CC1)=C3\c4ccccc4CC(=O)c2sccc23 |  | - | - | - | - |
| 82-02-0 | COc3c1c(OC(C)=CC1=O)c(OC)c2occc23 |  | 68.8 | - | 3.000 | 1040 |
| 525-79-1 | n1cnc3ncnc3c1NCc2ccco2 |  | - | - | 0.600 | - |
| 501-30-4 | O=C1C=C(CO)OC=C1O |  | - | - | -0.64 | 9.35E+05 |
| 36894-69-6 | O=C(N)c1cc(ccc1O)[C@@H](O)CN[C@@H](C)CCc2ccccc2 |  | 2000 | - | 3.09 | 117 |
| 103890-78-4 | CC=1NC(C)=C(C(C=1C(=O)OCC)c2ccccc2/C=C/C(=O)OC(C)(C)C)C(=O)OCC |  | 880 | - | 5.2 | 0.507 |
| 4618-18-2 | O[C@H]2[C@H](O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O)[C@@H](CO)O[C@]2(O)CO |  | 18160 | - | -4.670 | 7.64E+05 |
| 84057-84-1 | Clc1cccc(c1Cl)c2nnc(N)nc2N |  | 205 | - | - | - |
| 84-79-7 | C/C(C)=C\CC=2C(=O)c1ccccc1C(=O)C=2O |  | - | - | 3.130 | - |
| 2688-77-9 | COc1ccc(cc1OC)C[C@H]2c3cc(OC)c(cc3CCN2C)OC |  | - | - | 3.370 | - |
| 135-43-3 | N=C(N)Nc1ccc(OCCCCCCCCCCCC)c(c1)NC(=N)N |  | - | - | - | - |
| 7262-75-1 | CN(C)[C@H](Cc1ccccc1)c2ccccc2 |  | - | - | - | - |
| 86273-18-9 | N[C@H](c1ccccc1)C(=O)N[C@@H]4C(=O)N3[C@@H](C(=O)OCC=2OC(=O)OC=2C)C(C)(C)S[C@@H]34 |  | - | - | - | - |
| 53943-88-7 | OC(=O)[C@@H]1N[C@@H](CCSCC(=O)OCC)SC1 |  | - | - | -2.010 | - |
| 61-90-5 | CC(C)C[C@H](N)C(=O)O |  | - | - | -1.52E+00 | 2.15E+04 |
| 14769-73-4 | N1=C3SCCN3C[C@@H]1c2ccccc2 |  | 480 | - | 1.84 | 1120 |
| 47141-42-4 | CC(C)(C)NC[C@H](O)COc2cccc1c2CCCC1=O |  | - | - | 2.4 | 1250 |
| 79516-68-0 | Fc1ccc(cc1)[C@@]2(CC[C@H](CC2)N4CC[C@@](c3ccccc3)(C(=O)O)[C@H](C)C4)C#N |  | - | - | - | - |
| 137-58-6 | O=C(Nc1c(C)cccc1C)CN(CC)CC |  | 317 | - | 2.44 | 4100 |
| 59160-29-1 | O=C(Nc1c(C)cccc1C)CN(CC(=O)O)CC(=O)O |  | - | - | -2.430 | - |
| 88852-12-4 | C[C@@H](CCCC)C[C@H](O)/C=C/[C@@H]1[C@@H](CCC/C=C/C(=O)O)C(=O)C[C@H]1O.O[C@@H]2[C@H](O)[C@@H]1O[C@H]7O[C@H](CO)[C@@H](O[C@H]6O[C@H](CO)[C@@H](O[C@H]5O[C@H](CO)[C@@H](O[C@H]4O[C@H](CO)[C@@H](O[C@H]3O[C@H](CO)[C@@H](O[C@H]2O[C@@H]1CO)[C@H](O)[C@H]3O)[C@H](O)[C@H]4O)[C@@H](O)[C@H]5O)[C@H](O)[C@H]6O)[C@H](O)[C@H]7O |  | 19 | - | - | - |
| 154-21-2 | O[C@@H]1[C@@H](O)[C@@H](O)[C@@H](O[C@@H]1SC)[C@@H](NC(=O)[C@@H]2C[C@@H](CCC)CN2C)[C@@H](C)O |  | 1000 | - | 0.56 | 927 |
| 330-55-2 | Clc1ccc(NC(=O)N(C)OC)cc1Cl |  | 1146 | - | 3.2 | 75 |
| 90-69-7 | CN2[C@H](CCC[C@H]2C[C@@H](O)c1ccccc1)CC(=O)c3ccccc3 |  | - | - | 3.740 | 48.4 |
| 63329-53-3 | OC(=O)c2ccc(Cl)cc2Nc1ccccc1C(=O)O |  | - | - | - | - |
| 53882-12-5 | Clc1c(cc(cc1NC(=O)C(=O)O)C#N)NC(=O)C(=O)O |  | - | - | - | - |
| 31036-80-3 | Clc2cccc(Cl)c2O[C@H](C)C1=NCCN1 |  | - | - | 3.580 | - |
| 790-69-2 | Clc2cc(NC(=S)Nc1ccc(F)cc1)cc(Cl)c2 |  | - | - | 4.700 | - |
| 98079-51-7 | O=C(O)C2=CN(CC)c1c(F)c(c(F)cc1C2=O)N3C[C@H](C)NCC3 |  | 3800 | - | -0.3 | 2.72E+04 |
| 13010-47-4 | O=C(NC1CCCCC1)N(CCCl)N=O |  | 70 | - | 2.83 | 111 |
| 91431-42-4 | CC(=O)Oc2c1cc(Cl)ccc1c(OC(C)=O)c(OC)c2OC |  | - | - | 3.26 | 11.9 |
| 53808-88-1 | O=C(O)Cc1cn(nc1c2ccc(Cl)cc2)c3ccccc3 |  | - | - | 3.670 | - |
| 50264-69-2 | O=C(O)c3nn(Cc1ccc(Cl)cc1Cl)c2ccccc23 |  | 1700 | - | 4.660 | - |
| 53179-11-6 | CN(C)C(=O)C(CCN1CCC(O)(CC1)c2ccc(Cl)cc2)(c3ccccc3)c4ccccc4 |  | 98 | - | 5.150 | - |
| 61197-73-7 | CN5CCN(/C=C3/N=C4CN=C(c1ccccc1Cl)c2cc(ccc2N4C3=O)[N+]([O-])=O)CC5 |  | - | - | - | - |
| 47562-08-3 | O=C(OCCl)[C@H]6[C@]34C[C@H]5N1[C@H](O)[C@@H](CC)[C@@H](C[C@H]1[C@@H]4N(C)c2ccccc23)[C@@H]56 |  | - | - | - | - |
| 846-49-1 | Clc3ccccc3C2=NC(O)C(=O)Nc1ccc(Cl)cc12 |  | 4500 | - | 2.39 | 80 |
| 59729-31-6 | CC(C)N1CCC(CC1)N(c2ccc(Cl)cc2)C(=O)Cc3ccccc3 |  | 395 | - | 4.85 | 0.334 |
| 848-75-9 | Clc3ccccc3C2=N[C@@H](O)C(=O)N(C)c1ccc(Cl)cc12 |  | 10000 | - | 2.230 | - |
| 75330-75-5 | C[C@@H](CC)C(=O)O[C@H]3C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@H]23 |  | - | - | 4.26 | 2.140 |
| 1977-10-2 | CN1CCN(CC1)C3=Nc4ccccc4Oc2ccc(Cl)cc23 |  | 151 | - | 3.600 | 5.650 |
| 80382-23-6 | [Na+].O.O.[O-]C(=O)C(C)c2ccc(CC1CCCC1=O)cc2 |  | 145 | - | - | - |
| 73-22-3 | O=C(O)[C@@H](N)Cc2cnc1ccccc12 |  | 16000 | - | -1.06E+00 | 1.34E+04 |
| 487-21-8 | Oc2nc(O)nc1nccnc12 |  | - | - | -0.410 | 1250 |
| 1086-80-2 | Cc1cc2nc3NC(=O)NC(=O)c3nc2cc1C |  | - | - | 1.860 | - |
| 52-76-6 | C[C@]32CC[C@@H]1[C@H]4CCCC=C4CC[C@H]1[C@@H]3CC[C@@]2(O)C#C |  | - | - | 4.750 | - |
| 56341-08-3 | Nc1c(cc(cc1Cl)[C@@H](O)CNC(C)(C)C)C(F)(F)F |  | - | - | - | - |
| 59937-28-9 | CC(C)OC(=O)C(/C(=O)OC(C)C)=C1/SC=CS1 |  | 2065 | - | 3.75 | 9.000 |
| 69-79-4 | O[C@H]2[C@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)[C@@H](CO)O[C@@H](O)[C@@H]2O |  | 34800 | - | -5.030 | 7.80E+05 |
| 591-27-5 | Nc1cccc(O)c1 |  | 924 | - | 0.21 | 2.70E+04 |
| 532-28-5 | O[C@H](C#N)c1ccccc1 |  | - | - | 0.020 | - |
| 10262-69-8 | CNCCCC24CCC(c1ccccc12)c3ccccc34 |  | 760 | - | 4.520 | - |
| 22232-71-9 | Clc1ccc(cc1)[C@]4(O)c2ccccc2C3=NCCN34 |  | 36.3 | - | 4.090 | - |
| 13085-08-0 | O=C(CN1CCN(C)CC1)[C@@]4(O)CC[C@@H]3[C@@H]5CCC2=CC(=O)C=C[C@]2(C)[C@H]5[C@@H](O)C[C@@]34C |  | - | - | - | - |
| 31431-39-7 | O=C(OC)Nc1nc2cc(ccc2n1)C(=O)c3ccccc3 |  | 714 | - | 2.83 | 71.3 |
| 78266-06-5 | Cc1cc(C)c(Br)c(C)c1NC(=O)CN(CC(=O)O)CC(=O)O |  | - | - | 0.11 | 1.230 |
| 569-65-3 | Cc1cccc(c1)CN2CCN(CC2)[C@@H](c3ccc(Cl)cc3)c4ccccc4 |  | 1750 | 230 | 5.870 | - |
| 2013-58-3 | NC(=O)C=4C(=O)[C@]3(O)C(O)=C2C(=O)c1c(O)ccc(Cl)c1C(=C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C |  | 2000 | - | - | - |
| 51-68-3 | Clc1ccc(OCC(=O)OCCN(C)C)cc1 |  | 2600 | - | 1.960 | - |
| 5668-06-4 | Clc1ccc(cc1)[C@](C)(O[C@H](C)CN(C)C)c2ccccc2 |  | - | - | - | - |
| 137-05-3 | N#CC(=C)C(=O)OC |  | 1600 | - | 0.930 | 9480 |
| 2898-12-6 | Clc1ccc2c(c1)C(=NCCN2C)c3ccccc3 |  | 900 | - | 4.41 | 3.100 |
| 53-31-6 | c1cc(cc2OCOc12)CN3CCN(CC3)C(c4ccccc4)c5ccccc5 |  | - | - | 4.610 | - |
| 32359-34-5 | CN(C)CC(Oc1ccccc1)Oc2ccccc2 |  | - | - | - | - |
| 977-79-7 | CC(=O)[C@@]3(C)CC[C@H]2[C@@H]4C=C(C)C1=CC(=O)CC[C@]1(C)[C@H]4CC[C@@]23C |  | - | - | 4.450 | 1.82 |
| 520-85-4 | CC(=O)[C@@]3(O)CC[C@H]2[C@@H]4C[C@H](C)C1=CC(=O)CC[C@]1(C)[C@H]4CC[C@@]23C |  | - | - | 3.500 | - |
| 7195-27-9 | C[C@@]2(CN(C)S(=O)(=O)c1ccc(Cl)c(c1)S(N)(=O)=O)CCCO2 |  | 10000 | - | 1.54 | 16.8 |
| 5633-18-1 | CC(=O)[C@@]3(O)C(=C)C[C@H]2[C@@H]4C=C(C)C1=CC(=O)CC[C@]1(C)[C@H]4CC[C@@]23C |  | - | - | 3.830 | - |
| 5118-29-6 | CN(C)CC\C=C2/c1ccccc1C(C)(C)c3ccccc23 |  | 170 | - | 4.810 | - |
| 517-60-2 | OC(=O)c1c(c(c(c(c1C(=O)O)C(=O)O)C(=O)O)C(=O)O)C(=O)O |  | - | - | 1.5 | 362 |
| 71125-38-7 | Cc3cnc(NC(=O)C2=C(O)c1ccccc1S(=O)(=O)N2C)s3 |  | - | - | 3.43 | 7.150 |
| 481-85-6 | Oc1cc(C)c(O)c2ccccc12 |  | - | - | 2.760 | - |
| 58-27-5 | O=C2C=C(C)C(=O)c1ccccc12 |  | - | - | 2.2 | 160 |
| 71628-96-1 | CN(C)[C@H]6[C@H](O)[C@@H]5Oc3c(cc(O)c4C(=O)c2c(O)c1c(C[C@](C)(O)C[C@H]1OC)cc2C(=O)c34)[C@](C)(O5)[C@H]6O |  | 1788 | - | - | - |
| 1490-04-6 | CC(C)[C@H]1CC[C@H](C)C[C@H]1O |  | - | - | 3.380 | 420 |
| 46464-11-3 | COc1ccc(CNC(=N\C)\NC)cc1 |  | - | - | - | - |
| 60-89-9 | CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23 |  | - | - | 5.360 | 5.59 |
| 57-42-1 | CN1CCC(CC1)(C(=O)OCC)c2ccccc2 |  | 162 | - | 2.72 | 3220 |
| 70-07-5 | COc2ccccc2OC[C@@H]1CNC(=O)O1 |  | 3820 | - | 3.220 | - |
| 100-92-5 | CC(C)(NC)Cc1ccccc1 |  | - | - | 2.670 | - |
| 20326-12-9 | Cc3cc(CCN1CCN(CC1)c2cccc(Cl)c2)nn3 |  | - | - | - | - |
| 17854-59-0 | O=C3c4ccccc4Oc2c3ccc(OC)c2CN1CCCCC1 |  | 183 | - | 5.040 | - |
| 1247-42-3 | OCC(=O)[C@@]3(O)C(C)C[C@H]2[C@@H]4CCC1=CC(=O)C=C[C@]1(C)[C@H]4C(=O)C[C@@]23C |  | - | - | 2.010 | - |
| 57-53-4 | O=C(N)OCC(C)(COC(=O)N)CCC |  | 794 | - | 0.7 | 4700 |
| 495-70-5 | CC(C)(COC(=O)c1ccccc1)NCCC |  | - | - | - | - |
| 89-57-6 | OC(=O)c1cc(N)ccc1O |  | 2800 | - | 0.980 | - |
| 54-04-6 | COc1c(cc(cc1OC)CCN)OC |  | - | - | 0.78 | 8.41E+04 |
| 1424-00-6 | O=C4C[C@H]3CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]3(C)[C@@H](C)C4 |  | - | - | 3.480 | - |
| 72-33-3 | COc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)c4cc3 |  | 10000 | - | 4.680 | - |
| 135-58-0 | Cc1ccc2Sc3ccc(C)cc3Sc2c1 |  | - | - | 5.920 | - |
| 57837-19-1 | C[C@@H](N(C(=O)COC)c1c(C)cccc1C)C(=O)OC |  | 566 | 295.9 dec | 1.65 | 8400 |
| 15351-09-4 | O=C(c1ccccc1)[C@H](C)N(C)C |  | - | - | 2.060 | - |
| 5001-33-2 | Oc1ccc(cc1OC)[C@H](O)CNC |  | - | - | -0.64 | 1.00E+06 |
| 21730-16-5 | CNC2Cc1ccccc1N(C)c3ccccc23 |  | - | - | - | - |
| 586-06-1 | Oc1cc(cc(O)c1)[C@H](O)CNC(C)C |  | 3370 | - | 0.210 | - |
| 17692-51-2 | O=C(OCc1ccccc1)NC[C@@H]3C[C@@H]4c5cccc2c5c(cn2C)C[C@H]4N(C)C3 |  | - | - | - | - |
| 914-00-1 | NC(=O)C=4C(=O)[C@@]3(O)C(O)=C2C(=O)c1c(O)cccc1C(=C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C |  | - | - | -1.370 | 7550 |
| 517-18-0 | O=C(O)C(C)(C)[C@H](CC)c1ccc2cc(ccc2c1)OC |  | - | - | 5.320 | - |
| 926-93-2 | C[C@@H](NC(=S)NNC(=S)NC)C=C |  | 1000 | - | 0.320 | - |
| 521-10-8 | C[C@]4(O)CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C |  | - | - | 4.350 | - |
| 67-56-1 | CO |  | 5628 | 64.6 | -0.77 | 1.00E+06 |
| 91-80-5 | CN(C)CCN(Cc1cccs1)c2ccccn2 |  | - | - | 2.87 | 601 |
| 72-44-6 | Cc1ccccc1N3C(C)=Nc2ccccc2C3=O |  | 185 | - | 4.330 | 4.730 |
| 554-57-4 | CN1N=C(S/C1=N/C(C)=O)S(=O)(N)=O |  | - | - | 0.13 | 3500 |
| 100-97-0 | C1N3CN2CN(CN1C2)C3 |  | - | - | -4.150 | 4.49E+05 |
| 153-00-4 | O=C3C[C@@H]4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)C(C)=C3 |  | - | - | 3.690 | - |
| 950-37-8 | O=C1SC(=NN1CSP(=S)(OC)OC)OC |  | 20 | - | 2.2 | 187 |
| 63-68-3 | O=C(O)[C@@H](N)CCSC |  | 36000 | - | -1.87E+00 | 5.66E+04 |
| 467-43-6 | O=C1NC(=S)NC(=O)C1(CCSC)[C@H](C)CCC |  | - | - | - | - |
| 4969-02-2 | CN1CCC[C@@H](C1)CC2c4ccccc4Sc3ccccc23 |  | - | - | 5.670 | - |
| 16752-77-5 | C\C(=N\OC(=O)NC)SC |  | 14.7 | - | 0.6 | 5.80E+04 |
| 59-05-2 | O=C(O)[C@H](CCC(=O)O)NC(=O)c1ccc(cc1)N(C)Cc2nc3c(nc2)nc(N)nc3N |  | 135 | - | -1.85E+00 | 2600 |
| 298-81-7 | COc1c3occc3cc2C=CC(=O)Oc12 |  | 791 | - | 2.140 | 47.6 |
| 76-38-0 | ClC(Cl)C(F)(F)OC |  | 3600 | 105 | 2.21 | 2.83E+04 |
| 93-30-1 | COc1ccccc1C[C@H](C)NC |  | - | - | 2.300 | - |
| 77-41-8 | C[C@@]1(CC(=O)N(C)C1=O)c2ccccc2 |  | - | - | 1.450 | 5190 |
| 134-20-3 | Nc1ccccc1C(=O)OC |  | 2910 | 256 | 1.88 | 2850 |
| 93-58-3 | COC(=O)c1ccccc1 |  | 1177 | 199 | 2.12 | 2100 |
| 93-60-7 | COC(=O)c1cccnc1 |  | - | 204 | 0.83 | 4.76E+04 |
| 502-02-3 | OS(=O)(=O)c2ccc(/N=N/c1ccc(cc1)N(C)C)cc2 |  | - | - | 1.130 | 42.1 |
| 493-52-7 | CN(C)c2ccc(/N=N/c1ccccc1C(=O)O)cc2 |  | - | - | 3.830 | 3.670 |
| 74-89-5 | CN |  | 100 | -6.30E+00 | -0.57 | 1.08E+06 |
| 60-34-4 | CNN |  | 32 | 87.5 | -1.05E+00 | 1.00E+06 |
| 113-45-1 | O=C(OC)[C@@H](c1ccccc1)[C@@H]2CCCCN2 |  | 367 | - | 0.2 | 2.01E+05 |
| 1084-65-7 | NS(=O)(=O)c2cc1c(CCCS1(=O)=O)cc2C |  | 16000 | - | 1.260 | - |
| 17692-22-7 | Cc3sc1ccccc1c3CC2=NCCN2 |  | - | - | - | - |
| 364-62-5 | Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC |  | 750 | - | 2.62 | 200 |
| 51218-45-2 | ClCC(=O)N(c1c(C)cccc1CC)[C@H](C)COC |  | 2200 | - | 3.13 | 530 |
| 17560-51-9 | NS(=O)(=O)c2cc3C(=O)N(c1ccccc1C)[C@H](C)Nc3cc2Cl |  | 5000 | - | 1.840 | 60.3 |
| 5377-20-8 | C[C@H](c1ccccc1)n2cncc2C(=O)OC |  | - | - | 2.570 | - |
| 51384-51-1 | CC(C)NCC(O)COc1ccc(cc1)CCOC |  | - | - | - | - |
| 1178-28-5 | O=C(OC)[C@H]2[C@@H](OC)[C@@H](C[C@H]3CN4CCc1c5ccc(OC)cc5nc1[C@H]4C[C@@H]23)OC |  | - | - | - | - |
| 54188-38-4 | COc1cc4c(cc1)n3CCN(C)C2=NCCc4c23 |  | - | - | - | - |
| 21087-64-9 | O=C1C(=NN=C(SC)N1N)C(C)(C)C |  | 1100 | - | 1.7 | 1050 |
| 31112-62-6 | O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]2NC(=O)c1c(I)c(NC(C)=O)c(I)c(N(C)C(C)=O)c1I |  | 20000 | - | -1.89E+00 | 5.00E+05 |
| 114-91-0 | COCCc1ccccn1 |  | - | 203 | 1.080 | - |
| 73573-88-3 | C[C@@H](CC)C(=O)O[C@H]3CCC=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@@H]23 |  | - | - | 3.95 | 4.800 |
| 7786-34-7 | O=P(OC)(OC)OC(/C)=C/C(=O)OC |  | 3 | - | 0.13 | 6.00E+05 |
| 31868-18-5 | Clc1ccccc1[C@@]34OC[C@@H](C)N4CC(=O)Nc2ccc(Cl)cc23 |  | 4500 | - | - | - |
| 24219-97-4 | CN1C[C@H]3N(CC1)c4ccccc4Cc2ccccc23 |  | 925 | - | - | - |
| 3704-09-4 | C[C@@H]4CC1=CC(=O)CC[C@@H]1[C@H]3CC[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@@H]34 |  | - | - | 3.19 | 72.5 |
| 22916-47-8 | Clc1ccc(c(Cl)c1)[C@H](OCc2ccc(Cl)cc2Cl)Cn3ccnc3 |  | 550 | - | 6.250 | - |
| 59467-70-8 | Fc4ccccc4C2=NCc1cnc(C)n1c3ccc(Cl)cc23 |  | 215 | - | 4.330 | - |
| 84371-65-3 | CN(C)c1ccc(cc1)[C@H]5C[C@@]2(C)[C@@H](CC[C@@]2(O)C#CC)[C@@H]4CCC3=CC(=O)CCC3=C45 |  | - | - | - | - |
| 72432-03-2 | OCCN1C[C@@H](O)[C@H](O)[C@@H](O)[C@H]1CO |  | - | - | - | - |
| 78415-72-2 | N#CC1=CC(=C(C)NC1=O)c2ccncc2 |  | 91 | - | 1.170 | - |
| 2116-55-4 | N[C@@H](CN1C=CC(=O)C(O)=C1)C(=O)O |  | - | - | - | - |
| 25905-77-5 | Cc2cc(nnc2NCCN1CCOCC1)c3ccccc3 |  | - | - | 2.03 | 2360 |
| 10118-90-8 | CN(C)c2ccc(O)c1C(=O)C3=C(O)[C@]4(O)C(=O)C(=C(O)[C@@H](N(C)C)[C@@H]4C[C@@H]3Cc12)C(N)=O |  | - | - | 0.05 | 5.20E+04 |
| 2385-85-5 | ClC53C1(Cl)C4(Cl)C2(Cl)C1(Cl)C(Cl)(Cl)C5(Cl)C2(Cl)C3(Cl)C4(Cl)Cl |  | 235 | - | 6.89 | 0.085 |
| 50924-49-7 | NC(=O)c1ncn(c1O)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O |  | 2847 | - | - | - |
| 99-09-2 | O=[N+]([O-])c1cccc(N)c1 |  | 535 | 306 | 1.37 | 1200 |
| 554-84-7 | O=[N+]([O-])c1cccc(O)c1 |  | 328 | - | 2 | 1.35E+04 |
| 68693-11-8 | O=S(CC(N)=O)C(c1ccccc1)c2ccccc2 |  | - | - | - | - |
| 2210-63-1 | O=C2NN(c1ccccc1)C(=O)[C@H]2CCCC |  | 1750 | - | 1.900 | - |
| 7416-34-4 | O=C2c3c(CC)c(C)nc3CC[C@H]2CN1CCOCC1 |  | - | - | 2.310 | - |
| 103-16-2 | Oc2ccc(OCc1ccccc1)cc2 |  | - | - | 3.300 | 251 |
| 5741-22-0 | CC(C)NC[C@H](O)COc1ccccc1OC |  | - | - | 1.69 | 9940 |
| 20574-50-9 | Cc2ccsc2/C=C/C1=NCCCN1C |  | - | - | 3.690 | - |
| 6536-18-1 | CC4=C(CN2CCO[C@H](c1ccccc1)[C@@H]2C)C(=O)N(c3ccccc3)N4C |  | 250 | - | 2.010 | - |
| 480-16-0 | Oc3ccc(C=2Oc1cc(O)cc(O)c1C(=O)C=2O)c(O)c3 |  | - | - | 1.54 | 250 |
| 3731-59-7 | N=C(N)NC(=N)N1CCOCC1 |  | - | - | -3.030 | - |
| 57-27-2 | Oc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 |  | 335 | - | 0.89 | 149 |
| 110-91-8 | C1CNCCO1 |  | 1450 | 128 | -0.86 | 1.00E+06 |
| 56281-36-8 | Cc1c(C)c(/C=CC(\C)=C\C=C\C(\C)=C\C(=O)NCC)c(C)cc1OC |  | - | - | 6.900 | - |
| 85856-54-8 | OC(=O)[C@H]2CCCN2C(=O)[C@@H](C)CSC(=O)[C@@H](C)NC(=O)C1CCCCC1 |  | - | - | - | - |
| 54-32-0 | CC(=O)Oc1cc(C(C)C)c(OCCN(C)C)cc1C |  | - | - | 3.17 | 323 |
| 108-45-2 | Nc1cccc(N)c1 |  | 280 | 285 | -0.33 | 2.38E+05 |
| 3051-09-0 | [NH4+].O=C2NC(=O)NC(=O)/C2=N/C1=C([O-])NC(=O)NC1=O |  | - | - | -3.970 | - |
| 55294-15-0 | O=C1CC(N)=NN1[C@H](C)c2ccc(Cl)c(Cl)c2 |  | 1559 | - | - | - |
| 529-44-2 | Oc1cc(cc(O)c1O)C=3Oc2cc(O)cc(O)c2C(=O)C=3O |  | - | - | 1.420 | - |
| 127-19-5 | CN(C)C(C)=O |  | 4300 | 165 | -0.77 | 1.00E+06 |
| 42924-53-8 | CC(=O)CCc1ccc2cc(ccc2c1)OC |  | 3880 | - | 3.08 | 72.8 |
| 42200-33-9 | CC(C)(C)NC[C@@H](O)COc2cccc1C[C@@H](O)[C@@H](O)Cc12 |  | 5300 | - | 0.81 | 8330 |
| 54063-51-3 | O\N=C(\N)C[C@@H](O)COc2cccc1ccccc12 |  | - | - | - | - |
| 2188-67-2 | Nc1ccc(cc1)C(=O)OCCNCCCCC |  | - | - | - | - |
| 65472-88-0 | CN(C\C=C\c1ccccc1)Cc3cccc2ccccc23 |  | - | - | - | - |
| 20594-83-6 | Oc5ccc1C[C@H]2N(CC[C@@]34c1c5O[C@@H]4[C@@H](O)CC[C@@]23O)CC6CCC6 |  | - | - | - | - |
| 62-67-9 | Oc5ccc1C[C@H]2N(CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23)CC=C |  | - | - | 1.86 | 2770 |
| 465-65-6 | O=C1CC[C@@]5(O)[C@H]2Cc4ccc(O)c3O[C@@H]1[C@]5(CCN2CC=C)c34 |  | - | - | 2.09 | 1420 |
| 434-22-0 | O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@H]1O)=C4 |  | - | - | 2.62 | 323 |
| 835-31-4 | c2cc(CC1=NCCN1)c3ccccc3c2 |  | - | - | 3.520 | 11.8 |
| 91-20-3 | c1cccc2ccccc12 |  | 490 | 217.9 | 3.3 | 31 |
| 15299-99-7 | CCN(CC)C(=O)C(C)Oc2cccc1ccccc12 |  | 5000 | - | 3.36 | 73 |
| 132-66-1 | O=C(O)c1ccccc1C(=O)Nc3cccc2ccccc23 |  | 8200 | - | 3.410 | 200 |
| 131-28-2 | O=C(O)c1c(OC)c(OC)ccc1C(=O)Cc2c(cc3OCOc3c2OC)CCN(C)C |  | - | - | 1.970 | 780 |
| 3947-65-7 | N[C@H]2C[C@@H](N)[C@H](O)[C@@H](O)[C@@H]2O[C@H]1O[C@H](CN)[C@@H](O)[C@H](O)[C@H]1N |  | - | - | - | - |
| 118457-14-0 | Fc1cc2CC[C@@H](Oc2cc1)[C@@H](O)CNC[C@H](O)[C@@H]3CCc4cc(F)ccc4O3 |  | - | - | - | - |
| 83366-66-9 | Clc1cccc(c1)N4CCN(CCCN3N=C(CC)N(CCOc2ccccc2)C3=O)CC4 |  | - | - | 5.000 | - |
| 463-82-1 | CC(C)(C)C |  | - | 9.4 | 3.11 | 33.2 |
| 13997-19-8 | O=C(OC)C3=CNc2cc(OCc1ccccc1)c(CCCC)cc2C3=O |  | - | - | 6.560 | - |
| 466-07-9 | O=C1C=C(CO1)[C@@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CC[C@@H]2C[C@H](CC[C@@]23C)O[C@@H]4O[C@@H](C)[C@@H](O)[C@H](OC)[C@H]4O |  | - | - | 2.1 | 6.890 |
| 128-53-0 | O=C1C=CC(=O)N1CC |  | 25 | - | 0.580 | - |
| 88255-01-0 | O=S(=O)(O)CCN\C(NC(=O)OC)=N\c1cc(SCCC)ccc1[N+]([O-])=O |  | - | - | - | - |
| 27848-84-6 | Brc1cc(cnc1)C(=O)OC[C@@H]3C[C@]4(OC)c5cccc2c5c(cn2C)C[C@H]4N(C)C3 |  | 1193 | - | - | - |
| 5868-05-3 | O=C(OCC(COC(=O)c1cccnc1)(COC(=O)c2cccnc2)COC(=O)c3cccnc3)c4cccnc4 |  | - | - | 1.910 | - |
| 10571-59-2 | Clc1ccc(cc1)[C@H](OC(=O)c2cccnc2)C(C)C |  | - | - | 4.320 | - |
| 31980-29-7 | Clc1ccc(cc1)OC(C)(C)C(=O)OCc2cccnc2 |  | - | - | 3.650 | - |
| 639-48-5 | O=C(Oc6ccc1C[C@H]2N(C)CC[C@@]35c1c6O[C@H]5[C@H](C=C[C@@H]23)OC(=O)c4cccnc4)c7cccnc7 |  | - | - | - | - |
| 54-11-5 | CN2CCC[C@H]2c1cnccc1 |  | 50 | 247 | 1.17 | 1.00E+06 |
| 59-67-6 | O=C(O)c1cccnc1 |  | 7000 | - | 0.36 | 1.80E+04 |
| 405-22-1 | O=[N+]([O-])c1ccc(/C=N/N(CCO)C(N)=O)o1 |  | - | - | -0.540 | 500 |
| 555-84-0 | O=[N+]([O-])c2ccc(/C=N/N1CCNC1=O)o2 |  | 1681 | - | 0.240 | 98.5 |
| 4936-47-4 | CSC[C@@H]2CN(/N=C\c1ccc(o1)[N+]([O-])=O)C(=O)O2 |  | - | - | 1.530 | - |
| 3363-58-4 | [O-][N+](=O)c1ccc(o1)/C=N/N3CC(=O)N(CN2CCOCC2)C3=O |  | - | - | -1.140 | - |
| 57474-29-0 | O=[N+]([O-])c1ccc(o1)c2cc(C(=O)O)[n+]([O-])c3ccccc23 |  | - | - | 1.230 | - |
| 6236-05-1 | O=[N+]([O-])c1ccc(\C=N\O)o1 |  | - | - | 0.3 | 1000 |
| 13411-16-0 | O=[N+]([O-])c2ccc(/C=C/c1cccc(CO)n1)o2 |  | - | - | 1.37 | 684 |
| 1614-20-6 | O=[N+]([O-])c2ccc(/C=C/c1ccc(N)nn1)o2 |  | - | - | 1.600 | - |
| 23256-30-6 | O=S2(=O)C[C@H](C)N(/N=C/c1ccc(o1)[N+]([O-])=O)CC2 |  | 4050 | - | -0.340 | - |
| 1088-92-2 | O=[N+]([O-])c2ccc(/C=N/N1CC(=O)N(CO)C1=O)o2 |  | - | - | -1.420 | - |
| 75530-68-6 | CC=1NC(C#N)=C(C(C=1C(=O)OC(C)C)c2cccc(c2)[N+]([O-])=O)C(=O)OC |  | 1560 | - | - | - |
| 2011-67-8 | [O-][N+](=O)c1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3 |  | 970 | - | 2.16 | 76.2 |
| 50435-25-1 | Clc2cc(C)c(\N=C1/SCS1)cc2 |  | - | - | - | - |
| 66085-59-4 | CC=1NC(C)=C(C(C=1C(=O)OC(C)C)c2cccc(c2)[N+]([O-])=O)C(=O)OCCOC |  | 2738 | - | 3.05 | 24.3 |
| 63675-72-9 | CC=1NC(C)=C(C(C=1C(=O)OCC(C)C)c2ccccc2[N+]([O-])=O)C(=O)OC |  | 1257 | - | 3.26 | 24.6 |
| 98-95-3 | [O-][N+](=O)c1ccccc1 |  | 349 | 210.8 | 1.85 | 2090 |
| 962-02-7 | [O-][N+](=O)c1ccc(cc1)/N=N\[C@@H]2SC(=S)N(C)C2=O |  | - | - | - | - |
| 79-24-3 | [O-][N+](=O)CC |  | 1100 | 114 | 0.18 | 4.70E+04 |
| 75-52-5 | [O-][N+](C)=O |  | 940 | 101.1 | -0.35 | 1.11E+05 |
| 19881-18-6 | [O-][N+](=O)c1ccc(cc1)Oc2ccc(cc2)\N=C=S |  | - | - | 5.200 | - |
| 76963-41-2 | CN(C)Cc1nc(CSCCNC(=C\[N+]([O-])=O)\NC)cs1 |  | 1653 | - | -0.430 | - |
| 54533-85-6 | Clc1ccccc1C(=O)c2cc(ccc2n3ccnc3CN(CC)CC)[N+]([O-])=O |  | - | - | - | - |
| 6384-92-5 | OC(=O)C[C@@H](NC)C(=O)O |  | - | - | - | - |
| 579-10-2 | CN(C(C)=O)c1ccccc1 |  | - | 256 | 1.12 | 1.67E+04 |
| 62-75-9 | CN(C)N=O |  | 37 | 154 | -0.57 | 1.00E+06 |
| 59-89-2 | O=NN1CCOCC1 |  | 282 | 225 | -0.44 | 1.00E+06 |
| 24526-64-5 | Nc3cccc1c3CN(C)C[C@@H]1c2ccccc2 |  | 267 | - | 2.380 | - |
| 1477-39-0 | C[C@H](NC)CC(c1ccccc1)(c2ccccc2)[C@@H](OC(C)=O)CC |  | - | - | 5.470 | - |
| 1235-15-0 | O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(CC)[C@H]2CC[C@@]1(O)CC)=C4 |  | - | - | - | - |
| 1088-11-5 | Clc1ccc2NC(=O)CN=C(c2c1)c3ccccc3 |  | - | - | 2.93 | 57 |
| 52-78-8 | O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@]1(O)CC)=C4 |  | - | - | 3.760 | - |
| 68-22-4 | O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)=C4 |  | - | - | 2.97 | 7.04 |
| 68-23-5 | O=C1CCC4=C(C1)CC[C@@H]3[C@@H]4CC[C@@]2(C)[C@H]3CC[C@@]2(O)C#C |  | - | - | 3.510 | - |
| 27314-13-2 | FC(F)(F)c1cc(ccc1)N2N=CC(NC)=C(Cl)C2=O |  | 8000 | - | 2.3 | 33.7 |
| 13563-60-5 | O=C1CCC4=C(C1)CC[C@@H]3[C@@H]4CC[C@@]2(C)[C@H]3CC[C@@]2(O)C=C |  | - | - | - | - |
| 6533-00-2 | O=C4CC[C@H]3C(CC[C@@H]2[C@H]3CC[C@]1(CC)[C@H]2CC[C@@]1(O)C#C)=C4 |  | 5010 | - | 3.480 | 1.73 |
| 848-21-5 | O=C3C=C4CC[C@@H]2C(C=C[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)=C4CC3 |  | - | - | 2.590 | - |
| 537-29-1 | OC[C@H](c1ccccc1)C(=O)O[C@@H]2C[C@H]3CC[C@H](C2)N3 |  | - | - | - | - |
| 1531-12-0 | Oc3ccc4C[C@H]1NCC[C@@]2(CCCC[C@@H]12)c4c3 |  | - | - | 3.200 | - |
| 467-85-6 | CCC(=O)C(CCN(C)C)(c1ccccc1)c2ccccc2 |  | - | - | 3.750 | - |
| 466-97-7 | Oc5ccc1C[C@H]2NCC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 |  | - | - | -0.17 | 2.56E+05 |
| 561-48-8 | CCC(=O)C(CCN1CCCCC1)(c2ccccc2)c3ccccc3 |  | - | - | 5.110 | - |
| 941-69-5 | O=C2C=CC(=O)N2c1ccccc1 |  | 58 | - | 1.09 | 6970 |
| 120-34-3 | Nc1ccc(cc1)S(=O)(=O)NC(=O)c2ccc(C)c(C)c2 |  | 2800 | - | 2.390 | - |
| 1843-05-6 | O=C(c1ccc(cc1O)OCCCCCCCC)c2ccccc2 |  | 10000 | - | 6.960 | - |
| 4684-87-1 | CCCCCC[C@H](C)NN |  | - | - | - | - |
| 71251-02-0 | CCCCCCCC\N=C1/C=CN(C=C1)CCCCCCCCCCN2C=C/C(C=C2)=N\CCCCCCCC |  | - | - | - | - |
| 95-50-1 | Clc1ccccc1Cl |  | 500 | 180 | 3.43 | 156 |
| 99614-02-5 | O=C3c4c1ccccc1n(C)c4CC[C@@H]3Cn2ccnc2C |  | - | - | - | - |
| 88-74-4 | O=[N+]([O-])c1ccccc1N |  | 1600 | 284 | 1.85 | 1470 |
| 35727-72-1 | O=C2CCCC(=O)C2C(=S)Nc1ccc(Cl)cc1 |  | - | - | - | - |
| 94-70-2 | CCOc1ccccc1N |  | - | 232.5 | 1.650 | 3370 |
| 90-43-7 | Oc2ccccc2c1ccccc1 |  | 2000 | 286 | 3.09 | 700 |
| 2779-55-7 | O=C(N/N=C/c1ccc(OC)c(OC)c1C(=O)O)c2ccncc2 |  | - | - | - | - |
| 16773-42-5 | Cc1ncc([N+]([O-])=O)n1C[C@H](O)CCl |  | 1780 | - | 0.6 | 4330 |
| 70-26-8 | NCCC[C@H](N)C(=O)O |  | - | - | -4.22E+00 | 1.00E+06 |
| 70667-26-4 | O[C@@H]1CC(=O)[C@H](CC(=O)CCCCC(=O)OC)[C@H]1/C=C/[C@@H](O)C[C@@H](C)CCCC |  | 44 | - | - | - |
| 119-93-7 | Cc1cc(ccc1N)c2ccc(N)c(C)c2 |  | - | 339 | 2.34 | 1300 |
| 529-20-4 | Cc1ccccc1C=O |  | - | 200 | 2.26 | 1180 |
| 529-19-1 | N#Cc1ccccc1C |  | 3200 | 205 | 2.21 | 724 |
| 508-52-1 | O[C@@H]3C[C@@]4(O)CC[C@@H]2[C@@]5(O)CC[C@H](C1=CC(=O)OC1)[C@@]5(C)C[C@@H](O)[C@@H]2[C@@]4(CO)[C@H](O)C3 |  | - | - | -0.02 | 1830 |
| 33996-33-7 | O[C@@H]1C[C@@H](C(=O)O)N(C1)C(=O)C |  | - | - | -1.550 | - |
| 66-79-5 | OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1ccccc1)[C@H]4SC3(C)C |  | - | - | 2.38 | 27.8 |
| 19666-30-9 | O=C2OC(=NN2c1cc(OC(C)C)c(Cl)cc1Cl)C(C)(C)C |  | 3500 | - | 4.8 | 0.7 |
| 26629-87-8 | CC(C)N1C[C@@H](OCC1)c2ccc(cc2)C(F)(F)F |  | - | - | - | - |
| 15301-80-1 | CCN(CC)CCOc1cc2c(cc1OCCN(CC)CC)OC(=O)C=C2C |  | - | - | - | - |
| 21738-42-1 | [O-][N+](=O)c1cc2N[C@H](CCc2cc1CO)CNC(C)C |  | 30 | - | 2.24 | 820 |
| 23135-22-0 | O=C(C(=N\OC(=O)NC)\SC)N(C)C |  | 2.5 | - | -0.48 | 2.80E+05 |
| 126-93-2 | O=C(N)[C@@]1(CC)O[C@H]1CCC |  | 1250 | - | 1.720 | 1.05E+04 |
| 53-39-4 | O=C2C[C@H]3CC[C@H]1[C@@H]4CC[C@](C)(O)[C@]4(C)CC[C@@H]1[C@@]3(C)CO2 |  | 10000 | - | 2.580 | - |
| 21256-18-8 | OC(=O)CCc1nc(c(o1)c2ccccc2)c3ccccc3 |  | 4470 | - | 4.19 | 8.800 |
| 60607-34-3 | O=C5Nc1ccccc1N5CCCN2CCN(CC2)C(c3ccccc3)c4ccccc4 |  | 1410 | - | 4.150 | - |
| 604-75-1 | Clc1ccc2NC(=O)[C@H](O)N=C(c2c1)c3ccccc3 |  | 8000 | - | 2.24 | 179 |
| 27591-42-0 | O=C3c4ccccc4C(=O)C3(CN1CCOCC1)c2ccccc2 |  | - | - | 2.090 | - |
| 24143-17-7 | Clc1ccc2NC(=O)CN3C[C@@H](C)O[C@]3(c2c1)c4ccccc4 |  | 4000 | - | - | - |
| 468-61-1 | CCC(CC)(C(=O)OCCOCCN(CC)CC)c1ccccc1 |  | 183 | - | 4.340 | - |
| 33765-68-3 | CC[C@H]3C[C@H]2[C@@H]4CCC1=CC(=O)CC[C@@H]1[C@H]4CC[C@]2(C)[C@H]3O |  | 12105 | - | - | - |
| 53716-50-0 | O=C(OC)Nc1nc2ccc(cc2n1)S(=O)c3ccccc3 |  | - | - | 1.630 | - |
| 62613-82-5 | O[C@H]1CC(=O)N(CC(=O)N)C1 |  | - | - | - | - |
| 959-14-8 | CCN(CC)CCc1nc(no1)c2ccccc2 |  | 2000 | - | 2.360 | - |
| 131-57-7 | O=C(c1ccc(cc1O)OC)c2ccccc2 |  | 7400 | - | 3.79 | 68.6 |
| 485-89-2 | O=C(O)c1c3ccccc3nc(c1O)c2ccccc2 |  | - | - | 4.160 | - |
| 2277-92-1 | Clc2c(C(=O)Nc1cc(Cl)cc(Cl)c1O)c(O)c(Cl)cc2Cl |  | 1000 | - | 6.040 | - |
| 15687-41-9 | COc1cc(ccc1)C(=O)CCN[C@H](C)[C@H](O)c2ccccc2 |  | - | - | - | - |
| 145-12-0 | OC=4C(=O)CC[C@@]3(C)C=4CC[C@@H]2[C@@H]3CC[C@]1(C)[C@H]2CC[C@]1(C)O |  | - | - | 4.160 | - |
| 1491-59-4 | CC(C)(C)c2cc(C)c(CC1=NCCN1)c(C)c2O |  | - | - | 4.870 | - |
| 434-07-1 | O=C3C[C@@H]4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@]1(C)O)[C@@]4(C)C/C3=C\O |  | - | - | 3.610 | - |
| 76-41-5 | O=C1CC[C@@]5(O)[C@H]2Cc4ccc(O)c3O[C@@H]1[C@]5(CCN2C)c34 |  | - | - | 0.83 | 2.40E+04 |
| 5585-93-3 | OCCN1CCN(CC1)CCCN2c4ccccc4Sc3cccnc23 |  | - | - | - | - |
| 153-87-7 | COc3cc4nc(C)c(CCN1CCN(CC1)c2ccccc2)c4cc3OC |  | 1000 | - | 3.850 | - |
| 129-20-4 | Oc1ccc(cc1)N3C(=O)[C@@H](CCCC)C(=O)N3c2ccccc2 |  | 329 | - | 2.72 | 60 |
| 125-53-1 | CN3CCCN=C3COC(=O)[C@@](O)(c1ccccc1)C2CCCCC2 |  | - | - | 3.520 | - |
| 2439-01-2 | Cc1ccc2nc3SC(=O)Sc3nc2c1 |  | 1100 | - | 3.78 | 1 |
| 82571-53-7 | O=C(O)/C=C/c2ccc(Cn1ccnc1)cc2 |  | - | - | - | - |
| 491-92-9 | CCN(CC)CCC[C@@H](C)Nc1cc(cc2cccnc12)OC |  | - | - | 4.730 | - |
| 123-30-8 | Nc1ccc(O)cc1 |  | 375 | 284 | 0.04 | 1.60E+04 |
| 130-85-8 | O=C(O)c4cc1ccccc1c(Cc2c3ccccc3cc(C(=O)O)c2O)c4O |  | - | - | 6.870 | 1.09E+05 |
| 100-09-4 | COc1ccc(cc1)C(=O)O |  | - | 276.5 | 1.96 | 530 |
| 522-57-6 | COc1ccc(cc1OC)C(=O)c3nccc2cc(OC)c(cc23)OC |  | - | - | - | - |
| 123-63-7 | CC1OC(C)OC(C)O1 |  | 1530 | 124.3 | 0.67 | 1.12E+05 |
| 53-33-8 | OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@H]2[C@@H](C[C@H](F)C1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C |  | - | - | 1.680 | - |
| 1729-61-9 | N=C(N)c1ccc(cc1)\C=C4/c2ccccc2c3ccccc34 |  | - | - | - | - |
| 14255-87-9 | O=C(OC)Nc1nc2ccc(cc2n1)CCCC |  | 40 | - | 3.570 | - |
| 7542-37-2 | N[C@@H]4[C@@H](O)[C@H](O)[C@@H](CO)O[C@@H]4O[C@@H]3[C@@H](N)C[C@H](N)[C@H](O)[C@H]3O[C@H]2O[C@H](CO)[C@@H](O[C@H]1O[C@@H](CN)[C@@H](O)[C@H](O)[C@H]1N)[C@H]2O |  | 21620 | - | -6.920 | - |
| 61869-08-7 | Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2 |  | - | - | 3.950 | - |
| 70-70-2 | O=C(CC)c1ccc(O)cc1 |  | - | - | 2.03 | 345 |
| 508-59-8 | O=C2C=C[C@@]3(O)[C@@H](C)CC[C@H]1C(=C)C(=O)O[C@H]1[C@@]23C |  | - | - | 0.77 | 1.44E+04 |
| 4042-30-2 | OC2=C(C(=O)c1ccccc1C2=O)C3CCCCC3 |  | - | - | 3.590 | - |
| 103-88-8 | Brc1ccc(NC(C)=O)cc1 |  | - | - | 2.29 | 410 |
| 99-91-2 | O=C(C)c1ccc(Cl)cc1 |  | - | 232 | 2.32 | 111 |
| 106-37-6 | Brc1ccc(Br)cc1 |  | - | 218.5 | 3.79 | 20 |
| 540-36-3 | Fc1ccc(F)cc1 |  | - | 89 | 2.13 | 1220 |
| 70458-92-3 | CN1CCN(CC1)c2cc3N(CC)C=C(C(=O)O)C(=O)c3cc2F |  | - | - | 0.27 | 1.14E+04 |
| 2152-34-3 | NC1=NC(=O)[C@@H](O1)c2ccccc2 |  | 436 | - | 0.540 | - |
| 79-55-0 | CC1(C)CCCC(C)(C)N1C |  | - | 147 | 2.690 | - |
| 983-85-7 | CC(=O)OCOC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)Cc1ccccc1)[C@H]3SC2(C)C |  | - | - | 0.620 | - |
| 40487-42-1 | [O-][N+](=O)c1c(C)c(C)cc([N+]([O-])=O)c1NC(CC)CC |  | 1050 | 330 | 5.18 | 0.3 |
| 135-48-8 | c1c3cc4cc5ccccc5cc4cc3cc2ccccc12 |  | - | - | 7.11 | 1.08E-03 |
| 87-86-5 | Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl |  | 27 | 309.5 | 5.12 | 14 |
| 115-77-5 | OCC(CO)(CO)CO |  | 19500 | - | -1.69E+00 | 7.23E+04 |
| 7001-56-1 | CC(=O)[C@@]5(O)CC[C@H]4[C@]5(C)CC[C@H]2[C@H]4CC=C1C=C(CC[C@@]12C)OC3CCCC3 |  | - | - | - | - |
| 100-33-4 | N=C(N)c1ccc(cc1)OCCCCCOc2ccc(cc2)C(=N)N |  | - | - | 2.790 | - |
| 109-66-0 | CCCCC |  | 400 | 36 | 3.39 | 38 |
| 62087-72-3 | O=C(N[C@@H](CCCNC(=N)N)C(=O)O)[C@@H]1CCCN1C(=O)[C@H](CC(=O)O)NC(=O)[C@H](CO)NC(=O)[C@@H](N)CC(=O)O |  | - | - | - | - |
| 96513-83-6 | CC(C)N(CC[C@@](CC(C)C)(c1ccccn1)C(N)=O)C(C)C |  | 1100 | - | - | - |
| 76-74-4 | O=C1NC(=O)NC(=O)C1(CC)C(C)CCC |  | 125 | - | 2.1 | 679 |
| 53910-25-1 | O[C@@H]3CNC=Nc1c3ncn1[C@H]2C[C@@H](O)[C@H](CO)O2 |  | - | - | -2.540 | - |
| 84-97-9 | CN1CCN(CC1)CCCN2c4ccccc4Sc3ccccc23 |  | 500 | - | 4 | 2.170 |
| 37924-13-3 | O=S(=O)(c1ccccc1)c2cc(C)c(NS(=O)(=O)C(F)(F)F)cc2 |  | 633 | - | 4.240 | 60 |
| 6621-47-2 | C(C(C1CCCCC1)C2CCCCC2)[C@@H]3CCCCN3 |  | - | - | 7.540 | - |
| 52645-53-1 | Cl/C(Cl)=C/[C@H]3[C@@H](C(=O)OCc2cccc(Oc1ccccc1)c2)C3(C)C |  | 383 | - | 6.5 | 0.006 |
| 58-39-9 | OCCN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 |  | 318 | - | 4.2 | 28.3 |
| 1182-87-2 | O=C1C=C(CO1)[C@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CC[C@@H]2C[C@@H](CC[C@@]23C=O)O[C@H]4O[C@@H](C)[C@@H](O)[C@H](OC)[C@H]4O |  | - | - | 1.05 | 400 |
| 371-40-4 | Fc1ccc(N)cc1 |  | 417 | 182 | 1.15 | 1.12E+04 |
| 85-01-8 | c2cc3ccc1ccccc1c3cc2 |  | - | 340 | 4.46 | 1.15 |
| 84-11-7 | O=C2c3ccccc3c1ccccc1C2=O |  | - | 360 | 2.52 | 7.5 |
| 92-82-0 | n1c3ccccc3nc2ccccc12 |  | - | 360 | 2.84 | 16 |
| 3735-90-8 | CCN(CC)CCSC(=O)N(c1ccccc1)c2ccccc2 |  | 370 | - | 3.600 | - |
| 77-10-1 | C1CC(CCC1)(c2ccccc2)N3CCCCC3 |  | - | - | 4.69 | - |
| 51-71-8 | NNCCc1ccccc1 |  | - | - | 0.970 | - |
| 60-12-8 | OCCc1ccccc1 |  | 1790 | 218.2 | 1.36 | 2.22E+04 |
| 103-73-1 | CCOc1ccccc1 |  | - | 169.8 | 2.51 | 569 |
| 103-03-7 | NC(=O)NNc1ccccc1 |  | - | - | 0.13 | 2840 |
| 82-88-2 | CN1CC3=C(CC1)c2ccccc2[C@H]3c4ccccc4 |  | - | - | 4.220 | - |
| 86-21-5 | CN(C)CC[C@H](c1ccccn1)c2ccccc2 |  | - | - | 3.170 | - |
| 554-24-5 | O=C(O)[C@@H](CC)Oc1c(I)cc(I)cc1I |  | - | - | 5.740 | - |
| 108-95-2 | Oc1ccccc1 |  | 317 | 181.8 | 1.46 | 8.28E+04 |
| 77-09-8 | Oc1ccc(cc1)C3(OC(=O)c2ccccc23)c4ccc(O)cc4 |  | - | - | 2.41 | 400 |
| 143-74-8 | Oc1ccc(cc1)C3(OS(=O)(=O)c2ccccc23)c4ccc(O)cc4 |  | - | - | 3.02 | 770 |
| 92-84-2 | c1ccc2Sc3ccccc3Nc2c1 |  | - | 371 | 4.15 | 1.59 |
| 26002-80-2 | C/C(C)=C/[C@@H]3[C@H](C(=O)OCc2cccc(Oc1ccccc1)c2)C3(C)C |  | 10000 | - | 7.540 | 0.0097 |
| 135-67-1 | c1ccc2Oc3ccccc3Nc2c1 |  | - | - | 3.85 | 2.130 |
| 59-96-1 | C[C@H](COc1ccccc1)N(Cc2ccccc2)CCCl |  | 2500 | - | 4.640 | - |
| 3818-37-9 | C[C@@H](COc1ccccc1)NN |  | - | - | 1.200 | - |
| 673-31-4 | NC(=O)OCCCc1ccccc1 |  | 1110 | - | 1.96 | 1180 |
| 435-97-2 | OC=1c3ccccc3OC(=O)C=1[C@H](CC)c2ccccc2 |  | 200 | - | 3.62 | 12.9 |
| 86-34-0 | O=C2N(C)C(=O)C[C@@H]2c1ccccc1 |  | - | - | 0.990 | 7020 |
| 122-09-8 | NC(C)(C)Cc1ccccc1 |  | - | 205 | 1.9 | 1.86E+04 |
| 122-79-2 | O=C(C)Oc1ccccc1 |  | 1.63mL/kg | 196 | 1.49 | 4640 |
| 101-84-8 | c1ccccc1Oc2ccccc2 |  | 2450 | 258 | 4.21 | 18 |
| 139-66-2 | c1ccccc1Sc2ccccc2 |  | - | 296 | 4.45 | 8.120 |
| 122-78-1 | O=CCc1ccccc1 |  | 1550 | 195 | 1.78 | 3030 |
| 103-82-2 | OC(=O)Cc1ccccc1 |  | 2250 | 265.5 | 1.41 | 1.66E+04 |
| 63-91-2 | N[C@@H](Cc1ccccc1)C(=O)O |  | - | - | -1.38E+00 | 2.69E+04 |
| 50-33-9 | O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2 |  | 245 | - | 3.16 | 47.5 |
| 100-63-0 | NNc1ccccc1 |  | 188 | 243.5 | 1.25 | 1.27E+05 |
| 92-12-6 | CN(C)CCOc2ccccc2Cc1ccccc1 |  | 1400 | - | 3.790 | - |
| 64-10-8 | O=C(N)Nc1ccccc1 |  | 2000 | 238 | 0.83 | 1.70E+04 |
| 553-69-5 | O[C@H](CNc1ccccn1)c2ccccc2 |  | 756 | - | 1.740 | - |
| 509-67-1 | CN5CC[C@@]32c6c4ccc(OCCN1CCOCC1)c6O[C@H]2[C@@H](O)C=C[C@H]3[C@H]5C4 |  | - | - | 0.590 | 2.00E+04 |
| 2310-17-0 | CCOP(=S)(OCC)SCN1c2ccc(Cl)cc2OC1=O |  | 85 | - | 4.38 | 3.05 |
| 732-11-6 | COP(=S)(OC)SCN2C(=O)c1ccccc1C2=O |  | 92.5 | - | 2.78 | 24.4 |
| 13171-21-6 | O=P(OC)(OC)OC(\C)=C(/Cl)C(=O)N(CC)CC |  | 8 | - | 0.79 | 1.00E+06 |
| 253-52-1 | c1cccc2cnncc12 |  | - | 316 | 0.57 | 5.00E+04 |
| 85-41-6 | O=C1NC(=O)c2ccccc12 |  | - | - | 1.15 | 360 |
| 131-67-9 | O=C(O)c1ccccc1C(=O)O[C@](C)(C#C)CC |  | - | - | - | - |
| 131-69-1 | O=S(=O)(NC(C)=O)c2ccc(NC(=O)c1ccccc1C(=O)O)cc2 |  | - | - | 1.260 | - |
| 57-47-6 | CNC(=O)Oc1cc2c(cc1)N(C)[C@H]3N(C)CC[C@]23C |  | 4.5 | - | 1.58 | 7760 |
| 62510-56-9 | Clc1ccc(cc1)[C@@H]2C[C@@H](N[C@@H]2C)C3CC3 |  | - | - | - | - |
| 98-98-6 | O=C(O)c1ccccn1 |  | - | - | 0.72 | 9.60E+05 |
| 21755-66-8 | C(CN1CCCCC1)N(Cc2ccccn2)c3ccccc3 |  | 806 | - | - | - |
| 32828-81-2 | O=C(NCc1cccnc1)c3cc(C(=O)NCc2cccnc2)c(OC)cc3 |  | 3000 | - | 1.530 | - |
| 39577-19-0 | Clc1ccc(cc1)CN2CCN(CC2)CCCOc3ccc4c(c3)OC(=O)C(C)=C4C |  | - | - | - | - |
| 56208-01-6 | C/C(C)=C\CCC(\C)=C\CCC(\C)=C\CN1CCN(CC1)Cc2ccc3OCOc3c2 |  | - | - | - | - |
| 60576-13-8 | O=C(Nc1cc(C)ccn1)[C@H](C)c2cccc(c2)C(=O)c3ccccc3 |  | - | - | - | - |
| 64000-73-3 | CN(C[C@H](C)O)c1ccc(NN)nn1 |  | - | - | - | - |
| 10001-43-1 | O=C2c1n(cnc1N(C)C(=O)N2C)CCNCc3cccnc3 |  | - | - | - | - |
| 13495-09-5 | O=C(OCC)C2(CCN(CCCNc1ccccc1)CC2)c3ccccc3 |  | - | - | 4.800 | - |
| 75-97-8 | CC(C)(C)C(C)=O |  | 610 | 106.1 | 1.2 | 1.90E+04 |
| 52463-83-9 | Clc1ccc2c(c1)C(=NCC(=O)N2CC#C)c3ccccc3 |  | 5819 | - | 2.910 | - |
| 13523-86-9 | CC(C)NCC(O)COc2cccc1nccc12 |  | 263 | - | 1.75 | 7880 |
| 540-38-5 | Ic1ccc(O)cc1 |  | - | - | 2.91 | 428 |
| 111025-46-8 | CCc1ccc(nc1)CCOc3ccc(C[C@H]2SC(=O)NC2=O)cc3 |  | - | - | - | - |
| 84-04-8 | NC(=O)C1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 |  | 620 | - | 4.44 | 0.037 |
| 1893-33-0 | Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)(C(N)=O)N3CCCCC3 |  | 160 | - | 2.02 | 81.7 |
| 2167-85-3 | O=C(OCCOCCN1CCCCC1)N2c4ccccc4Sc3cccnc23 |  | - | - | 4.940 | - |
| 27315-91-9 | CN1CCN(CC1)CC3(CCCC)C(=O)N(c2ccccc2)N(C3=O)c4ccccc4 |  | - | - | - | - |
| 3819-00-9 | CC(=O)c2cc3N(CCCN1CCC(CCO)CC1)c4ccccc4Sc3cc2 |  | 390 | - | 5.050 | - |
| 110-85-0 | C1CNCCN1 |  | 1900 | 146 | -1.50E+00 | 1.00E+06 |
| 110-89-4 | C1CCCCN1 |  | 400 | 106.2 | 0.84 | 1.00E+06 |
| 4546-39-8 | OC(c1ccccc1)(c2ccccc2)C(=O)OCCN3CCCCC3 |  | - | - | - | - |
| 94-62-2 | O=C(/C=C/C=C/c1ccc2OCOc2c1)N3CCCCC3 |  | 514 | - | 3.690 | 40 |
| 120-57-0 | O=Cc1ccc2OCOc2c1 |  | 2700 | 263 | 1.05 | 3500 |
| 94-53-1 | O=C(O)c1ccc2OCOc2c1 |  | - | - | 1.940 | - |
| 59-39-2 | c1ccc2O[C@H](COc2c1)CN3CCCCC3 |  | - | - | - | - |
| 2531-04-6 | CN1CCC(CC1)N2NC(=C(CC)C2=O)c3ccccc3 |  | - | - | 1.720 | 509 |
| 54-91-1 | O=C(CCBr)N1CCN(CC1)C(=O)CCBr |  | 220 | - | 0.42 | 2490 |
| 467-60-7 | OC(c1ccccc1)(c2ccccc2)[C@@H]3CCCCN3 |  | 180 | - | 3.450 | - |
| 17243-64-0 | O=C(OCC)/C=C2/S[C@H](N1CCCCC1)C(=O)N2CC |  | 3256 | - | 2.850 | - |
| 7491-74-9 | O=C1CCCN1CC(=O)N |  | - | - | -1.54E+00 | 8.30E+04 |
| 71002-09-0 | Clc1ccc(cc1)c2cn(nc2CC(=O)O)c3ccc(F)cc3 |  | - | - | - | - |
| 38677-81-5 | Oc1ccc(nc1CO)[C@H](O)CNC(C)(C)C |  | - | - | - | - |
| 1043-21-6 | O=C(O)c1cc(O)c2C3=Nc4ccccc4OC3=CC(=O)c2n1 |  | - | - | 1.430 | - |
| 55837-27-9 | O=C(O)c2cc(c(Oc1ccccc1)c(c2)N3CCCC3)S(N)(=O)=O |  | 5601 | - | 3.92 | 2.340 |
| 87-21-8 | Nc1ccccc1C(=O)OCC[C@@H]2CCCCN2 |  | - | - | 3.530 | - |
| 55285-45-5 | Clc1ccc(cc1)OC(C)(C)C(=O)OCc2cccc(CO)n2 |  | - | - | - | - |
| 302-41-0 | N#CC(CCN1CCC(CC1)(C(N)=O)N2CCCCC2)(c3ccccc3)c4ccccc4 |  | 320 | - | 3.91 | 0.491 |
| 72732-56-0 | COc3cc(Cc1cnc2nc(N)nc(N)c2c1C)c(OC)cc3 |  | 1168 | - | 2.13 | 132 |
| 79548-73-5 | O[C@@H]1[C@@H](O)[C@@H](O)[C@H](O[C@@H]1SC)[C@H](NC(=O)[C@@H]2C[C@@H](CC)CCN2)[C@H](C)Cl |  | - | - | - | - |
| 68252-19-7 | C[C@H]3CCC[C@@H](C)N3CCC[C@@](O)(c1ccccc1)c2ccccn2 |  | - | - | - | - |
| 50650-76-5 | CC=1C=C(C[C@H](C)CC(C)(C)C)N(O)C(=O)C=1 |  | - | - | 3.710 | - |
| 16378-21-5 | CCN4CC/C(=C1\c3ccccc3CCc2ccccc12)C4C |  | - | - | - | - |
| 36322-90-4 | OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 |  | 216 | - | 3.06 | 23 |
| 31793-07-4 | O=C(O)[C@@H](C)c1cc(Cl)c(cc1)N2CC=CC2 |  | 351 | - | 3.320 | - |
| 33817-20-8 | CC(C)(C)C(=O)OCOC(=O)[C@@H]2N3C(=O)[C@H](NC(=O)[C@H](N)c1ccccc1)[C@H]3SC2(C)C |  | 6000 | - | - | - |
| 63394-05-8 | Clc1ccc(cc1)OC(C)(C)C(=O)NC(=O)NCN2CCOCC2 |  | 4000 | - | - | - |
| 64218-02-6 | OC\C=C(/C)CC\C=C(/CC\C=C(/C)CC\C=C(/C)C)CO |  | 10900 | - | - | - |
| 100-01-6 | O=[N+]([O-])c1ccc(N)cc1 |  | 750 | 332 | 1.39 | 728 |
| 100-02-7 | O=[N+]([O-])c1ccc(O)cc1 |  | 202 | 279 | 1.91 | 1.16E+04 |
| 5947-49-9 | O=C(O)[C@@]2(C)CCC[C@]1(C)c3cc(O)ccc3CC[C@H]12 |  | - | - | 4.590 | - |
| 801-52-5 | NC(=O)OC[C@@H]3C=1C(=O)C(N)=C(C)C(=O)C=1N2C[C@@H]4N(C)[C@@H]4[C@]23OC |  | 68 | - | -0.960 | - |
| 156-43-4 | CCOc1ccc(N)cc1 |  | 540 | 254 | 1.24 | 7510 |
| 106-50-3 | Nc1ccc(N)cc1 |  | 80 | 267 | -0.3 | 3.70E+04 |
| 92-69-3 | Oc1ccc(cc1)c2ccccc2 |  | - | 305 | 3.2 | 56.2 |
| 104632-26-0 | CCCN[C@@H]1Cc2sc(N)nc2CC1 |  | - | - | - | - |
| 68497-62-1 | O=C1CCCN1CC(=O)NCCN(C(C)C)C(C)C |  | - | - | - | - |
| 140-65-8 | CCCCOc1ccc(cc1)OCCCN2CCOCC2 |  | - | - | 3.430 | - |
| 52549-17-4 | O=C(O)[C@@H](C)c1cc2Cc3cccnc3Oc2cc1 |  | 59.5 | - | - | - |
| 55268-74-1 | O=C1CN(C[C@@H]2c3ccccc3CCN12)C(=O)C4CCCCC4 |  | 2840 | - | 2.420 | 400 |
| 19216-56-9 | O=C(N1CCN(CC1)c3nc2cc(OC)c(OC)cc2c(N)n3)c4ccco4 |  | - | - | 1.280 | - |
| 53-03-2 | OCC(=O)[C@@]3(O)CC[C@H]2[C@@H]4CCC1=CC(=O)C=C[C@]1(C)[C@H]4C(=O)C[C@@]23C |  | - | - | 1.46 | 312 |
| 599-33-7 | OCC(=O)[C@@]4(O)C(=C)C[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3CCC1=CC(=O)C=C[C@@]12C |  | - | - | 1.810 | - |
| 145-13-1 | CC(=O)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C |  | - | - | 4.22 | 7.06 |
| 57526-81-5 | CC(C)NC[C@H](O)COc1ccc(O)cc1 |  | - | - | 0.940 | - |
| 511-45-5 | OC(CCN1CCCCC1)(c2ccccc2)c3ccccc3 |  | - | - | 4.220 | 33 |
| 90-34-6 | CC(CCCN)Nc1cc(cc2cccnc12)OC |  | - | - | 3.150 | - |
| 23288-49-5 | CC(C)(C)c2cc(SC(C)(C)Sc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C)cc(c2O)C(C)(C)C |  | 5000 | - | 10.91 | - |
| 59-46-1 | Nc1ccc(cc1)C(=O)OCCN(CC)CC |  | - | - | 2.14 | 9450 |
| 671-16-9 | CC(C)NC(=O)c1ccc(CNNC)cc1 |  | - | - | 0.08 | 1420 |
| 72332-33-3 | CC(C)N[C@@H](CC)[C@@H](O)c2ccc(O)c1NC(=O)C=Cc12 |  | - | - | - | - |
| 67747-09-5 | O=C(N(CCOc1c(Cl)cc(Cl)cc1Cl)CCC)n2ccnc2 |  | 1600 | - | 4.1 | 34 |
| 58-38-8 | CN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 |  | 1800 | - | 4.88 | 15 |
| 23249-97-0 | O=C(O)CCc1nc2ccccc2n1 |  | 1700 | - | - | - |
| 77-37-2 | O[C@](CCN1CCCC1)(c2ccccc2)C3CCCCC3 |  | - | - | 4.780 | - |
| 13931-64-1 | NC(=O)O[C@@H](CC)C1CCCCC1 |  | - | - | 3.160 | - |
| 32809-16-8 | Clc1cc(cc(Cl)c1)N2C(=O)[C@]3(C)C[C@@]3(C)C2=O |  | 7000 | - | 3.08 | 4.5 |
| 31314-38-2 | CC(C)N1CCC(CC1)(c2ccccc2)c3ccccc3 |  | - | - | 5.100 | - |
| 26399-36-0 | CCCN(CC1CC1)c2c(cc(cc2[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O |  | 1808 | - | 5.58 | 0.1 |
| 62666-20-0 | Clc1ccc(cc1)/C(=N\CCCC(N)=O)c2cc(F)ccc2O |  | 1350 | - | 3.06 | 70.9 |
| 57-83-0 | CC(=O)[C@H]3CC[C@H]2[C@@H]4CCC1=CC(=O)CC[C@]1(C)[C@H]4CC[C@]23C |  | - | - | 3.87 | 8.81 |
| 77-14-5 | C[C@@H]2CN(C)CCC[C@]2(OC(=O)CC)c1ccccc1 |  | - | - | 3.940 | - |
| 147-85-3 | O=C(O)[C@@H]1CCCN1 |  | - | - | -2.54E+00 | 1.62E+05 |
| 34184-77-5 | CCC(=O)[C@@]3(C)CC[C@H]2[C@@H]4CCC1=CC(=O)CCC1=C4CC[C@@]23C |  | - | - | - | - |
| 66532-85-2 | O=C(Oc1ccc(cc1)NC(C)=O)CN(CC)CC |  | - | - | - | - |
| 1918-16-7 | CC(C)N(C(=O)CCl)c1ccccc1 |  | 710 | - | 2.18 | 700 |
| 54063-53-5 | CCCNC[C@@H](O)COc2ccccc2C(=O)CCc1ccccc1 |  | - | - | 3.370 | - |
| 493-76-5 | CCN(CC)CCC(OC(=O)c1ccccc1)c2ccccc2 |  | - | - | 4.630 | - |
| 499-67-2 | CCN(CC)CCOC(=O)c1ccc(OCCC)c(N)c1 |  | - | - | 3.050 | - |
| 4354-45-4 | CN3CCC[C@H](OC(=O)[C@@](O)(c1ccccc1)C2CCCCC2)C3 |  | - | - | 3.510 | - |
| 551-27-9 | OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)C(CC)Oc1ccccc1)[C@H]3SC2(C)C |  | - | - | 2.65 | 22.7 |
| 362-29-8 | CCC(=O)c1cc2N(CC(C)N(C)C)c3ccccc3Sc2cc1 |  | - | - | 4.79 | 0.454 |
| 123-38-6 | CCC=O |  | 1410 | 48 | 0.59 | 3.06E+05 |
| 79-05-0 | CCC(N)=O |  | - | 213 | -0.66 | 4.91E+05 |
| 107-12-0 | CCC#N |  | 39 | 97.1 | 0.16 | 1.03E+05 |
| 93-55-0 | O=C(CC)c1ccccc1 |  | 4.49mL/kg | 217.5 | 2.19 | 2000 |
| 3670-68-6 | CCCOc1ccc(cc1)C(=O)CCN2CCCCC2 |  | - | - | - | - |
| 60569-19-9 | CN3CCC(OC(=O)C(OCCC)(c1ccccc1)c2ccccc2)CC3 |  | - | - | - | - |
| 2078-54-8 | CC(C)c1cccc(C(C)C)c1O |  | 500 | 256 | 3.79 | 124 |
| 525-66-6 | CC(C)NC[C@@H](O)COc2cccc1ccccc12 |  | 660 | - | 3.48 | 61.7 |
| 121-79-9 | Oc1cc(cc(O)c1O)C(=O)OCCC |  | 2100 | - | 1.8 | 3500 |
| 107-10-8 | CCCN |  | 370 | 47.2 | 0.48 | 1.00E+06 |
| 115-07-1 | C=CC |  | - | -4.76E+01 | 1.77 | 200 |
| 101-40-6 | C[C@H](NC)CC1CCCCC1 |  | 83 | 205 | 3.500 | - |
| 22760-18-5 | CC(C)N2c1cc(C)ccc1C(=NC2=O)c3ccccc3 |  | 759 | - | 3.020 | - |
| 466-06-8 | O=C1C=CC(=CO1)[C@@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CCC2=C[C@H](CC[C@@]23C)O[C@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O |  | 56 | - | 2.48 | 58.8 |
| 59-58-5 | Nc1nc(C)ncc1CN(C=O)C(/C)=C(/CCO)SSCCC |  | - | - | 1.850 | - |
| 303-69-5 | CN(C)CCCN1c3ccccc3Sc2cccnc12 |  | - | - | 4.010 | - |
| 136-70-9 | Oc1ccc(cc1O)[C@@H](O)CN[C@@H](C)Cc2ccc3OCOc3c2 |  | - | - | 1.760 | - |
| 438-60-8 | CNCCCC2c3ccccc3C=Cc1ccccc12 |  | 240 | - | 4.890 | 1.040 |
| 5696-09-3 | CC[C@@H](c1nc(CCN(CC)CC)on1)c2ccccc2 |  | - | - | - | - |
| 2537-29-3 | O=C1NC(=O)NC(=O)C1(C[C@@H](C)O)CC=C |  | - | - | -0.05 | 3.52E+04 |
| 603-00-9 | C[C@@H](O)Cn2cnc1c2C(=O)N(C)C(=O)N1C |  | 460 | - | -0.77 | 1.00E+06 |
| 3426-08-2 | C(CN1CCCCCC1)C(c2ccccc2)c3ccccc3 |  | - | - | 5.700 | - |
| 66-97-7 | O=C1C=Cc2cc3ccoc3cc2O1 |  | - | - | 1.67 | 1930 |
| 91-18-9 | n1ccnc2ncncc12 |  | - | - | -0.58 | 1.43E+05 |
| 53-79-2 | COc1ccc(cc1)C[C@@H](N)C(=O)N[C@H]4[C@@H](CO)O[C@@H](n3cnc2c3ncnc2N(C)C)[C@@H]4O |  | - | - | 0.03 | 50.3 |
| 81-54-9 | O=C2c1ccccc1C(=O)c3c2c(O)cc(O)c3O |  | - | - | 3.460 | 6.4 |
| 569-77-7 | Oc1cccc2C=C(O)C(O)=C(O)C(=O)c12 |  | - | - | 1.850 | - |
| 24691-76-7 | CC=2OCCCC=2C(=O)Nc1ccccc1 |  | 15000 | - | 2.080 | 600 |
| 15686-83-6 | CN2CCCN=C2/C=C/c1cccs1 |  | 170 | - | 3.140 | - |
| 290-37-9 | c1cnccn1 |  | - | 115 | -0.26 | 2.18E+05 |
| 13457-18-6 | O=C(OCC)c1cn2nc(cc2nc1C)OP(=S)(OCC)OCC |  | 218 | - | 3.8 | 4.2 |
| 129-00-0 | c1ccc2ccc3cccc4ccc1c2c34 |  | 2700 | 404 | 4.88 | 0.135 |
| 289-80-5 | c1cccnn1 |  | - | 208 | -0.72 | 1.00E+06 |
| 110-86-1 | c1ccccn1 |  | 891 | 115.2 | 0.65 | 1.00E+06 |
| 58-14-0 | CCc1nc(N)nc(N)c1c2ccc(Cl)cc2 |  | 440 | - | 2.69 | 121 |
| 1740-22-3 | OC(C=1C=C/C(C=1)=C(/c2ccccn2)c3ccccn3)(c4ccccn4)c5ccccn5 |  | - | - | 2.890 | - |
| 77-04-3 | CCC1(CC)C(=O)C=CNC1=O |  | 780 | - | 1.030 | - |
| 3563-49-3 | CCC[C@H](C(=O)c1ccc(C)cc1)N2CCCC2 |  | - | - | - | - |
| 91-82-7 | Clc3ccc(C/C(=C\CN1CCCC1)c2ccccc2)cc3 |  | - | - | 6.280 | - |
| 123-75-1 | C1CCCN1 |  | 300 | 86.5 | 0.46 | 1.00E+06 |
| 1018-71-9 | Clc2cncc2c1cccc(Cl)c1[N+]([O-])=O |  | 2000 | - | 3.750 | - |
| 36735-22-5 | Fc3ccccc3C2=NCC(=S)N(CC(F)(F)F)c1ccc(Cl)cc12 |  | 5000 | - | 4.03 | 1.340 |
| 1596-63-0 | OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c1nc2ccccc2nc1C(=O)O)[C@H]4SC3(C)C |  | - | - | 1.490 | - |
| 91-63-4 | Cc1ccc2ccccc2n1 |  | 1230 | 246.5 | 2.59 | 499 |
| 85441-61-8 | O=C(OCC)[C@H](CCc1ccccc1)N[C@@H](C)C(=O)N2Cc3ccccc3C[C@H]2C(=O)O |  | - | - | 3.720 | - |
| 152-43-2 | C#C[C@]5(O)CC[C@@H]2[C@]5(C)CC[C@@H]3c4ccc(OC1CCCC1)cc4CC[C@@H]23 |  | - | - | 6.460 | - |
| 73-49-4 | NS(=O)(=O)c1cc2C(=O)N[C@@H](Nc2cc1Cl)CC |  | - | - | 0.160 | 150 |
| 62265-68-3 | ClC(Cl)C(=O)N2CCCc1cc(ccc12)OC(=O)c3ccco3 |  | - | - | - | - |
| 130-95-0 | COc1cc2c(cc1)nccc2[C@@H](O)[C@@H]4C[C@@H]3CCN4C[C@@H]3C=C |  | - | - | 3.44 | 500 |
| 81-64-1 | O=C2c1ccccc1C(=O)c3c2c(O)ccc3O |  | 5000 | - | 3.940 | 0.0961 |
| 91-22-5 | c1cccc2cccnc12 |  | 331 | 237.1 | 2.03 | 6110 |
| 91-19-0 | c1cccc2nccnc12 |  | - | 229.5 | 1.32 | 6.60E+05 |
| 100-76-5 | C1CN2CCC1CC2 |  | 81.2 | - | 1.38 | 7.28E+04 |
| 22662-39-1 | Clc2cc(ccc2Oc1ccc(Cl)cc1)NC(=O)c3cc(I)cc(I)c3O |  | - | - | 8.140 | - |
| 84449-90-1 | Oc1ccc(cc1)c3sc2cc(O)ccc2c3C(=O)c5ccc(OCCN4CCCCC4)cc5 |  | - | - | - | - |
| 3615-24-5 | CC(C)NC=2C(=O)N(c1ccccc1)N(C)C=2C |  | - | - | 1.300 | - |
| 58994-96-0 | O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CNC(=O)N(CCCl)N=O)O[C@@H]1OC |  | 46.4 | - | -1.290 | 9000 |
| 66357-35-5 | [O-][N+](=O)\C=C(/NC)NCCSCc1ccc(CN(C)C)o1 |  | 5000 | - | 0.27 | 2.47E+04 |
| 80125-14-0 | CCN2CCC[C@H]2CNC(=O)c1c(OC)ccc(Br)c1OC |  | - | - | 2.1 | 74 |
| 73573-42-9 | Oc1ccc(cc1OC)/C=C/C(=O)O[C@@H]3C[C@@H]4CN5CCc2c6ccc(OC)cc6nc2[C@H]5C[C@H]4[C@H](C(=O)OC)[C@H]3OC |  | 15000 | - | - | - |
| 20788-07-2 | Brc2ccc(NC(=O)c1c(O)cccc1O)cc2 |  | - | - | 4.480 | - |
| 480-85-3 | O[C@@H]2CCN1CC=C(CO)[C@@H]12 |  | - | - | -0.560 | - |
| 3615-41-6 | O[C@@H](C)[C@H](O)[C@@H](O)[C@@H](O)C=O |  | - | - | -1.560 | - |
| 155-58-8 | COc1ccc(cc1O)/C=C/c2cc(cc(O)c2)O[C@@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O |  | - | - | - | - |
| 81-88-9 | [Cl-].O=C(O)c4ccccc4C=1c3ccc(cc3OC2=CC(\C=CC=12)=[N+](/CC)CC)N(CC)CC |  | - | - | 1.95 | 1.20E+04 |
| 36791-04-5 | NC(=O)c1ncn(n1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O |  | 2700 | - | -1.85E+00 | 4.74E+04 |
| 25546-65-0 | N[C@@H]3[C@@H](O)[C@H](O)[C@@H](CN)O[C@@H]3O[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O)[C@H]2O[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O |  | 10000 | - | -8.050 | - |
| 13392-28-4 | C[C@H](N)C12CC3CC(C1)CC(C2)C3 |  | - | - | - | - |
| 49697-38-3 | CCC(=O)[C@]3(C)[C@@]4(C)C[C@H](O)[C@H]2[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C |  | - | - | - | - |
| 77287-05-9 | O[C@@H]1CC(=O)[C@H](CCCCCCCO)[C@H]1/C=C\C[C@@](C)(O)CCCC |  | - | - | - | - |
| 106266-06-2 | CC=5N=C1CCCCN1C(=O)C=5CCN2CCC(CC2)c4noc3cc(F)ccc34 |  | 56.6 | - | 3.490 | - |
| 26652-09-5 | O[C@H](c1ccc(O)cc1)[C@H](C)NCCc2ccc(O)cc2 |  | - | - | - | - |
| 53716-44-2 | O[C@@]1(CCCC[C@H]1C(=O)O[C@@H](C)CN(CC)CC)C2CCCCC2 |  | - | - | 4.920 | - |
| 61413-54-5 | COc2ccc(cc2OC1CCCC1)[C@H]3CC(=O)NC3 |  | - | - | - | - |
| 84057-95-4 | CCCN2CCCC[C@@H]2C(=O)Nc1c(C)cccc1C |  | - | - | 2.9 | 57.6 |
| 84088-42-6 | CN(c1ccccc1)C(=O)C3=C(O)c2ccccc2N(C)C3=O |  | - | - | - | - |
| 35834-26-5 | CN(C)[C@H]3C[C@@H](C)O[C@@H](O[C@@H]1[C@@H](C)[C@H](O)CC(=O)O[C@H](CC)[C@@H](C)[C@@H]2O[C@@]2(C)C=CC(=O)[C@H](C)C[C@@H]1CC=O)[C@H]3O |  | - | - | 2.19 | 29.1 |
| 40034-42-2 | O=C(O)C2=CN(CC)c1cc(ccc1C2=O)c3ccncc3 |  | - | - | 2.220 | - |
| 83-79-4 | C=C(C)[C@@H]2Oc3ccc1C(=O)[C@H]4c5cc(OC)c(OC)cc5OC[C@H]4Oc1c3C2 |  | 60 | - | 4.1 | 0.2 |
| 92071-51-7 | NC[C@@H]1CC[C@H](CC1)C(=O)c2ccc(CCC(=O)O)cc2 |  | - | - | - | - |
| 101363-10-4 | CN1CCN(CC1)c4c(F)cc2c3N(C=C(C2=O)C(=O)O)CCSc34 |  | - | - | - | - |
| 104383-17-7 | Fc1ccc(cc1)OC[C@H](O)CN2CCC(CC2)N(C)c3nc4ccccc4s3 |  | - | - | 4.61 | - |
| 81-07-2 | O=C2NS(=O)(=O)c1ccccc12 |  | - | - | 0.91 | 4000 |
| 94-59-7 | C=CCc1ccc2OCOc2c1 |  | 1950 | 234.5 | 3.450 | 121 |
| 2315-08-4 | O=S(=O)(Nc1nc(C)cc(C)n1)c3ccc(/N=N/c2cc(C(=O)O)c(O)cc2)cc3 |  | - | - | - | - |
| 138-52-3 | OCc2ccccc2O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O |  | - | - | -1.22E+00 | 4.00E+04 |
| 90-02-8 | O=Cc1ccccc1O |  | 520 | 197 | 1.81 | 1.70E+04 |
| 94-67-7 | Oc1ccccc1\C=N\O |  | - | - | 1.390 | - |
| 87-17-2 | O=C(Nc1ccccc1)c2ccccc2O |  | - | - | 3.27 | 55 |
| 89-73-6 | O=C(NO)c1ccccc1O |  | 5000 | - | 0.910 | - |
| 63-36-5 | O=C([O-])c1ccccc1O |  | - | - | - | - |
| 69-72-7 | OC(=O)c1ccccc1O |  | 891 | - | 2.26 | 2240 |
| 89365-50-4 | OCc1cc(ccc1O)[C@H](O)CNCCCCCCOCCCCc2ccccc2 |  | - | - | - | - |
| 552-94-3 | O=C(Oc1ccccc1C(=O)O)c2ccccc2O |  | - | - | 3.360 | 110 |
| 89-31-6 | COc1cc2C(C)NCCc2cc1O |  | - | - | 1.510 | - |
| 6376-26-7 | CCN(CCOc2ccccc2C(=O)Nc1ccccc1)CC |  | - | - | 3.460 | - |
| 107-97-1 | CNCC(=O)O |  | - | - | -2.78E+00 | 3.00E+05 |
| 92-61-5 | COc1cc2C=CC(=O)Oc2cc1O |  | 3800 | - | 0.860 | - |
| 3366-95-8 | Cc1ncc([N+]([O-])=O)n1CC(O)C |  | - | - | 0.22 | 1.37E+04 |
| 101526-83-4 | O=S(C)(=O)Nc1ccc(cc1)C(=O)NCCN(CC)CC |  | - | - | - | - |
| 50-67-9 | Oc1cc2c(cc1)ncc2CCN |  | - | - | 0.21 | 2.00E+04 |
| 99592-32-2 | Clc1ccc(c(Cl)c1)[C@@H](Cn2ccnc2)OCc4csc3c(Cl)cccc34 |  | - | - | - | - |
| 28523-86-6 | FC(F)(F)C(OCF)C(F)(F)F |  | 10800 | 58.5 | 1.750 | - |
| 138-59-0 | O[C@@H]1CC(=C[C@@H](O)[C@H]1O)C(=O)O |  | - | - | -1.340 | 1.50E+05 |
| 69353-22-6 | Cc1cc2O[C@@]4(C)CC[C@@]5(C)[C@@H](C)CCC[C@@]53CO[C@@H](c2c(O)c1)[C@@H]34 |  | 1000 | - | - | - |
| 93-72-1 | Clc1cc(OC(C)C(=O)O)c(Cl)cc1Cl |  | 650 | - | 3.8 | 71 |
| 154-82-5 | O=C(COc1ccc(CCC)cc1OC)N2CCN(CC2)C(=O)COc3ccc(CCC)cc3OC |  | 1025 | - | - | - |
| 79902-63-9 | CC(C)(CC)C(=O)O[C@H]3C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@H]23 |  | 4438 | - | 4.68 | 0.765 |
| 532-32-1 | [Na+].[O-]C(=O)c1ccccc1 |  | 4070 | - | -2.270 | 5.56E+05 |
| 3930-20-9 | O=S(C)(=O)Nc1ccc(cc1)[C@H](O)CNC(C)C |  | - | - | 0.24 | 5510 |
| 1404-64-4 | CC=1NC(=O)NC(=O)C=1/C=C/C(=O)N[C@H](CO)CS(=O)CSC |  | - | - | -1.71E+00 | 7470 |
| 90-39-1 | C3CCCN4C[C@H]2C[C@H](CN1CCCC[C@@H]12)[C@H]34 |  | 960 | 325 | 2.730 | 3040 |
| 52-01-7 | CC(=O)S[C@@H]4CC1=CC(=O)CC[C@]1(C)[C@H]5CC[C@@]3(C)[C@@H](CC[C@]23CCC(=O)O2)[C@H]45 |  | 1000 | - | 2.78 | 22 |
| 111-01-3 | CC(C)CCC[C@@H](C)CCC[C@@H](C)CCCC[C@@H](C)CCC[C@H](C)CCCC(C)C |  | - | 350 | 14.63 | - |
| 111-02-4 | C\C(C)=C\CCC(\C)=C\CCC(\C)=C\CC\C=C(/C)CC\C=C(\C)CC\C=C(/C)C |  | - | - | 14.12 | - |
| 636-47-5 | O=C(Nc1cc(C(=O)NCCC(=N)N)n(C)c1)c3cc(NC(=O)c2cc(NC=O)cn2C)cn3C |  | - | - | - | - |
| 521-18-6 | O=C3C[C@H]4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)CC3 |  | - | - | 3.55 | 5.25E+05 |
| 10418-03-8 | C[C@]2(O)CC[C@H]1[C@@H]3CC[C@H]4Cc5nncc5C[C@]4(C)[C@H]3CC[C@]12C |  | - | - | - | - |
| 5197-58-0 | O=C3C[C@@H]4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)C=C3C |  | - | - | - | - |
| 83-48-7 | CC(C)[C@H](CC)/C=C/[C@@H](C)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C |  | - | - | 9.430 | - |
| 3930-19-6 | O=C(O)c3nc(c1nc2c(cc1)C(=O)C(OC)=C(N)C2=O)c(N)c(c3C)c4ccc(OC)c(OC)c4O |  | - | - | -0.560 | - |
| 18883-66-4 | O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1NC(=O)N(C)N=O |  | - | - | -1.45E+00 | 5070 |
| 57-24-9 | O=C2C[C@H]7OCC=C6CN4CC[C@@]53c1ccccc1N2[C@@H]3[C@H]7[C@H]6C[C@@H]45 |  | 2.35 | - | 1.93 | 160 |
| 94-35-9 | O[C@H](COC(N)=O)c1ccccc1 |  | - | - | 0.150 | - |
| 100-42-5 | C=Cc1ccccc1 |  | 2650 | 145 | 2.95 | 310 |
| 121-55-1 | O=S(=O)(CC)c1ccc(/C=N/NC(N)=S)cc1 |  | - | - | 1.040 | - |
| 30279-49-3 | NS(=O)(=O)c1cc(Cl)c(cc1)N2C(=O)C[C@@H](C2=O)c3ccccc3 |  | - | - | 0.690 | - |
| 56030-54-7 | CCC(=O)N(c1ccccc1)C2(COC)CCN(CC2)CCc3cccs3 |  | - | - | 3.95 | 76 |
| 68373-14-8 | O=S2(=O)C(C)(C)[C@@H](N1C(=O)C[C@H]12)C(=O)O |  | - | - | - | - |
| 41744-40-5 | OC(=O)[C@@H]2N3C(=O)[C@H](NC(=O)[C@@H](c1ccccc1)S(=O)(=O)O)[C@H]3SC2(C)C |  | - | - | 0.59 | 69.4 |
| 58095-31-1 | NC(=O)N[C@@H]2CCC(=O)c1sccc12 |  | 5000 | - | - | - |
| 350-12-9 | S=C3SCN(Cc1ccccc1)CN3Cc2ccccc2 |  | - | - | 4.350 | - |
| 485-41-6 | O=S(N)(=O)c2ccc(/N=N/c1c(cc(N)cc1N)C(=O)O)cc2 |  | - | - | 0.040 | - |
| 17784-12-2 | O=C1N=C(C=CN1CC)NS(=O)(=O)c2ccc(N)cc2 |  | - | - | -0.730 | 1750 |
| 115-68-4 | Nc1ccc(cc1)S(=O)(=O)NC(=O)/C=C(\C)C |  | - | - | 0.710 | - |
| 2447-57-6 | O=S(=O)(Nc1ncnc(OC)c1OC)c2ccc(N)cc2 |  | - | - | 0.7 | 2700 |
| 94-19-9 | O=S(=O)(Nc1nnc(CC)s1)c2ccc(N)cc2 |  | - | 185.75 | 1.01 | 3250 |
| 57-67-0 | Nc1ccc(cc1)S(=O)(=O)/N=C(\N)N |  | - | - | -1.22E+00 | 2200 |
| 27031-08-9 | Nc1ccc(cc1)S(=O)(=O)NC(=N)Nc2nc(C)c(C)o2 |  | - | - | - | - |
| 95-06-7 | C=C(Cl)CSC(=S)N(CC)CC |  | 850 | - | 3.150 | 100 |
| 57-68-1 | O=S(=O)(Nc1nc(C)cc(C)n1)c2ccc(N)cc2 |  | - | - | 0.89 | 1500 |
| 723-46-6 | Cc2cc(NS(=O)(=O)c1ccc(N)cc1)no2 |  | 6200 | - | 0.89 | 610 |
| 80-35-3 | O=S(=O)(Nc1ccc(OC)nn1)c2ccc(N)cc2 |  | 2739 | - | 0.32 | 147 |
| 32909-92-5 | COc2nsnc2NS(=O)(=O)c1ccc(N)cc1 |  | - | - | 1.880 | - |
| 63-74-1 | Nc1ccc(cc1)S(=O)(N)=O |  | 3900 | - | -0.62 | 7500 |
| 121-57-3 | Nc1ccc(cc1)S(O)(=O)=O |  | 12300 | - | -2.16E+00 | 1.08E+04 |
| 98-62-4 | Nc1ccc(cc1)S(=O)(F)=O |  | - | - | 1.710 | - |
| 116-42-7 | Nc1ccc(cc1)S(=O)(=O)NC(=O)c2ccc(OC(C)C)cc2 |  | - | - | 2.290 | - |
| 144-83-2 | O=S(=O)(Nc1ccccn1)c2ccc(N)cc2 |  | 15800 | - | 0.35 | 268 |
| 59-40-5 | Nc1ccc(cc1)S(=O)(=O)Nc2cnc3ccccc3n2 |  | 1370 | - | 1.68 | 7.5 |
| 599-79-1 | O=S(=O)(Nc1ccccn1)c3ccc(/N=N/c2cc(C(=O)O)c(O)cc2)cc3 |  | 15600 | - | 3.810 | - |
| 72-14-0 | O=S(=O)(Nc1nccs1)c2ccc(N)cc2 |  | - | - | 0.05 | 373 |
| 515-49-1 | Nc1ccc(cc1)S(=O)(=O)NC(N)=S |  | 3000 | - | -1.280 | 1.10E+04 |
| 852-19-7 | Nc1ccc(cc1)S(=O)(=O)Nc3cc(C)nn3c2ccccc2 |  | - | - | 2.090 | - |
| 66264-77-5 | Oc1ccc(cc1S(=O)C)[C@H](O)CN[C@H](C)CCc2ccc(OC)cc2 |  | - | - | - | - |
| 57-96-5 | O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3 |  | 358 | - | 2.3 | 31.2 |
| 95-05-6 | CCN(CC)C(=S)SC(=S)N(CC)CC |  | - | - | 2.710 | - |
| 515-64-0 | Cc2cc(NS(=O)(=O)c1ccc(N)cc1)nc(C)n2 |  | - | - | -0.33 | 1620 |
| 38194-50-2 | CS(=O)c1ccc(cc1)/C=C3/c2ccc(F)cc2C(CC(=O)O)=C3C |  | 264 | - | 3.42 | 3000 |
| 29334-07-4 | O=S(=O)(O)Oc1cc2c(cc1OS(=O)(=O)O)OC(=O)C=C2C |  | - | - | -3.870 | - |
| 73384-60-8 | CS(=O)c3ccc(c1nc2cccnc2n1)c(OC)c3 |  | 315 | - | 1.18 | 1430 |
| 54767-75-8 | CC(C)Sc1ccc(cc1)[C@H](O)[C@H](C)NCCCCCCCC |  | 1740 | - | - | - |
| 60325-46-4 | O[C@@H]2CC(=O)[C@@H](C/C=C\CCCC(=O)NS(C)(=O)=O)[C@H]2/C=C/[C@@H](O)COc1ccccc1 |  | - | - | 1.580 | - |
| 53583-79-2 | CCN2CCC[C@@H]2CNC(=O)c1cc(ccc1OC)S(=O)(=O)CC |  | - | - | 1.06 | 724 |
| 103628-46-2 | CNS(=O)(=O)Cc1cc2c(cc1)ncc2CCN(C)C |  | - | - | 0.93 | 2.14E+04 |
| 40828-46-4 | O=C(c1ccc(cc1)[C@H](C)C(=O)O)c2cccs2 |  | 70.6 | - | 2.820 | - |
| 53813-83-5 | CN1CCN(CC1)C(=O)O[C@@H]5C=2SCCSC=2C(=O)N5c3ccc4ccc(Cl)nc4n3 |  | - | - | 2.180 | - |
| 27470-51-5 | O=C(O)CCC(=O)OCC2(CCCC)C(=O)N(c1ccccc1)N(C2=O)c3ccccc3 |  | 1700 | - | - | - |
| 87-90-1 | ClN1C(=O)N(Cl)C(=O)N(Cl)C1=O |  | 406 | - | 0.940 | 1.20E+04 |
| 134-96-3 | COc1cc(cc(OC)c1O)C=O |  | - | - | 0.880 | - |
| 321-64-2 | Nc1c3ccccc3nc2CCCCc12 |  | 70 | - | 2.71 | 217 |
| 47747-56-8 | N[C@H](c1ccccc1)C(=O)N[C@@H]5C(=O)N4[C@@H](C(=O)OC3OC(=O)c2ccccc23)C(C)(C)S[C@@H]45 |  | - | - | 1.700 | - |
| 16188-61-7 | CN(C)CCN2N=C(Cc1ccccc1)c3ccccc3C2=O |  | - | - | - | - |
| 82989-25-1 | O=C(OCCCC)C(=O)Nc1cccc(c1)c2nnnn2 |  | 4000 | - | - | - |
| 4267-05-4 | NS(=O)(=O)c2cc1c(N[C@@H](NS1(=O)=O)C(Cl)(Cl)Cl)cc2Cl |  | - | - | 0.82 | 43.8 |
| 5560-78-1 | ClC(Cl)C(=O)N(CCOCC)Cc1ccc(CN(CCOCC)C(=O)C(Cl)Cl)cc1 |  | - | - | 3.030 | - |
| 124-72-1 | FC(F)(F)[C@H](Br)F |  | - | 8.6 | 1.950 | 2270 |
| 80880-90-6 | CN1CCN(CC1)CC(=O)N3c2c(csc2C)C(=O)Nc4ccccc34 |  | - | - | - | - |
| 66148-78-5 | OC(=O)[C@@H]2N3C(=O)[C@](NC(=O)[C@@H](c1ccsc1)C(=O)O)(OC)[C@H]3SC2(C)C |  | - | - | - | - |
| 85622-93-1 | NC(=O)c1ncn2C(=O)N(C)N=Nc12 |  | - | - | - | - |
| 3810-35-3 | O=C(Nc1ncc(s1)[N+]([O-])=O)c2cccs2 |  | - | - | 2.090 | - |
| 59804-37-4 | OC=2c1sccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 |  | 79 | - | 2.400 | - |
| 63590-64-7 | O=C(N1CCN(CC1)c3nc2cc(OC)c(OC)cc2c(N)n3)C4CCCO4 |  | - | - | 1.470 | - |
| 5902-51-2 | O=C1NC(C)=C(Cl)C(=O)N1C(C)(C)C |  | 1700 | - | 1.89 | 710 |
| 23031-25-6 | Oc1cc(cc(O)c1)[C@@H](O)CNC(C)(C)C |  | - | - | 0.9 | 2.13E+05 |
| 67915-31-5 | CC(C)N1CCN(CC1)c2ccc(cc2)OC[C@H]4CO[C@@](Cn3ncnc3)(O4)c5ccc(Cl)cc5Cl |  | - | - | - | - |
| 37686-84-3 | CCN(CC)C(=O)N[C@H]1C[C@@H]2c3cccc4ncc(C[C@@H]2N(C)C1)c34 |  | 100 | - | - | - |
| 15793-40-5 | CC(C)(C)N[C@@H](C)CC(c1ccccc1)c2ccccc2 |  | - | - | 5.420 | - |
| 83688-84-0 | CC(C)(C)NC[C@@H](O)COc1cccc2CCCSc12 |  | - | - | - | - |
| 968-93-4 | O=C3C=C4CC[C@@H]1[C@H](CC[C@]2(C)OC(=O)CC[C@@H]12)[C@@]4(C)C=C3 |  | - | - | 2.090 | - |
| 58-22-0 | O=C4CC[C@@]3(C)C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@H]1O)=C4 |  | - | - | 3.32 | 23.4 |
| 76-23-3 | O=C1NC(=O)NC(=O)C1(CC)[C@@H](CC)CCC |  | - | - | 2.500 | - |
| 58-46-8 | CC(C)C[C@@H]2CN3CCc1cc(OC)c(OC)cc1[C@H]3CC2=O |  | - | - | 2.660 | - |
| 60-54-8 | NC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@]2(O)C1=O)C(=O)c3c(O)cccc3[C@@]4(C)O |  | 807 | - | -1.30E+00 | 231 |
| 116-29-0 | Clc1cc(c(Cl)cc1Cl)S(=O)(=O)c2ccc(Cl)cc2 |  | 566 | - | 4.61 | 0.078 |
| 109-99-9 | C1CCCO1 |  | 1650 | 65 | 0.46 | 1.00E+06 |
| 4747-99-3 | Oc1ccc(cc1O)C[C@H]3NCCc2cc(O)c(O)cc23 |  | - | - | - | - |
| 142-68-7 | C1CCCCO1 |  | - | 88 | 0.95 | 8.02E+04 |
| 632-22-4 | CN(C)C(=O)N(C)C |  | 794 | 176.5 | 0.19 | 1.00E+06 |
| 10379-14-3 | Clc1ccc2c(c1)C(=NCC(=O)N2C)C3=CCCCC3 |  | - | - | 3.2 | 26.4 |
| 319-89-1 | OC=1C(=O)C(O)=C(O)C(=O)C=1O |  | - | - | 1.210 | - |
| 50-35-1 | O=C1NC(=O)CCC1N3C(=O)c2ccccc2C3=O |  | 113 | - | 0.33 | 545 |
| 115-37-7 | COC1=CC=C3[C@H]2Cc4ccc(OC)c5O[C@@H]1[C@]3(CCN2C)c45 |  | 114 | - | 2.020 | 680 |
| 467-98-1 | O=C3C=CC4[C@H]2Cc1ccc(OC)c(O)c1[C@@]4(CCN2C)C3 |  | - | - | 1.260 | 4000 |
| 91-79-2 | CN(C)CCN(Cc1ccsc1)c2ccccn2 |  | - | - | 2.550 | 4440 |
| 83-67-0 | Cn1cnc2c1C(=O)NC(=O)N2C |  | 1265 | - | -0.78 | 330 |
| 54504-70-0 | Clc1ccc(cc1)OC(C)(C)C(=O)OCCn3cnc2c3C(=O)N(C)C(=O)N2C |  | 17000 | - | - | - |
| 58-55-9 | O=C2c1ncnc1N(C)C(=O)N2C |  | 225 | - | -0.02 | 7360 |
| 148-79-8 | n1c3ccccc3nc1c2cscn2 |  | 2080 | - | 2.47 | 50 |
| 5581-52-2 | O=[N+]([O-])c3ncn(C)c3Sc2nc(N)nc1ncnc12 |  | - | - | 0.960 | - |
| 77-27-0 | O=C1NC(=S)NC(=O)C1(CC=C)[C@H](C)CCC |  | - | - | 3.23 | 49.4 |
| 5845-26-1 | CN(C)CCN1c3ccccc3S[C@H](CC1=O)c2ccccc2 |  | - | - | - | - |
| 288-47-1 | c1cncs1 |  | - | 118 | 0.44 | 5.38E+04 |
| 473-30-3 | O=S(=O)(c1cnc(N)s1)c2ccc(N)cc2 |  | - | - | 0.520 | 400 |
| 59669-26-0 | CN(SN(C)C(=O)O\N=C(\C)SC)C(=O)O\N=C(\C)SC |  | 66 | - | 1.7 | 35 |
| 154-42-7 | NC2=Nc1ncnc1C(=S)N2 |  | - | - | -0.07 | 3.63E+04 |
| 110-02-1 | c1cccs1 |  | 1400 | 84 | 1.81 | 3010 |
| 108-98-5 | Sc1ccccc1 |  | 46.2 | 169.1 | 2.52 | 835 |
| 84-06-0 | CC(=O)OCCN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 |  | - | - | 4.820 | 8.92 |
| 316-81-4 | CN(C)S(=O)(=O)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 |  | - | - | 2.950 | - |
| 50-52-2 | CN4CCCCC4CCN1c3ccccc3Sc2ccc(SC)cc12 |  | 995 | - | 5.9 | 0.034 |
| 7283-41-2 | SC(=O)c1ccccc1O |  | - | - | - | - |
| 5591-45-7 | CN(C)S(=O)(=O)c2cc3C(=C\CCN1CCN(C)CC1)\c4ccccc4Sc3cc2 |  | 720 | - | 3.780 | 0.760 |
| 62-56-6 | NC(N)=S |  | 125 | - | -1.08E+00 | 1.42E+05 |
| 492-22-8 | O=C1c3ccccc3Sc2ccccc12 |  | - | 373 | 3.99 | 1.150 |
| 82-99-5 | CCN(CC)CCSC(=O)C(c1ccccc1)c2ccccc2 |  | - | - | - | - |
| 137-26-8 | CN(C)C(=S)SSC(=S)N(C)C |  | 560 | - | 1.73 | 30 |
| 655-05-0 | CN(C)C1=NC(=O)[C@@H](O1)c2ccccc2 |  | 3000 | - | -0.230 | - |
| 72-19-5 | O=C(O)[C@@H](N)[C@@H](C)O |  | - | - | -2.94E+00 | 9.70E+04 |
| 50-89-5 | CC1=CN(C(=O)NC1=O)[C@H]2C[C@H](O)[C@@H](CO)O2 |  | - | - | -0.93 | 7960 |
| 65-71-4 | CC1=CNC(=O)NC1=O |  | - | - | -0.62 | 3820 |
| 89-83-8 | CC(C)c1ccc(C)cc1O |  | 980 | 232.5 | 3.3 | 900 |
| 76-61-9 | CC(C)c1cc(c(C)cc1O)C3(OS(=O)(=O)c2ccccc23)c4cc(C(C)C)c(O)cc4C |  | - | - | 7.210 | 110 |
| 125-20-2 | CC(C)c1cc(c(C)cc1O)C3(OC(=O)c2ccccc23)c4cc(C(C)C)c(O)cc4C |  | - | - | 7.060 | - |
| 6964-20-1 | OCCSCCCCCCCCCCSCCO |  | - | - | 3.880 | - |
| 71116-82-0 | O[C@H](COc1ccsc1)/C=C/[C@H]2[C@@H](C\C=C\CCCC(=O)O)[C@@H](O)C[C@@H]2O |  | - | - | - | - |
| 32527-55-2 | OCCN1CCN(CC1)C(=O)CN2c3cc(Cl)ccc3SC2=O |  | 3600 | - | 1.04 | 739 |
| 31932-09-9 | C[C@H]2CCC[C@@H](C)N2C(=S)Nc1cc(ccc1)C(F)(F)F |  | - | - | - | - |
| 34787-01-4 | OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)[C@@H](c1ccsc1)C(=O)O)[C@H]3SC2(C)C |  | - | - | 1.010 | - |
| 40180-04-9 | O=C(c1ccc(OCC(=O)O)c(Cl)c1Cl)c2cccs2 |  | - | - | 3.590 | - |
| 102507-71-1 | Nc1nc(cs1)\C(=N\OCC(=O)O)C(=O)N[C@@H]2C(=O)N(OS(=O)(=O)O)C2(C)C |  | - | - | - | - |
| 51931-66-9 | CN(C)[C@@H]2C=CCC[C@]2(C(=O)OCC)c1ccccc1 |  | - | - | - | - |
| 85136-71-6 | CC(C)(C)NC[C@@H](O)COC1=CN(C)C(=O)c2ccccc12 |  | - | - | - | - |
| 27591-97-5 | CCN(CC)CCOc2ccc3c1ccc(cc1C(=O)c3c2)OCCN(CC)CC |  | - | - | - | - |
| 57648-21-2 | Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)N3c4ccccc4NC3=S |  | 232 | - | 4.510 | - |
| 26839-75-8 | O[C@H](COc1nsnc1N2CCOCC2)CNC(C)(C)C |  | - | - | 1.83 | 2740 |
| 444-27-9 | O=C(O)C1CSCN1 |  | 875 | - | -3.040 | - |
| 22619-35-8 | Clc1ccc(s1)[C@@H](C[C@H](O)c2ccc(Cl)cc2)C3=C(O)c4ccccc4OC3=O |  | - | - | 5.480 | - |
| 65899-73-2 | Clc3sccc3CO[C@H](Cn1ccnc1)c2ccc(Cl)cc2Cl |  | 770 | - | - | - |
| 2205-73-4 | CC(=O)S[C@@H]3CC1=CC(=O)C[C@H](SC(C)=O)[C@]1(C)[C@H]4CC[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@H]34 |  | 10000 | - | 2.360 | - |
| 4991-65-5 | Oc1cc2OC(=O)Sc2cc1 |  | 633 | - | 1.670 | - |
| 5169-78-8 | CN1CCC\C(C1)=C(/c2sccc2)c3cccs3 |  | - | - | - | - |
| 51-24-1 | O=C(O)Cc2cc(I)c(Oc1cc(I)c(O)cc1)c(I)c2 |  | - | - | 5.670 | - |
| 55837-29-1 | CCCN(CCC)C(=O)[C@@H](NC(=O)c1ccccc1)Cc2ccc(OCCN(CC)CC)cc2 |  | 800 | - | - | - |
| 61951-99-3 | SCC(=O)[C@@]4(O)CC[C@H]2[C@]4(C)C[C@H](O)[C@@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 |  | - | - | - | - |
| 14679-73-3 | O=C(OCC)NNc2nncc1ccccc12 |  | 318 | - | - | - |
| 15301-93-6 | Cc1ccccc1[C@H](OCCNC)c2ccccc2 |  | - | - | 3.440 | - |
| 22345-47-7 | COc1ccc(cc1OC)C3=NN=C(C)[C@@H](CC)c2cc(OC)c(cc23)OC |  | 825 | - | 5.390 | - |
| 1156-19-0 | Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2CCCCCC2 |  | 5000 | - | 2.69 | 65.4 |
| 59-98-3 | c2cc(CC1=NCCN1)ccc2 |  | - | - | 2.65 | 373 |
| 64-77-7 | Cc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC |  | 2490 | - | 2.34 | 109 |
| 50838-36-3 | Cc1cc(ccc1)N(C)C(=S)Oc2ccc4c(c2)[C@@H]3CC[C@@H]4C3 |  | 1800 | - | 6.490 | - |
| 2933-94-0 | CC(C)NC[C@@H](O)COc1cc(C)ccc1 |  | - | - | 1.970 | - |
| 4201-22-3 | Cc2cc(Cl)c(NC1=NCCN1)cc2 |  | - | - | 1.8 | 1.15E+04 |
| 29218-27-7 | OC[C@@H]2CN(c1cccc(C)c1)C(=O)O2 |  | 1225 | - | 1.880 | - |
| 728-88-1 | C[C@H](CN1CCCCC1)C(=O)c2ccc(C)cc2 |  | 1450 | - | 3.65 | 195 |
| 69004-03-1 | O=C3N(c2cc(C)c(Oc1ccc(SC(F)(F)F)cc1)cc2)C(=O)NC(=O)N3C |  | - | - | - | - |
| 108-88-3 | Cc1ccccc1 |  | 636 | 110.6 | 2.73 | 526 |
| 3686-58-6 | O=C(Nc1c(C)cccc1C(=O)OC)CN(CC)CC |  | - | - | 2.300 | - |
| 97240-79-4 | NS(=O)(=O)OC[C@]23OC[C@H]1OC(C)(C)O[C@H]1[C@@H]3OC(C)(C)O2 |  | - | - | - | - |
| 89778-26-7 | CN(C)CCOc1ccc(cc1)\C(c2ccccc2)=C(/CCCl)c3ccccc3 |  | 1700 | - | - | - |
| 100490-36-6 | O=C(O)C2=CN(c1nc(c(F)cc1C2=O)N3CCC(N)C3)c4ccc(F)cc4F |  | - | - | - | - |
| 606-58-6 | Nc3ncnc1c3c(cn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C#N |  | - | - | -0.420 | - |
| 27203-92-5 | O[C@@]1(CCCC[C@@H]1CN(C)C)c2cc(OC)ccc2 |  | 228 | - | 3.010 | - |
| 1082-57-1 | C2CCCc3cccc(NC1=NCCN1)c23 |  | - | - | 2.530 | - |
| 53902-12-8 | COc1cc(ccc1OC)/C=C/C(=O)Nc2ccccc2C(=O)O |  | 1100 | - | 3.620 | - |
| 15421-84-8 | CCN(CC)c1cc(C)nc2ncnn12 |  | 235 | - | 1.620 | - |
| 19794-93-5 | Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O |  | 690 | - | 3.210 | - |
| 10161-33-8 | O=C3C=C4CC[C@@H]2C(C=C[C@@]1(C)[C@H]2CC[C@H]1O)=C4CC3 |  | - | - | - | - |
| 5192-84-7 | CC(=O)[C@H]2CC[C@H]3[C@@H]4C=C(Cl)C1=CC(=O)C=C[C@@]1(C)[C@@H]4CC[C@]23C |  | - | - | 3.730 | - |
| 30418-38-3 | COc1cc(cc(OC)c1OC)C[C@@H]3NCCc2cc(O)c(O)cc23 |  | - | - | - | - |
| 68-76-8 | O=C1C=C(C(=O)C(=C1N2CC2)N3CC3)N4CC4 |  | - | 357.5 | -0.13 | 3.94E+05 |
| 24017-47-8 | CCOP(=S)(OCC)Oc1ncn(n1)c2ccccc2 |  | 57 | - | 3.34 | 39 |
| 10310-32-4 | O[C@H]2[C@@H](OCc1ccccc1)[C@H](O[C@H]2OCC)[C@H](COCc3ccccc3)OCc4ccccc4 |  | 20000 | - | 4.940 | - |
| 87-10-5 | Oc1c(cc(Br)cc1Br)C(=O)Nc2ccc(Br)cc2 |  | 410 | - | 5.970 | - |
| 133-67-5 | NS(=O)(=O)c2cc1c(N[C@H](NS1(=O)=O)C(Cl)Cl)cc2Cl |  | 5600 | - | 0.62 | 800 |
| 101-20-2 | Clc2ccc(NC(=O)Nc1ccc(Cl)cc1)cc2Cl |  | 34600 | - | 4.900 | - |
| 112-24-3 | NCCNCCNCCN |  | 2500 | 266.5 | -2.650 | 4.77E+06 |
| 121-44-8 | CCN(CC)CC |  | 460 | 89 | 1.45 | 7.37E+04 |
| 280-57-9 | C1CN2CCN1CC2 |  | 1700 | 174 | -0.490 | 4.50E+05 |
| 51-18-3 | n1c(nc(nc1N2CC2)N3CC3)N4CC4 |  | 13 | - | 2.560 | 4.00E+05 |
| 1420-06-0 | c1ccccc1C(N2CCOCC2)(c3ccccc3)c4ccccc4 |  | 83 | - | 4.210 | 0.02 |
| 2622-37-9 | FC(F)(F)c1cc2N(CC(C)CN(C)C)c3ccccc3Sc2cc1 |  | - | - | - | - |
| 117-89-5 | FC(F)(F)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 |  | - | - | 5.03 | 12.2 |
| 749-13-3 | FC(F)(F)c1cccc(c1)C3(O)CCN(CCCC(=O)c2ccc(F)cc2)CC3 |  | 140 | - | 4.520 | - |
| 146-54-3 | FC(F)(F)c1cc2N(CCCN(C)C)c3ccccc3Sc2cc1 |  | 185 | - | 5.54 | 0.175 |
| 1582-09-8 | [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)C(F)(F)F |  | 1930 | - | 5.34 | 0.184 |
| 70-00-8 | FC(F)(F)C1=CN(C(=O)NC1=O)[C@H]2C[C@H](O)[C@@H](CO)O2 |  | - | - | -0.46 | 1560 |
| 322-79-2 | O=C(C)Oc1cc(ccc1C(=O)O)C(F)(F)F |  | 402 | - | 2.090 | - |
| 13647-35-3 | N#C[C@@H]2C[C@]4(C)C5CC[C@@]1(C)C(CC[C@@H]1O)C5CC[C@]43O[C@@H]3C2=O |  | 15000 | - | 2.020 | - |
| 616-68-2 | O=C(Nc1c(C)cc(C)cc1C)CN(CC)CC |  | - | - | 2.41 | 211 |
| 552-30-7 | O=C(O)c1ccc2C(=O)OC(=O)c2c1 |  | - | 390 | 1.950 | 1040 |
| 84-96-8 | CN(C)CC(C)CN1c3ccccc3Sc2ccccc12 |  | 210 | - | 4.71 | 0.942 |
| 5011-34-7 | COc2ccc(CN1CCNCC1)c(OC)c2OC |  | - | - | 0.630 | - |
| 738-70-5 | Nc2nc(N)ncc2Cc1cc(OC)c(OC)c(OC)c1 |  | 5300 | - | 0.91 | 400 |
| 635-41-6 | O=C(c1cc(OC)c(OC)c(OC)c1)N2CCOCC2 |  | 1800 | - | -0.150 | - |
| 52128-35-5 | COc1cc(cc(OC)c1OC)NCc2ccc3nc(N)nc(N)c3c2C |  | - | - | 2.55 | 31.4 |
| 739-71-9 | CN(C)C[C@@H](C)CN2c3ccccc3CCc1ccccc12 |  | - | - | 5.430 | - |
| 69900-72-7 | O[C@H](/C=C\[C@@H]1[C@H](C\C=C\CCCC(=O)O)C(=O)C[C@@H]1C)C(C)(C)CCCC |  | 22 | - | - | - |
| 73803-48-2 | NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN3C[C@@H]4[C@@H]2CC[C@H](C2)[C@@H]4C3 |  | 8000 | - | - | - |
| 91-81-6 | CN(C)CCN(Cc1ccccc1)c2ccccn2 |  | - | - | 2.730 | 587 |
| 217-59-4 | c3cccc4c1ccccc1c2ccccc2c34 |  | - | 425 | 5.49 | 0.0411 |
| 519-73-3 | c1ccccc1C(c2ccccc2)c3ccccc3 |  | - | 359 | 5.370 | 0.664 |
| 486-12-4 | Cc1ccc(cc1)C(=C\CN2CCCC2)\c3ccccn3 |  | - | - | 3.92 | 74.9 |
| 477-75-8 | c1ccc3c(c1)C4c2ccccc2C3c5ccccc45 |  | - | - | 4.870 | - |
| 14504-73-5 | COc1c5OCOc5cc2CCN(C)[C@@H](c12)[C@H]4OC(=O)c3c(N)c(OCC)c(OCC)c(OCC)c34 |  | 15000 | - | - | - |
| 22089-22-1 | O=P1(OCCCN1CCCl)N(CCCl)CCCl |  | 202 | - | 2.270 | - |
| 53783-83-8 | CN(C)CCOCC(=O)NC12CC3CC(C1)CC(C2)C3 |  | - | - | 1.790 | - |
| 552-63-6 | OC[C@@H](C(=O)O)c1ccccc1 |  | - | - | 0.380 | 2.00E+04 |
| 88669-04-9 | CCCC[C@@H]1O[C@H]2O[C@H]3[C@H](O[C@@]2(O)C(=O)C1)[C@@H](NC)[C@@H](O)[C@@H](NC)[C@@H]3O |  | - | - | - | - |
| 61-54-1 | NCCc2cnc1ccccc12 |  | - | - | 1.55 | 3.30E+04 |
| 526-55-6 | OCCc2cnc1ccccc12 |  | - | - | 1.630 | - |
| 69-33-0 | Nc3ncnc1c3ccn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O |  | 16 | - | -0.8 | 3000 |
| 2501-37-3 | COc1ccc(/C=C/NC=O)cc1 |  | - | - | - | - |
| 41570-61-0 | OC(CNC(C)(C)C)c1ccccc1Cl |  | - | - | - | - |
| 51-67-2 | Oc1ccc(CCN)cc1 |  | - | - | 0.860 | 1.04E+04 |
| 60-18-4 | Oc1ccc(C[C@H](N)C(=O)O)cc1 |  | - | - | -2.26E+00 | 479 |
| 118-78-5 | NC1C(=O)NC(=O)NC1=O |  | - | - | -1.990 | - |
| 302-49-8 | O=P(NC(=O)OCC)(N1CC1)N2CC2 |  | - | - | -0.370 | - |
| 58-96-8 | O=C1NC(=O)N(C=C1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O |  | - | - | -1.98E+00 | 6.12E+04 |
| 4171-13-5 | CC[C@@H](C(N)=O)[C@H](C)CC |  | 760 | - | 1.640 | - |
| 124027-47-0 | Nc1c3ccccc3nc2CCC[C@H](O)c12 |  | - | - | - | - |
| 93413-69-5 | OC1(CCCCC1)[C@H](CN(C)C)c2ccc(OC)cc2 |  | - | - | 3.280 | - |
| 66644-81-3 | C=CCN2CCC[C@@H]2CNC(=O)c1cc(cc(OC)c1OC)S(N)(=O)=O |  | - | - | 1.47 | 215 |
| 52-53-9 | COc1cc(ccc1OC)[C@@](C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C |  | 163 | - | 3.79 | 4.470 |
| 93-47-0 | O=C(N/N=C/c1ccc(OC)c(OC)c1)c2ccncc2 |  | - | - | - | - |
| 1929-77-7 | O=C(SCCC)N(CCC)CCC |  | 1200 | - | 3.84 | 90 |
| 18542-37-5 | O[C@H]3C[C@@]1(COC(=O)C(=C)[C@@H]1[C@H]2OC(=O)C(=C)[C@@H]23)C=C |  | - | - | 0.31 | 2.96E+04 |
| 81840-15-5 | O=C(c1ccc(OC)c(OC)c1)N2CCN(CC2)c3cc4CCC(=O)Nc4cc3 |  | 7594 | - | - | - |
| 46817-91-8 | CCOc2ccccc2OC[C@@H]1CNCCO1 |  | 2000 | - | 1.750 | - |
| 21363-18-8 | C[C@@H](CC)N(C[C@H](O)c2cccn2Cc1ccccc1Cl)[C@@H](C)CC |  | - | - | 5.280 | - |
| 50471-44-8 | O=C1N(C(=O)O[C@@]1(C)C=C)c2cc(Cl)cc(Cl)c2 |  | 10000 | - | 3.1 | 2.6 |
| 70704-03-9 | O=C(OC)C1=CC[C@@H]2c3n1c4ccccc4c3CCN2CC |  | - | - | - | - |
| 2430-49-1 | O=C1NC(=O)NC(=O)C1(C=C)[C@H](C)CCC |  | - | - | 1.870 | - |
| 59-02-9 | CC(C)CCC[C@H](C)CCC[C@H](C)CCC[C@@]1(C)CCc2c(O1)c(C)c(C)c(O)c2C |  | - | - | 12.18 | - |
| 58-95-7 | CC(=O)Oc2c(C)c(C)c1O[C@](C)(CCc1c2C)CCC[C@H](C)CCC[C@H](C)CCCC(C)C |  | - | - | 12.26 | - |
| 81-81-2 | CC(=O)CC(C1=C(O)c2ccccc2OC1=O)c3ccccc3 |  | 1.6 | - | 2.6 | 17 |
| 69-89-6 | O=C1NC(=O)Nc2ncnc12 |  | - | - | -0.73 | 69 |
| 580-74-5 | Oc2ccc(/C=C(\[N+]#[C-])/C(/[N+]#[C-])=C\c1ccc(O)cc1)cc2 |  | - | - | - | - |
| 90-47-1 | O=C1c3ccccc3Oc2ccccc12 |  | - | 351 | 3.39 | 4.520 |
| 146-80-5 | Oc3nc1c(ncn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)c(O)n3 |  | - | - | -1.800 | - |
| 30187-90-7 | CC(C)(C)NC[C@H](O)COc1cccc(C)c1C |  | - | - | - | - |
| 56187-89-4 | O=C(O)[C@H](C)c1ccc(cc1)[C@H]2C/C(CCC2)=N\O |  | - | - | 2.400 | - |
| 14293-44-8 | O=S(N)(=O)c1cc(c(O)cc1Cl)C(=O)Nc2c(C)cccc2C |  | 1640 | - | 2.19 | 58 |
| 7361-61-7 | Cc2cccc(C)c2NC1=NCCCS1 |  | 130 | - | 4.520 | - |
| 526-36-3 | CC(C)(C)c2cc(C)c(CC1=NCCN1)c(C)c2 |  | - | - | 5.350 | - |
| 146-48-5 | O=C(OC)[C@H]2[C@@H](O)CC[C@H]3CN4CCc1c5ccccc5nc1[C@@H]4C[C@@H]23 |  | - | - | 2.73 | 277 |
| 56775-88-3 | Brc1ccc(cc1)C(=C\CN(C)C)/c2cccnc2 |  | 900 | - | 3.180 | - |
| 1222-57-7 | CS(=O)(=O)c1ccc(cc1)c2cn3ccccc3n2 |  | 3710 | - | 2.090 | - |
| 82626-48-0 | CN(C)C(=O)Cc1c(nc2ccc(C)cn12)c3ccc(C)cc3 |  | - | - | 3.850 | - |
| 43200-80-2 | CN1CCN(CC1)C(=O)O[C@H]4c2nccnc2C(=O)N4c3ccc(Cl)cn3 |  | 827 | - | 1.540 | - |
| 26615-21-4 | CN(C)CCOC1=Cc3ccccc3Sc2ccc(Cl)cc12 |  | 306 | - | - | - |

**Evolution of optimal descriptors: solved, unsolved, and unsoluble tasks**

**Supplementary materials 2**

**Splits of available data on normal boiling point, octanol/water partition coefficient, water solubility, and toxicity towards rat can be used as input file for the CORAL software (**[**http://www.insilico.eu/coral**](http://www.insilico.eu/coral)**).**

**Important**

**In the case of traditional scheme “training – calibration – validation”:**

**‘+’ is indicator for the training set;**

**‘#‘ is indicator for the calibration set;**

**‘\*’ is indicator of the validation set.**

**In the case of balance of correlations scheme “training – calibration – test-validation”:**

**‘+’ is indicator for the training set;**

**‘-’ is indicator for the calibration set;**

**‘#‘ is indicator for the test set;**

**‘\*’ is indicator of the validation set.**

**Table S1**

**The numerical data on boiling points (‘C) for drug-like substances. Split 1**

\*79-00-5 ClCC(Cl)Cl 113.800

+87-61-6 Clc1cccc(Cl)c1Cl 218.500

+108-70-3 Clc1cc(Cl)cc(Cl)c1 208.000

#106-99-0 C=CC=C -4.400

+534-07-6 ClCC(=O)CCl 173.400

#106-98-9 C=CCC -6.200

+112-53-8 CCCCCCCCCCCCO 259.000

+70-34-8 Fc1ccc(cc1[N+](=O)[O-])[N+]([O-])=O 296.000

+86-55-5 O=C(O)c2cccc1ccccc12 300.000

\*90-15-3 Oc2cccc1ccccc12 288.000

+108-03-2 [O-][N+](=O)CCC 131.100

+109-67-1 CCCC=C 29.900

+118-79-6 Brc1cc(Br)cc(Br)c1O 286.000

+87-40-1 COc1c(Cl)cc(Cl)cc1Cl 241.000

#88-06-2 Clc1cc(Cl)cc(Cl)c1O 246.000

+120-83-2 Clc1cc(Cl)c(O)cc1 210.000

+367-25-9 Fc1ccc(N)c(F)c1 170.000

+97-02-9 O=[N+]([O-])c1cc(ccc1N)[N+]([O-])=O 333.600

+87-65-0 Clc1cccc(Cl)c1O 220.000

#108-48-5 Cc1cccc(C)n1 144.100

\*110-43-0 CC(=O)CCCCC 151.000

#137-32-6 C[C@@H](CC)CO 128.000

+115-19-5 C#CC(C)(C)O 104.000

+91-60-1 Sc1ccc2ccccc2c1 288.000

\*135-19-3 Oc1ccc2ccccc2c1 285.000

\*79-46-9 CC(C)[N+]([O-])=O 120.200

+123-96-6 CC(O)CCCCCC 178.500

+6032-29-7 C[C@@H](O)CCC 119.300

+109-68-2 C\C=C\CC 37.000

+122-99-6 OCCOc1ccccc1 245.000

+95-76-1 Nc1cc(Cl)c(Cl)cc1 272.000

+13466-78-9 CC2(C)[C@H]1CC=C(C)C[C@@H]12 170.000

+536-78-7 CCc1cccnc1 165.000

+598-75-4 CC(C)[C@@H](C)O 112.000

+584-02-1 CCC(O)CC 116.200

\*536-75-4 CCc1ccncc1 168.300

+83-32-9 c1cc2cccc3CCc(c1)c23 279.000

#75-07-0 CC=O 20.100

+107-29-9 C\C=N\O 115.000

\*60-35-5 CC(N)=O 222.000

+103-84-4 O=C(C)Nc1ccccc1 304.000

+75-05-8 CC#N 81.600

+98-86-2 CC(=O)c1ccccc1 202.000

+74-86-2 C#C -84.700

+79-06-1 C=CC(N)=O 192.600

\*546-43-0 C[C@H]2CCC[C@]1(C)C[C@@H]3OC(=O)C(=C)[C@H]3C=C12 275.000

#107-11-9 C=CCN 53.300

+834-12-8 CSc1nc(NCC)nc(NC(C)C)n1 345.000

#300-62-9 NC(C)Cc1ccccc1 203.000

+538-68-1 CCCCCc1ccccc1 205.400

+62-53-3 Nc1ccccc1 184.100

\*100-66-3 COc1ccccc1 153.700

+120-12-7 c1ccc2cc3ccccc3cc2c1 339.900

\*60-80-0 O=C2C=C(C)N(C)N2c1ccccc1 319.000

+103-33-3 N(=N/c1ccccc1)\c2ccccc2 293.000

\*100-52-7 O=Cc1ccccc1 179.000

+55-21-0 NC(=O)c1ccccc1 290.000

+71-43-2 c1ccccc1 80.000

#134-81-6 O=C(C(=O)c1ccccc1)c2ccccc2 347.000

+51-17-2 c1cccc2ncnc12 360.000

+271-89-6 c1cccc2occc12 174.000

+65-85-0 O=C(O)c1ccccc1 249.200

+100-47-0 N#Cc1ccccc1 191.100

+119-61-9 O=C(c1ccccc1)c2ccccc2 305.400

+95-16-9 c1cccc2scnc12 231.000

#98-88-4 ClC(=O)c1ccccc1 197.200

#100-51-6 OCc1ccccc1 205.300

+103-41-3 O=C(OCc1ccccc1)/C=C/c2ccccc2 350.000

+103-50-4 C(OCc1ccccc1)c2ccccc2 298.000

+100-46-9 NCc1ccccc1 185.000

+103-29-7 C(Cc1ccccc1)c2ccccc2 284.000

\*108-86-1 Brc1ccccc1 156.000

+75-25-2 BrC(Br)Br 149.100

\*123-72-8 CCCC=O 74.800

+109-74-0 CCCC#N 117.600

+76-22-2 CC2(C)[C@@H]1CC(=O)[C@]2(C)CC1 204.000

+86-74-8 c1cccc2nc3ccccc3c12 354.700

+133-90-4 Clc1cc(C(=O)O)c(Cl)c(N)c1 312.000

+78-95-5 CC(=O)CCl 119.000

\*108-90-7 Clc1ccccc1 131.700

\*57-15-8 ClC(Cl)(Cl)C(C)(C)O 167.000

#67-66-3 ClC(Cl)Cl 61.100

+76-06-2 ClC(Cl)(Cl)[N+]([O-])=O 112.000

+57-88-5 CC(C)CCC[C@@H](C)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C 360.000

+218-01-9 c1cc4ccccc4c2ccc3ccccc3c12 448.000

-104-54-1 OC\C=C\c1ccccc1 250.000

+91-64-5 O=C1C=Cc2ccccc2O1 301.700

+460-19-5 N#CC#N -21.100

#108-93-0 OC1CCCCC1 160.800

+108-94-1 O=C1CCCCC1 155.400

+110-83-8 C1C=CCCC1 82.900

+120-92-3 O=C1CCCC1 130.500

+75-19-4 C1CC1 -32.800

+75-99-0 CC(Cl)(Cl)C(=O)O 187.500

\*124-02-7 C=CCNCC=C 111.000

+75-71-8 ClC(Cl)(F)F -29.800

+111-42-2 OCCNCCO 268.800

+109-89-7 CCNCC 55.500

+131-11-3 COC(=O)c1ccccc1C(=O)OC 283.700

+124-40-3 CNC 6.800

+88-85-7 O=[N+]([O-])c1cc(cc(c1O)[C@H](C)CC)[N+]([O-])=O 332.000

+122-39-4 c1ccccc1Nc2ccccc2 302.000

+101-81-5 c1ccccc1Cc2ccccc2 265.000

+299-42-3 O[C@H](c1ccccc1)[C@H](C)NC 255.000

+149-32-6 OC[C@H](O)[C@H](O)CO 330.500

+53-16-7 Oc3cc4CC[C@@H]1[C@H](CC[C@]2(C)C(=O)CC[C@@H]12)c4cc3 154.000

+75-08-1 CCS 35.100

+141-43-5 NCCO 171.000

#93-89-0 O=C(OCC)c1ccccc1 212.000

\*101-97-3 O=C(OCC)Cc1ccccc1 227.000

+118-61-6 Oc1ccccc1C(=O)OCC 232.500

\*75-04-7 CCN 16.500

+100-41-4 CCc1ccccc1 136.100

#107-15-3 NCCN 117.000

+470-82-6 CC2(C)OC1(C)CCC2CC1 176.400

+97-53-0 Oc1ccc(cc1OC)CC=C 253.200

+462-06-6 Fc1ccccc1 84.700

+110-00-9 c1ccco1 31.500

+98-01-1 O=Cc1ccco1 161.700

+106-24-1 C\C(C)=C\CCC(/C)=C\CO 230.000

+56-81-5 OCC(O)CO 290.000

+90-05-1 Oc1ccccc1OC 205.000

+76-44-8 ClC2=C(Cl)[C@]3(Cl)[C@@H]1C=C[C@H](Cl)[C@@H]1[C@@]2(Cl)C3(Cl)Cl 310.000

+118-74-1 Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl 325.000

+70-30-4 Clc2c(Cc1c(O)c(Cl)cc(Cl)c1Cl)c(O)c(Cl)cc2Cl 479.000

+123-31-9 Oc1ccc(O)cc1 287.000

+288-32-4 c1cncn1 257.000

\*496-11-7 c1cccc2CCCc12 177.900

#95-13-6 c1cccc2CC=Cc12 182.000

+120-72-9 c1cccc2nccc12 254.000

\*538-93-2 CC(C)Cc1ccccc1 172.700

+97-54-1 Oc1ccc(cc1OC)\C=C\C 266.000

+26675-46-7 FC(F)(F)[C@H](Cl)OC(F)F 48.500

+503-01-5 C[C@H](CC\C=C(\C)C)NC 177.000

+78-59-1 O=C1C=C(C)CC(C)(C)C1 215.200

+119-65-3 c1cccc2ccncc12 243.200

+27762-78-3 OC(O)C(=O)[C@H](C)OCC 145.000

+569-65-3 Cc1cccc(c1)CN2CCN(CC2)[C@@H](c3ccc(Cl)cc3)c4ccccc4 230.000

\*67-56-1 CO 64.600

#76-38-0 ClC(Cl)C(F)(F)OC 105.000

+134-20-3 Nc1ccccc1C(=O)OC 256.000

\*93-58-3 COC(=O)c1ccccc1 199.000

+93-60-7 COC(=O)c1cccnc1 204.000

#74-89-5 CN -6.300

+60-34-4 CNN 87.500

+114-91-0 COCCc1ccccn1 203.000

\*99-09-2 O=[N+]([O-])c1cccc(N)c1 306.000

+110-91-8 C1CNCCO1 128.000

+108-45-2 Nc1cccc(N)c1 285.000

+127-19-5 CN(C)C(C)=O 165.000

\*91-20-3 c1cccc2ccccc12 217.900

+463-82-1 CC(C)(C)C 9.400

+54-11-5 CN2CCC[C@H]2c1cnccc1 247.000

#98-95-3 [O-][N+](=O)c1ccccc1 210.800

+79-24-3 [O-][N+](=O)CC 114.000

#75-52-5 [O-][N+](C)=O 101.100

#579-10-2 CN(C(C)=O)c1ccccc1 256.000

+62-75-9 CN(C)N=O 154.000

+59-89-2 O=NN1CCOCC1 225.000

-95-50-1 Clc1ccccc1Cl 180.000

+88-74-4 O=[N+]([O-])c1ccccc1N 284.000

+94-70-2 CCOc1ccccc1N 232.500

#90-43-7 Oc2ccccc2c1ccccc1 286.000

+119-93-7 Cc1cc(ccc1N)c2ccc(N)c(C)c2 339.000

+529-20-4 Cc1ccccc1C=O 200.000

+529-19-1 N#Cc1ccccc1C 205.000

+123-30-8 Nc1ccc(O)cc1 284.000

+100-09-4 COc1ccc(cc1)C(=O)O 276.500

+123-63-7 CC1OC(C)OC(C)O1 124.300

+99-91-2 O=C(C)c1ccc(Cl)cc1 232.000

-106-37-6 Brc1ccc(Br)cc1 218.500

#540-36-3 Fc1ccc(F)cc1 89.000

+79-55-0 CC1(C)CCCC(C)(C)N1C 147.000

+40487-42-1 [O-][N+](=O)c1c(C)c(C)cc([N+]([O-])=O)c1NC(CC)CC 330.000

\*87-86-5 Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl 309.500

\*109-66-0 CCCCC 36.000

\*371-40-4 Fc1ccc(N)cc1 182.000

+85-01-8 c2cc3ccc1ccccc1c3cc2 340.000

\*84-11-7 O=C2c3ccccc3c1ccccc1C2=O 360.000

+92-82-0 n1c3ccccc3nc2ccccc12 360.000

#60-12-8 OCCc1ccccc1 218.200

+103-73-1 CCOc1ccccc1 169.800

\*108-95-2 Oc1ccccc1 181.800

#92-84-2 c1ccc2Sc3ccccc3Nc2c1 371.000

+122-09-8 NC(C)(C)Cc1ccccc1 205.000

+122-79-2 O=C(C)Oc1ccccc1 196.000

+101-84-8 c1ccccc1Oc2ccccc2 258.000

+139-66-2 c1ccccc1Sc2ccccc2 296.000

+122-78-1 O=CCc1ccccc1 195.000

#103-82-2 OC(=O)Cc1ccccc1 265.500

\*100-63-0 NNc1ccccc1 243.500

+64-10-8 O=C(N)Nc1ccccc1 238.000

#253-52-1 c1cccc2cnncc12 316.000

#75-97-8 CC(C)(C)C(C)=O 106.100

+110-85-0 C1CNCCN1 146.000

#110-89-4 C1CCCCN1 106.200

+120-57-0 O=Cc1ccc2OCOc2c1 263.000

+100-01-6 O=[N+]([O-])c1ccc(N)cc1 332.000

+100-02-7 O=[N+]([O-])c1ccc(O)cc1 279.000

+156-43-4 CCOc1ccc(N)cc1 254.000

#106-50-3 Nc1ccc(N)cc1 267.000

+92-69-3 Oc1ccc(cc1)c2ccccc2 305.000

\*123-38-6 CCC=O 48.000

+79-05-0 CCC(N)=O 213.000

\*107-12-0 CCC#N 97.100

+93-55-0 O=C(CC)c1ccccc1 217.500

+2078-54-8 CC(C)c1cccc(C(C)C)c1O 256.000

+107-10-8 CCCN 47.200

+115-07-1 C=CC -47.600

+101-40-6 C[C@H](NC)CC1CCCCC1 205.000

+290-37-9 c1cnccn1 115.000

+129-00-0 c1ccc2ccc3cccc4ccc1c2c34 404.000

+289-80-5 c1cccnn1 208.000

#110-86-1 c1ccccn1 115.200

+123-75-1 C1CCCN1 86.500

#91-63-4 Cc1ccc2ccccc2n1 246.500

\*91-22-5 c1cccc2cccnc12 237.100

\*91-19-0 c1cccc2nccnc12 229.500

+94-59-7 C=CCc1ccc2OCOc2c1 234.500

\*90-02-8 O=Cc1ccccc1O 197.000

+28523-86-6 FC(F)(F)C(OCF)C(F)(F)F 58.500

+90-39-1 C3CCCN4C[C@H]2C[C@H](CN1CCCC[C@@H]12)[C@H]34 325.000

+111-01-3 CC(C)CCC[C@@H](C)CCC[C@@H](C)CCCC[C@@H](C)CCC[C@H](C)CCCC(C)C 350.000

+100-42-5 C=Cc1ccccc1 145.000

+94-19-9 O=S(=O)(Nc1nnc(CC)s1)c2ccc(N)cc2 185.750

+124-72-1 FC(F)(F)[C@H](Br)F 8.600

+109-99-9 C1CCCO1 65.000

+142-68-7 C1CCCCO1 88.000

\*632-22-4 CN(C)C(=O)N(C)C 176.500

+288-47-1 c1cncs1 118.000

+110-02-1 c1cccs1 84.000

\*108-98-5 Sc1ccccc1 169.100

#492-22-8 O=C1c3ccccc3Sc2ccccc12 373.000

#89-83-8 CC(C)c1ccc(C)cc1O 232.500

\*108-88-3 Cc1ccccc1 110.600

+68-76-8 O=C1C=C(C(=O)C(=C1N2CC2)N3CC3)N4CC4 357.500

+112-24-3 NCCNCCNCCN 266.500

+121-44-8 CCN(CC)CC 89.000

+280-57-9 C1CN2CCN1CC2 174.000

#552-30-7 O=C(O)c1ccc2C(=O)OC(=O)c2c1 390.000

#217-59-4 c3cccc4c1ccccc1c2ccccc2c34 425.000

+519-73-3 c1ccccc1C(c2ccccc2)c3ccccc3 359.000

+90-47-1 O=C1c3ccccc3Oc2ccccc12 351.000

**Table S2**

**The numerical data on octanol/water partition coefficient for drug-like substances. Split 1**

+79-00-5 ClCC(Cl)Cl 1.890

+530-50-7 NN(c1ccccc1)c2ccccc2 2.800

+87-61-6 Clc1cccc(Cl)c1Cl 4.050

+150-61-8 C(CNc1ccccc1)Nc2ccccc2 2.910

\*524-42-5 O=C1c2ccccc2C=CC1=O 2.110

#108-70-3 Clc1cc(Cl)cc(Cl)c1 4.190

#106-99-0 C=CC=C 1.990

\*534-07-6 ClCC(=O)CCl 0.270

\*102-06-7 N=C(Nc1ccccc1)Nc2ccccc2 2.890

+130-15-4 O=C2C=CC(=O)c1ccccc12 1.710

+547-81-9 Oc3cc4CC[C@H]2[C@H](CC[C@]1(C)[C@H]2C[C@H](O)[C@@H]1O)c4cc3 2.320

+106-98-9 C=CCC 2.400

\*112-53-8 CCCCCCCCCCCCO 5.130

+70-34-8 Fc1ccc(cc1[N+](=O)[O-])[N+]([O-])=O 1.830

\*288-88-0 c1nncn1 -0.580

\*86-55-5 O=C(O)c2cccc1ccccc12 3.100

#90-15-3 Oc2cccc1ccccc12 2.850

+108-03-2 [O-][N+](=O)CCC 0.870

+131-91-9 O=Nc1c2ccccc2ccc1O 2.280

+109-67-1 CCCC=C 2.660

\*92-43-3 O=C1CCN(N1)c2ccccc2 0.890

+118-79-6 Brc1cc(Br)cc(Br)c1O 4.130

#87-40-1 COc1c(Cl)cc(Cl)cc1Cl 4.110

#88-06-2 Clc1cc(Cl)cc(Cl)c1O 3.690

\*118-96-7 Cc1c(cc(cc1[N+](=O)[O-])[N+]([O-])=O)[N+]([O-])=O 1.600

#120-83-2 Clc1cc(Cl)c(O)cc1 3.060

#367-25-9 Fc1ccc(N)c(F)c1 1.540

+97-02-9 O=[N+]([O-])c1cc(ccc1N)[N+]([O-])=O 1.840

\*51-28-5 O=[N+]([O-])c1cc(ccc1O)[N+]([O-])=O 1.670

+119-26-6 NNc1ccc(cc1[N+]([O-])=O)[N+]([O-])=O 1.470

+329-71-5 O=[N+]([O-])c1ccc(cc1O)[N+]([O-])=O 1.750

#1904-98-9 Nc1nc(N)nc2ncnc12 -0.790

+87-65-0 Clc1cccc(Cl)c1O 2.750

\*573-56-8 O=[N+]([O-])c1cccc([N+]([O-])=O)c1O 1.370

#108-48-5 Cc1cccc(C)n1 1.680

\*695-34-1 Cc1ccnc(N)c1 0.560

+136-95-8 Nc1nc2ccccc2s1 2.000

+96-50-4 Nc1nccs1 0.380

\*110-43-0 CC(=O)CCCCC 1.980

#149-30-4 Sc1nc2ccccc2s1 2.420

+137-32-6 C[C@@H](CC)CO 1.290

#115-19-5 C#CC(C)(C)O 0.280

+84-54-8 Cc2ccc3C(=O)c1ccccc1C(=O)c3c2 3.890

+91-60-1 Sc1ccc2ccccc2c1 3.860

+135-19-3 Oc1ccc2ccccc2c1 2.700

\*79-46-9 CC(C)[N+]([O-])=O 0.930

\*123-96-6 CC(O)CCCCCC 2.900

+6032-29-7 C[C@@H](O)CCC 1.190

+109-68-2 C\C=C\CC 2.580

\*122-99-6 OCCOc1ccccc1 1.160

-141-90-2 O=C1C=CNC(=S)N1 0.900

+54-96-6 Nc1ccncc1N -1.030

#95-76-1 Nc1cc(Cl)c(Cl)cc1 2.690

+300-38-9 Brc1cc(cc(Br)c1O)C[C@H](N)C(=O)O 0.020

+90-59-5 Oc1c(C=O)cc(Br)cc1Br 3.790

\*13466-78-9 CC2(C)[C@H]1CC=C(C)C[C@@H]12 4.380

\*536-78-7 CCc1cccnc1 1.660

+598-75-4 CC(C)[C@@H](C)O 1.280

#56-49-5 Cc2ccc3cc1c5ccccc5ccc1c4CCc2c34 6.420

#584-02-1 CCC(O)CC 1.210

+536-75-4 CCc1ccncc1 1.650

+104-91-6 O=Nc1ccc(O)cc1 1.290

\*537-47-3 O=C(Nc1ccccc1)NN 0.160

+51-20-7 BrC1=CNC(=O)NC1=O -0.210

+2435-76-9 N#N=C1/C=NC(=O)NC1=O -1.950

+608-07-1 COc1cc2c(cc1)ncc2CCN 1.350

\*480-68-2 O=C1NC(=O)NC(=O)C1[N+]([O-])=O -1.190

\*54-25-1 O=C1NC(=O)C=NN1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -2.140

+134-58-7 O=C1NC(N)=Nc2nnnc12 -0.710

#523-27-3 Brc2c1ccccc1c(Br)c3ccccc23 6.130

+37517-30-9 CC(C)NCC(O)COc1ccc(cc1C(C)=O)NC(=O)CCC 1.710

+32795-44-1 O=C(C)Nc1ccc(cc1)C(=O)NCCN(CC)CC 0.990

+77-46-3 O=S(=O)(c1ccc(NC(C)=O)cc1)c2ccc(NC(C)=O)cc2 0.820

+80-03-5 O=S(=O)(c1ccc(N)cc1)c2ccc(NCC(=O)O)cc2 0.570

#2490-97-3 O=C(C)N[C@H](CCC(N)=O)C(=O)O -2.110

+83-32-9 c1cc2cccc3CCc(c1)c23 3.920

#152-72-7 [O-][N+](=O)c1ccc(cc1)[C@@H](CC(C)=O)C2=C(O)c3ccccc3OC2=O 1.980

+807-31-8 Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)(CNC(C)=O)c3ccccc3 3.980

+33665-90-6 CC1=CC(=O)NS(=O)(=O)O1 -1.330

+75-07-0 CC=O -0.340

+107-29-9 C\C=N\O -0.130

+60-35-5 CC(N)=O -1.260

+103-84-4 O=C(C)Nc1ccccc1 1.160

#59-66-5 O=S(N)(=O)c1nnc(NC(C)=O)s1 -0.260

\*968-81-0 O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(cc2)C(C)=O 2.440

+75-05-8 CC#N -0.340

\*2751-68-0 CC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2 2.620

\*98-86-2 CC(=O)c1ccccc1 1.580

#616-91-1 CC(=O)N[C@@H](CS)C(O)=O -0.660

+74-86-2 C#C 0.370

+51037-30-0 [O-][n+]1cc(ncc1C)C(O)=O -0.520

\*55079-83-9 Cc1c(C)c(/C=CC(\C)=C\C=C\C(\C)=C\C(=O)O)c(C)cc1OC 6.400

+87848-99-5 O=C(O)/C=C/c1cccc(n1)/C(=C\CN2CCCC2)c3ccc(C)cc3 2.830

+79-06-1 C=CC(N)=O -0.670

+15301-40-3 O=S(=O)(O)c1ccc(OCC)c2ncccc12 -0.440

+59277-89-3 NC2=Nc1c(ncn1COCCO)C(=O)N2 -1.560

+281-23-2 C1C3CC2CC1CC(C2)C3 4.240

\*73-24-5 NC=1NC=NC2=NC=NC=12 -0.090

\*522-27-0 O\N=C(/C(=N/O)c1ccco1)c2ccco2 2.250

+3011-89-0 O=C(N)c1ccc(cc1Cl)[N+]([O-])=O 0.470

\*546-43-0 C[C@H]2CCC[C@]1(C)C[C@@H]3OC(=O)C(=C)[C@H]3C=C12 3.380

+54965-21-8 O=C(OC)Nc1nc2ccc(cc2n1)SCCC 3.140

#18559-94-9 OCc1cc(ccc1O)[C@@H](O)CNC(C)(C)C 0.640

+22131-79-9 Clc1cc(ccc1OCC=C)CC(=O)O 2.480

+116-06-3 CC(C)(\C=N\OC(=O)NC)SC 1.130

\*52-39-1 OCC(=O)[C@H]4CC[C@@H]2[C@@]4(C=O)C[C@H](O)[C@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 1.080

+309-00-2 ClC3=C(Cl)[C@@]4(Cl)[C@@H]2[C@@H]([C@@H]1C[C@H]2C=C1)[C@]3(Cl)C4(Cl)Cl 6.500

+22573-93-9 CCCC[C@@H](CC)CNC(=N)NC(=N)NCCCCCCNC(=N)NC(=N)NC[C@H](CC)CCCC 3.580

+595-77-7 CC(=O)[C@]2(O)[C@@]3(C)CC[C@@H]1[C@@]4(C)CCC(=O)C=C4CC[C@H]1[C@@H]3C[C@H]2O 3.150

+59338-93-1 C=CCN3CCC[C@@H]3CNC(=O)c1cc2nnnc2cc1OC 1.790

\*97-59-6 O=C1NC(=O)NC1NC(=O)N -3.140

\*5486-77-1 O=C(NCCN(CC)CC)c1ccc(Cl)cc1OCC=C 3.450

#107-11-9 C=CCN 0.030

#432-60-0 C[C@]32CC[C@H]1[C@H]4CCCC=C4CC[C@@H]1[C@@H]3CC[C@@]2(O)CC=C 5.880

+39718-89-3 O=C(O)[C@H](C)c1ccc(NCC(=C)C)cc1 2.870

#1415-73-2 O[C@H]1[C@H](O)[C@@H](O)[C@@H](O[C@@H]1CO)[C@@H]4c2cccc(O)c2C(=O)c3c(O)cc(CO)cc34 0.550

#77-20-3 C[C@@H]2CN(C)CC[C@]2(OC(=O)CC)c1ccccc1 2.830

#850-52-2 O=C3C=C4CC[C@@H]2C(C=C[C@@]1(C)[C@H]2CC[C@@]1(O)CC=C)=C4CC3 3.710

#150-59-4 CCN(CCCc1ccccc1)CCCc2ccccc2 5.910

+537-17-7 Nc2ncnc(Nc1ccccc1)n2 1.890

+768-94-5 NC12CC3CC(C1)CC(C2)C3 2.440

+539-21-9 N=C(N)N\N=C1\C=C/C(=N\NC(N)=S)C=C1 1.230

#519-88-0 COc1ccc(cc1)[C@H](C(N)=O)N(CCCC)CCCC 3.860

+3754-19-6 O=S(N)(=O)c1cc(c(cc1Cl)\N=C\C=C(/C)O)S(=O)(=O)NCC=C 1.600

#51022-69-6 CC(=O)OCC(=O)[C@]56OC1(CCCC1)O[C@@H]6C[C@H]4C3CCC2=CC(=O)C=C[C@]2(C)[C@@]3(F)[C@@H](O)C[C@@]45C 3.780

\*32887-01-7 OC(=O)[C@@H]2N3C(=O)[C@@H](/N=C/N1CCCCCC1)[C@H]3SC2(C)C 3.090

\*834-12-8 CSc1nc(NCC)nc(NC(C)C)n1 2.980

+37517-28-5 NCC[C@H](O)C(=O)N[C@@H]3C[C@H](N)[C@@H](O[C@H]1O[C@H](CN)[C@@H](O)[C@H](O)[C@H]1O)[C@H](O)[C@H]3O[C@H]2O[C@H](CO)[C@@H](O)[C@H](N)[C@H]2O -8.780

#125-84-8 CC[C@@]1(CCC(=O)NC1=O)c2ccc(N)cc2 0.820

#642-44-4 O=C1N(CC=C)C(N)=CC(=O)N1CC 0.080

#60-46-8 NC(=O)C(CC(C)N(C)C)(c1ccccc1)c2ccccc2 2.750

+58-37-7 CN(C)CC(CN1c3ccccc3Sc2ccccc12)N(C)C 4.760

+54-62-6 O=C(O)[C@H](CCC(=O)O)NC(=O)c1ccc(cc1)NCc2nc3c(nc2)nc(N)nc3N -1.820

\*58-15-1 CN(C)C=2C(=O)N(c1ccccc1)N(C)C=2C 1.000

+2207-50-3 NC1=NC[C@@H](O1)c2ccccc2 1.150

+1951-25-3 CCN(CC)CCOc1c(I)cc(cc1I)C(=O)c2c3ccccc3oc2CCCC 7.570

\*50-48-6 CN(C)CC\C=C1\c3ccccc3CCc2ccccc12 4.920

\*88150-42-9 O=C(OC)C1=C(C)NC(COCCN)=C(C(=O)OCC)[C@@H]1c2ccccc2Cl 3.000

#14028-44-5 Clc1ccc2Oc4ccccc4N=C(c2c1)N3CCNCC3 3.380

\*134-37-2 Nc1cc(ccc1)N2C=CC=CC2=O 0.450

#300-62-9 NC(C)Cc1ccccc1 1.760

\*1673-06-9 Nc1ccc(cc1)OCCCCCN3C(=O)c2ccccc2C3=O 3.800

+69-53-4 OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)[C@H](N)c1ccccc1)[C@H]3SC2(C)C 1.350

+51264-14-3 CS(=O)(=O)Nc4ccc(Nc1c3ccccc3nc2ccccc12)c(OC)c4 3.890

+29883-15-6 O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]3OC[C@H]2O[C@@H](O[C@H](C#N)c1ccccc1)[C@H](O)[C@@H](O)[C@@H]2O -4.340

\*538-68-1 CCCCCc1ccccc1 4.900

+31698-14-3 N=C1N=C2O[C@H]3[C@H](O)[C@@H](CO)O[C@H]3N2C=C1 -2.370

+53-41-8 O=C4CC[C@@H]3[C@]4(C)CC[C@H]1[C@H]3CC[C@H]2C[C@H](O)CC[C@]12C 3.690

+62-53-3 Nc1ccccc1 0.900

+117-37-3 COc1ccc(cc1)C3C(=O)c2ccccc2C3=O 2.880

\*100-66-3 COc1ccccc1 2.110

+91-75-8 C(c1ccccc1)N(CC2=NCCN2)c3ccccc3 3.380

\*120-12-7 c1ccc2cc3ccccc3cc2c1 4.450

+1143-38-0 Oc2cccc1Cc3cccc(O)c3C(=O)c12 4.400

#60-80-0 O=C2C=C(C)N(C)N2c1ccccc1 0.380

+2835-06-5 N[C@H](C(=O)O)c1ccccc1 -2.070

+52-46-0 C1CN1p2(np(np(n2)(N3CC3)N4CC4)(N5CC5)N6CC6)N7CC7 2.190

#520-36-5 Oc1ccc(cc1)C3=CC(=O)c2c(cc(O)cc2O)O3 3.020

+58-00-4 Oc3ccc2C[C@@H]1c4c(CCN1C)cccc4c2c3O 2.300

+37321-09-8 O[C@@H]4[C@@H](O)[C@H](N)[C@@H](CO)O[C@@H]4O[C@H]2O[C@@H]3C[C@@H](N)[C@@H](O[C@@H]1[C@@H](N)C[C@@H](N)[C@H](O)[C@H]1O)O[C@@H]3[C@H](O)[C@@H]2NC -8.120

#147-81-9 O[C@H](C=O)[C@H](O)[C@H](O)CO -3.020

+499-04-7 OC(=O)C=1CN(C)CCC=1 -1.210

+74-79-3 N[C@@H](CCCNC(=N)N)C(=O)O -4.200

+63968-64-9 O=C4O[C@H]2O[C@@]1(C)CC[C@@H]3[C@]2(OO1)[C@@H](CC[C@H]3C)[C@H]4C 2.900

+22839-47-0 O=C(O)C[C@@H](N)C(=O)N[C@H](Cc1ccccc1)C(=O)OC 0.070

\*466-49-9 CC(=O)N2c1c(cccc1OC)[C@]35CCN4CCC[C@@](CC[C@@H]23)(CC)[C@@H]45 3.680

+68844-77-9 Fc1ccc(cc1)Cn4c5ccccc5nc4NC3CCN(CCc2ccc(OC)cc2)CC3 6.430

\*29122-68-7 CC(C)NCC(O)COc1ccc(cc1)CC(N)=O 0.160

+479-20-9 O=Cc2c(O)cc(C)c(C(=O)Oc1cc(C)c(C(=O)OC)c(O)c1C)c2O 6.860

#51-55-8 CN3C1CCC3CC(C1)OC(=O)C(CO)c2ccccc2 1.830

#320-67-2 NC1=NC(=O)N(C=N1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -3.830

#115-46-8 OC(c1ccccc1)(C2CCNCC2)c3ccccc3 3.450

\*62973-76-6 Cn2c(cnc2/C=C/c1ccnc(N)n1)[N+]([O-])=O 0.850

#1649-18-9 Fc1ccc(cc1)C(=O)CCCN2CCN(CC2)c3ccccn3 3.300

#3964-81-6 CN1CC\C(CC1)=C2\c4ncccc4CCc3ccccc23 3.590

+17243-38-8 OC(=O)[C@H]2N3C(=O)[C@H](NC(=O)[C@@H](\N=N#N)c1ccccc1)[C@H]3SC2(C)C 2.650

#1830-32-6 CCN(CC)C(=O)CSc1ccc(Cl)nn1 1.310

+37091-66-0 OC(=O)[C@@H]3N4C(=O)[C@H](NC(=O)[C@H](NC(=O)N1CCNC1=O)c2ccccc2)[C@H]4SC3(C)C 1.710

+103-33-3 N(=N/c1ccccc1)\c2ccccc2 3.820

+527-73-1 [O-][N+](=O)c1nccn1 0.150

+27589-33-9 NS(=O)(=O)c2cc(c(NCc1cccs1)cc2Cl)c3nnnn3 0.060

#275-51-4 c1cccc2cccc2c1 3.200

+531-55-5 [Cl-].CN(C)c1cc2[s+]c3cc(NC)ccc3nc2cc1 3.480

+531-57-7 [Cl-].Nc1ccc2nc3ccc(cc3[s+]c2c1)NC 2.380

+1134-47-0 Clc1ccc(cc1)C(CN)CC(=O)O -0.960

\*3703-79-5 O[C@H](CNCCCC)c1ccc(O)cc1 1.260

#2016-63-9 CCN(CCO)CCn2c3C(=O)N(C)C(=O)N(C)c3nc2Cc1ccccc1 1.630

#4945-47-5 CN1CCC(CC1)N(Cc2ccccc2)c3ccccc3 4.070

+101-27-9 Clc1cc(NC(=O)OCC#CCCl)ccc1 3.410

#39552-01-7 CC(C)NC[C@@H](O)COc1cccc2cc(oc12)C(C)=O 2.020

+64-65-3 CCC1(C)CC(=O)NC(=O)C1 0.520

\*2179-37-5 CN(C)CCCOC1(CCCCCC1)Cc2ccccc2 5.180

\*20187-55-7 O=C(O)COc3nn(Cc1ccccc1)c2ccccc23 3.280

\*22781-23-3 CNC(=O)Oc1cccc2OC(C)(C)Oc12 1.700

\*73-48-3 FC(F)(F)c1cc2N[C@H](NS(=O)(=O)c2cc1S(N)(=O)=O)Cc3ccccc3 1.890

\*23602-78-0 FC(F)(F)c2cccc(C[C@H](C)NCCOC(=O)c1ccccc1)c2 4.670

+17804-35-2 O=C(OC)Nc2nc1ccccc1n2C(=O)NCCCC 2.120

#51234-28-7 O=C(O)[C@@H](C)c1cc2nc(oc2cc1)c3ccc(Cl)cc3 3.230

+2062-84-2 Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)N3c4ccccc4NC3=O 3.910

+100-52-7 O=Cc1ccccc1 1.480

+55-21-0 NC(=O)c1ccccc1 0.640

+93-98-1 O=C(Nc1ccccc1)c2ccccc2 2.620

+3562-84-3 Brc1cc(cc(Br)c1O)C(=O)c2c3ccccc3oc2CC 6.030

+71-43-2 c1ccccc1 2.130

+134-81-6 O=C(C(=O)c1ccccc1)c2ccccc2 3.380

#51-17-2 c1cccc2ncnc12 1.320

+22994-85-0 O=C(Cn1ccnc1[N+]([O-])=O)NCc2ccccc2 0.910

#17243-39-9 CNCC24CCC(c1ccccc12)c3ccccc34 3.540

#271-89-6 c1cccc2occc12 2.670

\*65-85-0 O=C(O)c1ccccc1 1.870

-104-31-4 O=C(OCCOCCOCCOCCOCCOCCOCCOCCOCCOC)c1ccc(NCCCC)cc1 2.450

\*100-47-0 N#Cc1ccccc1 1.560

+119-61-9 O=C(c1ccccc1)c2ccccc2 3.180

+95-16-9 c1cccc2scnc12 2.010

+86-75-9 O=C(Oc1cccc2cccnc12)c3ccccc3 3.190

\*98-88-4 ClC(=O)c1ccccc1 1.440

+519-09-5 CN1[C@@H]2CC[C@@H]1[C@@H](C(=O)O)[C@H](C2)OC(=O)c3ccccc3 -1.320

\*156-08-1 CN(Cc1ccccc1)[C@@H](C)Cc2ccccc2 4.140

\*53-89-4 CN1CCC(CC1)N3NC(=C(Cc2ccccc2)C3=O)c4ccccc4 2.930

\*100-51-6 OCc1ccccc1 1.100

+103-41-3 O=C(OCc1ccccc1)/C=C/c2ccccc2 4.060

+103-50-4 C(OCc1ccccc1)c2ccccc2 3.310

+100-46-9 NCc1ccccc1 1.090

\*483-49-8 C2c4ccccc4CN3CCc1ccccc1[C@H]23 4.030

#5638-76-6 CNCCc1ccccn1 0.680

+378-44-9 OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@@H]3C 1.940

\*83-46-5 C[C@@H](C)[C@@H](CC)CC[C@@H](C)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C 9.650

\*105-20-4 NCCc1ccnn1 -0.730

+55-73-2 C\N=C(\NCc1ccccc1)NC 1.560

+59170-23-9 COc1cc(ccc1OC)CCNC[C@H](O)COc2cc(C)ccc2 3.000

#41859-67-0 O=C(NCCc1ccc(OC(C)(C)C(=O)O)cc1)c2ccc(Cl)cc2 4.250

+15301-48-1 CCC(=O)N5c1ccccc1N(C4CCN(CCC(C#N)(c2ccccc2)c3ccccc3)CC4)C5=O 4.800

#493-75-4 Oc1c(cc(cc1CN(CC)CC)c2cc(CC=C)c(O)c(CN(CC)CC)c2)CC=C 7.050

+103-29-7 C(Cc1ccccc1)c2ccccc2 4.790

+42576-02-3 Clc2cc(Cl)ccc2Oc1cc(C(=O)OC)c(cc1)[N+]([O-])=O 4.480

+60628-96-8 c1cc(ccc1c2ccccc2)[C@H](c3ccccc3)n4ccnc4 4.770

#28434-01-7 C/C(C)=C/[C@@H]3C(C(=C)CCC=2C=C(Cc1ccccc1)CC=2)C3(C)C 7.110

+58-85-5 O=C1N[C@H]2[C@@H](CCCCC(=O)O)SC[C@@H]2N1 0.390

#514-65-8 OC(CCN1CCCCC1)(c2ccccc2)C4CC3C=CC4C3 4.250

+3572-52-9 Oc1c(cccc1C(=O)OCCN(CC)CC)c2ccccc2 5.050

+66722-44-9 CC(C)NC[C@H](O)COc1ccc(cc1)COCCOC(C)C 1.870

+4044-65-9 S=C=N\c1ccc(cc1)\N=C=S 4.670

+1605-89-6 C[C@@H]4CC1=CC(=O)CC[C@]1(C)[C@H]3CC[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@@H]34 4.140

+846-48-0 O=C3C=C4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)C=C3 3.050

+56518-41-3 Nc2nc(N)ncc2Cc1cc(OC)c(Br)c(OC)c1 2.010

+314-40-9 CC[C@@H](C)N1C(=O)C(Br)=C(C)NC1=O 2.110

\*1812-30-2 Brc1ccc2NC(=O)CN=C(c2c1)c3ccccn3 2.050

#1146-98-1 Brc1ccc(cc1)C3C(=O)c2ccccc2C3=O 3.760

+496-67-3 CC(C)[C@@H](Br)C(=O)NC(N)=O 1.140

+108-86-1 Brc1ccccc1 2.990

+75-25-2 BrC(Br)Br 2.400

#2104-96-3 Clc1cc(OP(=S)(OC)OC)c(Cl)cc1Br 5.210

#4093-35-0 Nc1cc(OC)c(cc1Br)C(=O)NCCN(CC)CC 2.830

+10457-90-6 Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Br)cc3 4.450

+521-74-4 Oc1c(Br)cc(Br)c2cccnc12 3.440

+357-57-3 COc1cc2c(cc1OC)N3C(=O)C[C@@H]7OCC=C6CN4CC[C@@]25C3[C@H]7[C@H]6C[C@H]45 0.980

+362-74-3 CCCC(=O)Nc4ncnc1c4ncn1[C@@H]3O[C@H]2COP(=O)(O)O[C@H]2[C@H]3OC(=O)CCC 0.450

+841-73-6 O=C2N(C1CCCCC1)C(=O)NC(=O)[C@H]2CCCC 3.120

#51333-22-3 OCC(=O)[C@@]45O[C@@H](O[C@H]5C[C@@H]3[C@@H]2CCC1=CC(=O)C=C[C@]1(C)[C@H]2[C@@H](O)C[C@@]34C)CCC 2.180

+57982-78-2 CC(C)(C)N1CCC(CC1)(c2ccccc2)c3ccccc3 5.100

#22103-14-6 Ic1cc(cc(I)c1O)[C@@H](O)[C@@H](C)N[C@H](C)CCc2ccccc2 5.640

+54340-62-4 CC(C)(C)NC[C@@H](O)c1cc2cccc(CC)c2o1 3.500

+41483-43-6 CCNc1nc(C)c(CCCC)c(OS(=O)(=O)N(C)C)n1 2.700

+14556-46-8 Clc1ccc(C)cc1OC[C@H](O)CNC(C)(C)C 2.970

+52485-79-7 CC(C)(C)[C@@](C)(O)[C@H]1C[C@]74CC[C@]1(OC)[C@@H]5Oc3c(O)ccc2C[C@H]7N(CC[C@@]45c23)CC6CC6 4.980

+36505-84-7 O=C4CC1(CCCC1)CC(=O)N4CCCCN2CCN(CC2)c3ncccn3 2.630

+149-16-6 Nc1ccc(cc1)C(=O)OCCCN(CCCC)CCCC 4.440

+23184-66-9 ClCC(=O)N(COCCCC)c1c(cccc1CC)CC 4.500

\*22131-35-7 CCCCN(CCCC)CCNc1nc(no1)c2ccccc2 4.380

+3785-21-5 Clc1cccc(C)c1NC(=O)CNCCCC 2.040

#653-03-2 CCCC(=O)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 4.810

+2090-89-3 Nc1ccc(cc1)C(=O)OCCNCC(C)C 2.190

+2043-38-1 NS(=O)(=O)c2cc1c(N[C@H](NS1(=O)=O)CC(C)C)cc2Cl 1.200

#55837-18-8 CC[C@H](C(=O)O)c1ccc(cc1)CC(C)C 4.280

#42408-82-2 Oc3ccc4C[C@H]1N(CC[C@@]2(CCCC[C@]12O)c4c3)CC5CCC5 3.680

+33629-47-9 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N[C@H](C)CC)C(C)(C)C 4.930

+123-72-8 CCCC=O 0.880

+109-74-0 CCCC#N 0.530

#58-08-2 O=C2c1n(C)cnc1N(C)C(=O)N2C -0.070

#32222-06-3 C=C1C(\C[C@@H](O)CC1O)=C\C=C3\CCC[C@@]2(C)C3CC[C@@H]2C(C)CCCC(C)(C)O 7.600

+36104-80-0 CN(C)C(=O)OC2N=C(c1cc(Cl)ccc1N(C)C2=O)c3ccccc3 2.660

+26097-80-3 CC(C)OC(=O)Nc1ccc2nc(nc2c1)c3cscn3 2.670

#76-22-2 CC2(C)[C@@H]1CC(=O)[C@]2(C)CC1 2.380

+7689-03-4 CC[C@]1(O)C=2C=C3c4nc5ccccc5cc4CN3C(=O)C=2COC1=O 1.740

+298-46-4 NC(=O)N2c3ccccc3C=Cc1ccccc12 2.450

+86-74-8 c1cccc2nc3ccccc3c12 3.720

\*10605-21-7 O=C(OC)Nc1nc2ccccc2n1 1.520

\*77-23-6 CCN(CC)CCOCCOC(=O)C1(CCCC1)c2ccccc2 4.150

+486-16-8 Clc1ccc(cc1)[C@@H](OCCN(C)C)c2ccccn2 2.560

\*15687-16-8 CN(CCc1ccccc1)CCN(C)C(=O)C(OCC)(c2ccccc2)c3ccccc3 4.710

+541-79-7 O[C@@H](NC(=O)OCC)C(Cl)(Cl)Cl 1.840

+638-23-3 OC(=O)[C@@H](N)CSCC(O)=O -4.240

#1563-66-2 CNC(=O)Oc1cccc2CC(C)(C)Oc12 2.320

\*24279-91-2 NC(=O)OC[C@@H](OC)C=1C(=O)C(=C(C)C(=O)C=1N2CC2)N3CC3 -0.150

+339-43-5 Nc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC 1.010

+1260-17-9 O[C@H]1[C@H](O)[C@@H](O)[C@H](O[C@@H]1CO)c4c(O)c3C(=O)c2c(C)c(C(=O)O)c(O)cc2C(=O)c3c(O)c4O 0.970

+61422-45-5 O=C1NC(=O)C(F)=CN1C(=O)NCCCCCC 2.630

#2622-30-2 CCC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2 3.340

-5942-95-0 NC(=O)C4(CCN(CCCN2c3ccccc3CCc1ccccc12)CC4)N5CCCCC5 5.230

+53716-49-7 O=C(O)C(C)c1ccc2c3cc(Cl)ccc3nc2c1 3.790

#72956-09-3 COc4ccccc4OCCNC[C@@H](O)COc2cccc3nc1ccccc1c23 4.190

\*138-41-0 O=S(N)(=O)c1ccc(cc1)C(=O)O 0.500

#53994-73-3 ClC=3CS[C@H]2N(C(=O)[C@@H]2NC(=O)[C@H](N)c1ccccc1)C=3C(=O)O 0.350

#34444-01-4 O[C@H](c1ccccc1)C(=O)N[C@H]4C(=O)N3C(=C(CSc2nnnn2C)CS[C@@H]34)C(=O)O 0.500

#51627-14-6 Oc1ccc(cc1)[C@@H](N)C(=O)N[C@H]4C(=O)N3C(=C(CSc2cnnn2)CS[C@@H]34)C(=O)O -1.210

+25953-19-9 O=C(O)C=3N4C(=O)[C@@H](NC(=O)Cn1cnnn1)[C@H]4SCC=3CSc2nnc(C)s2 -0.580

+79350-37-1 Nc1scc(n1)/C(=N\OCC(=O)O)C(=O)N[C@@H]3C(=O)N2C(=C(C=C)CS[C@@H]23)C(=O)O 0.120

+63527-52-6 Nc1scc(n1)\C(=N\OC)C(=O)N[C@@H]3C(=O)N2C(=C(COC(C)=O)CS[C@H]23)C(=O)O 0.640

+35607-66-0 O=C(O)C=2N3C(=O)[C@](NC(=O)Cc1cccs1)(OC)[C@H]3SCC=2COC(N)=O -0.020

#51762-05-1 N[C@H](C1C=CCC=C1)C(=O)N[C@@H]3C(=O)N2C(=C(OC)CS[C@@H]23)C(=O)O -0.980

#55268-75-2 CO\N=C(\c1ccco1)C(=O)N[C@H]3C(=O)N2C(=C(COC(N)=O)CS[C@@H]23)C(=O)O -0.160

+153-61-7 O=C(O)C=2N3C(=O)[C@@H](NC(=O)Cc1cccs1)[C@H]3SCC=2COC(C)=O 0.000

+38821-53-3 CC=3CS[C@H]2N(C(=O)[C@@H]2NC(=O)[C@H](N)C1=CCC=CC1)C=3C(=O)O 0.410

+14176-10-4 O=C(OCCN1CCCCCC1)[C@@H](C2CCCCC2)c3ccsc3 6.140

+83881-51-0 O=C(O)COCCN1CCN(CC1)[C@@H](c2ccc(Cl)cc2)c3ccccc3 -0.610

#103-47-9 O=S(=O)(O)CCNC1CCCCC1 -0.630

+791-35-5 O[C@](CCN(C)C)(c1ccccc1Cl)c2ccccc2 3.500

\*133-90-4 Clc1cc(C(=O)O)c(Cl)c(N)c1 1.900

+305-03-3 O=C(O)CCCc1ccc(cc1)N(CCCl)CCCl 1.700

+56-75-7 O=[N+]([O-])c1ccc(cc1)[C@@H](O)[C@@H](CO)NC(=O)C(Cl)Cl 1.140

\*5588-20-5 O=C1N[C@@H](C(=O)N1SC(Cl)(Cl)Cl)[C@H](CC)CCCC 3.690

+58-25-3 Clc1ccc2N=C(C[N+]([O-])=C(c2c1)c3ccccc3)NC 2.440

+6164-98-3 Clc1cc(C)c(/N=C/N(C)C)cc1 2.890

+85-34-7 Clc1c(CC(=O)O)c(Cl)ccc1Cl 3.200

+3563-58-4 ClC(Cl)(Cl)[C@H](O)O[C@H](C)CC(O)(C)C 1.590

+145-94-8 Oc1ccc(Cl)c2CCCc12 3.630

+80-77-3 O=C1CCS(=O)(=O)C(N1C)c2ccc(Cl)cc2 -0.260

+3689-76-7 Clc1ccc(cc1)Cn2c3ccccc3nc2C 4.680

\*78-95-5 CC(=O)CCl 0.020

+502-98-7 Cl\N=C(\N)/N=NC(\N)=N\Cl -0.470

#108-90-7 Clc1ccccc1 2.840

#510-15-6 OC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)C(=O)OCC 4.740

#57-15-8 ClC(Cl)(Cl)C(C)(C)O 2.030

\*67-66-3 ClC(Cl)Cl 1.970

+76-06-2 ClC(Cl)(Cl)[N+]([O-])=O 2.090

+59-32-5 Clc1ccc(cc1)CN(CCN(C)C)c2ccccn2 3.370

\*148-65-2 Clc2ccc(CN(CCN(C)C)c1ccccn1)s2 3.190

+58-94-6 NS(=O)(=O)c2cc1c(N=CNS1(=O)=O)cc2Cl -0.240

+54749-90-5 O[C@H]1O[C@H](CO)[C@@H](O)[C@@H](O)[C@H]1NC(=O)N(CCCl)N=O -1.020

+104-29-0 Clc1ccc(OCC(O)CO)cc1 1.500

\*77-38-3 Clc1ccc(cc1)[C@](C)(OCCN(C)C)c2ccccc2 4.200

+461-78-9 Clc1ccc(CC(C)(C)N)cc1 2.600

+50-53-3 CN(C)CCCN1c3ccccc3Sc2ccc(Cl)cc12 5.410

+113-59-7 CN(C)CC\C=C1\c3ccccc3Sc2ccc(Cl)cc12 5.180

#72-80-0 Oc1c(Cl)cc(Cl)c2ccc(C)nc12 3.500

\*57-62-5 NC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@@]2(O)C1=O)C(=O)c3c(O)ccc(Cl)c3[C@@]4(C)O -0.620

+57-88-5 CC(C)CCC[C@@H](C)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C 8.740

\*218-01-9 c1cc4ccccc4c2ccc3ccccc3c12 5.810

\*481-74-3 Oc3cccc2C(=O)c1cc(C)cc(O)c1C(=O)c23 4.490

+53449-58-4 C[C@@H]2C[C@H](OC(=O)c1cccnc1)CC(C)(C)C2 4.200

+73963-72-1 O=C1CCc2cc(ccc2N1)OCCCCc4nnnn4C3CCCCC3 4.040

+51481-61-9 N#C\N=C(/NC)NCCSCc1ncnc1C 0.400

+118-10-5 O[C@H](C2CC1CCN2C[C@@H]1C=C)c4ccnc3ccccc34 2.680

\*132-60-5 O=C(O)c1cc(nc2ccccc12)c3ccccc3 3.790

#90-86-8 O[C@@H](c1ccccc1)[C@H](C)N(C)C/C=C/c2ccccc2 3.370

+104-54-1 OC\C=C\c1ccccc1 1.950

+298-57-7 c1ccccc1C(c2ccccc2)N3CCN(CC3)C/C=C/c4ccccc4 5.770

\*253-66-7 c1cnnc2ccccc12 0.930

+28657-80-9 O=C(O)C2=NN(CC)c1cc3OCOc3cc1C2=O 1.590

+104-28-9 COc1ccc(/C=C/C(=O)OCCOCC)cc1 2.650

+52214-84-3 ClC2(Cl)C[C@@H]2c1ccc(OC(C)(C)C(=O)O)cc1 3.940

\*85721-33-1 O=C(O)C2=CN(c1cc(c(F)cc1C2=O)N3CCNCC3)C4CC4 0.280

#81098-60-4 Clc1cc(c(OC)cc1N)C(=O)N[C@H]3CCN(CCCOc2ccc(F)cc2)C[C@H]3OC 3.090

#1195-16-0 O=C1SCC[C@H]1NC(=O)C -0.350

#372-75-8 N[C@@H](CCCNC(N)=O)C(=O)O -3.190

+30544-61-7 O=C(c1ccc(Cl)cc1)N(CCCC(=O)O)c2ccc(OC)cc2 2.700

+55905-53-8 Clc1cc(c(OC)cc1N)C(=O)NC3CCN(Cc2ccccc2)CC3 3.580

\*442-52-4 Clc1ccc(cc1)Cn3c4ccccc4nc3CN2CCCC2 4.400

#37148-27-9 Clc1cc(cc(Cl)c1N)C(O)CNC(C)(C)C 2.000

#18323-44-9 O[C@@H]1[C@@H](O)[C@@H](O)[C@H](O[C@@H]1SC)C(NC(=O)[C@@H]2C[C@@H](CCC)CN2C)[C@H](C)Cl 2.160

\*14437-41-3 Clc2ccc(NC(=O)c1cc(I)cc(I)c1OC(C)=O)cc2 5.280

+1159-93-9 CN(C)CCN2c3ccc(Cl)cc3Nc1ccccc1C2=O 3.730

#13364-32-4 Clc2ccccc2CN[C@H](C)Cc1ccccc1 4.570

+25122-41-2 ClCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@@H]3C 2.480

+54063-32-0 ClCC(=O)[C@]2(O)[C@@]3(C)CC(=O)[C@]1(F)[C@]4(C)C=CC(=O)C=C4CC[C@H]1[C@@H]3C[C@@H]2C 2.610

+22494-47-9 Clc1ccc(cc1)c2ccc(COC(C)(C)C(=O)O)cc2 4.310

+4828-27-7 OCC(=O)[C@@H]3[C@@]4(C)C[C@H](O)[C@@]2(Cl)C(C[C@H](F)C1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C 2.270

+2030-63-9 Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5 7.660

+671-95-4 O=S(N)(=O)c1cc(ccc1Cl)S(N)(=O)=O 0.410

\*369-77-7 FC(F)(F)c1cc(ccc1Cl)NC(=O)Nc2ccc(Cl)cc2 5.220

+37693-01-9 Clc2cc(Cl)ccc2Cc1cc(ccc1O)C(C)(C)CC(C)(C)C 8.590

\*14261-75-7 Clc1ccc(CC(C)(C)NC(=O)OCC)cc1 4.160

+25803-14-9 Clc1ccc(cc1)C(=O)c3c2ccc(cc2n(CC(=O)O)c3C)OC 3.530

+533-45-9 ClCCc1scnc1C 2.120

#1926-49-4 OC(=O)[C@H]2N3C(=O)[C@@H](NC(=O)[C@H](OC)c1ccc(Cl)c(Cl)c1)[C@H]3SC2(C)C 2.860

+911-45-5 CCN(CCOc1ccc(cc1)/C(c2ccccc2)=C(/Cl)c3ccccc3)CC 6.740

+1181-54-0 OCNC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@@]2(O)C1=O)C(=O)c3c(O)ccc(Cl)c3[C@]4(C)O -1.540

+1622-61-3 [O-][N+](=O)c1ccc2NC(=O)CN=C(c2c1)c3ccccc3Cl 2.410

+4205-90-7 Clc2cccc(Cl)c2NC1=NCCN1 1.590

\*3861-76-5 [O-][N+](=O)c2cc3nc(Cc1ccc(Cl)cc1)n(CCN(CC)CC)c3cc2 5.180

+636-54-4 O=C(NN1[C@@H](C)CCC[C@H]1C)c2ccc(Cl)c(c2)S(N)(=O)=O 1.870

\*3703-76-2 Clc1ccc(cc1)[C@H](OCCN2CCCCC2)c3ccccc3 5.110

#2971-90-6 Oc1c(Cl)c(C)nc(C)c1Cl 2.710

+5251-34-3 OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3C=C(Cl)C1=CC(=O)C=C[C@@]12C 1.680

#40665-92-7 O[C@H]2C[C@@H](O)[C@H](/C=C/[C@@H](O)COc1cccc(Cl)c1)[C@H]2C\C=C/CCCC(=O)O 3.950

\*120-32-1 Oc2ccc(Cl)cc2Cc1ccccc1 4.180

+3811-25-4 O[C@H](CNC(C)C)c1ccccc1Cl 1.820

+10389-73-8 Clc1ccccc1CC(C)(C)N 2.850

+57808-65-8 Clc2cc(NC(=O)c1cc(I)cc(I)c1O)c(C)cc2[C@H](C#N)c3ccc(Cl)cc3 8.110

+1093-58-9 ClC=4C(=O)CC[C@]3(C)C=4CC[C@@H]2[C@H]3CC[C@]1(C)[C@H]2CC[C@@H]1O 3.760

\*2058-52-8 CN1CCN(CC1)C3=Nc4ccccc4Sc2ccc(Cl)cc23 3.840

#33671-46-4 Clc3ccccc3C1=NCC(=O)N(C)c2sc(cc12)CC 3.180

+23593-75-1 Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4 6.260

\*61-72-3 OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1ccccc1Cl)[C@H]4SC3(C)C 2.480

+24166-13-0 Clc1ccccc1C34OCCN4CC(=O)Nc2ccc(Cl)cc23 3.910

#5786-21-0 CN1CCN(CC1)C2=Nc4cc(Cl)ccc4Nc3ccccc23 3.230

#76-57-3 COc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 1.190

+477-27-0 CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(O)C(=O)C=C12 1.200

\*64-86-8 CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12 1.300

+546-06-5 CN(C)[C@H]4CC5=CC[C@@H]1[C@@H](CC[C@@]23CN(C)[C@H](C)[C@@H]3CC[C@H]12)[C@]5(C)CC4 5.140

#458-35-5 Oc1ccc(cc1OC)/C=C\CO 1.190

\*50-22-6 OCC(=O)[C@H]4CC[C@@H]2[C@]4(C)C[C@H](O)[C@@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 1.940

+1110-40-3 CC(=O)OCC(=O)[C@@]3(O)[C@H](C)C[C@H]2[C@@H]4C=C(C)C1=Cc6c(C[C@]1(C)[C@H]4[C@@H](O)C[C@@]23C)cnn6c5ccccc5 5.480

+483-10-3 O=C(OC)[C@@H]2[C@@H](O)CC[C@@H]3CN4CCc1c5ccccc5nc1[C@H]4C[C@H]23 2.110

#486-56-6 CN2C(=O)CC[C@H]2c1cnccc1 0.070

+56-72-4 CCOP(=S)(OCC)Oc1ccc2c(c1)OC(=O)C(Cl)=C2C 4.130

#91-64-5 O=C1C=Cc2ccccc2O1 1.390

+4366-18-1 OC=1c4ccccc4OC(=O)C=1C(COC)C2=C(O)c3ccccc3OC2=O 1.380

#60-27-5 N=C1NC(=O)CN1C -1.760

#483-63-6 CCN(C(=O)\C=C\C)c1ccccc1C 2.730

#458-37-7 Oc1ccc(cc1OC)/C=C/C(=O)CC(=O)/C=C/c2ccc(O)c(OC)c2 3.290

+21725-46-2 Clc1nc(NCC)nc(NC(C)(C)C#N)n1 2.220

+460-19-5 N#CC#N 0.070

#456-59-7 O=C(O[C@H]1C[C@@H](C)CC(C)(C)C1)[C@H](O)c2ccccc2 4.100

+3572-80-3 Oc1ccc2C[C@@H]3N(CC[C@](C)(c2c1)[C@@H]3C)CC4CC4 4.510

+82-92-8 CN1CCN(CC1)C(c2ccccc2)c3ccccc3 2.970

#52-31-3 O=C1NC(=O)NC(=O)C1(CC)C2=CCCCC2 1.770

#31431-43-3 O=C(OC)Nc1nc2cc(ccc2n1)C(=O)C3CC3 2.030

+303-53-7 CN(C)CC\C=C2/c3ccccc3C=Cc1ccccc12 4.790

+512-16-3 OC1(CCCCC1)[C@H](CC)C(=O)O 2.250

+516-21-2 Clc1ccc(cc1)N2C(N)=NC(N)=NC2(C)C 0.960

#108-93-0 OC1CCCCC1 1.230

#108-94-1 O=C1CCCCC1 0.810

#110-83-8 C1C=CCCC1 2.860

\*139-62-8 C[C@@H]3CCCCN3CCCOC(=O)c2ccc(OC1CCCCC1)cc2 6.150

+120-92-3 O=C1CCCC1 0.630

#512-15-2 OC1(CCCC1)[C@H](C(=O)OCCN(C)C)c2ccccc2 2.470

\*75-19-4 C1CC1 1.720

+68-41-7 N[C@@H]1CONC1=O -1.720

+2259-96-3 NS(=O)(=O)c4cc1c(N[C@H](NS1(=O)=O)[C@@H]3C[C@H]2C=C[C@H]3C2)cc4Cl 1.950

+579-23-7 Oc1ccc(cc1OC)/C=C3\CCC\C(=C\c2cc(OC)c(O)cc2)C3=O 4.180

#7199-29-3 NC(=O)C2c3ccccc3CCc1ccccc12 3.160

+52-90-4 O=C(O)[C@@H](N)CS -2.490

\*485-35-8 O=C3C=CC=C2N3C[C@H]1C[C@H]2CNC1 0.600

+71-30-7 NC=1C=CNC(=O)N=1 -1.730

+486-66-8 Oc1ccc(cc1)C3=COc2cc(O)ccc2C3=O 2.550

\*75-99-0 CC(Cl)(Cl)C(=O)O 0.780

+17230-88-5 C#C[C@]3(O)CC[C@H]2[C@@H]4CCC1=Cc5oncc5C[C@]1(C)[C@H]4CC[C@]23C 4.210

+605-65-2 CN(C)c2cccc1c2cccc1S(Cl)(=O)=O 4.290

\*50-29-3 Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl 6.910

#1131-64-2 N=C(N)N1Cc2ccccc2CC1 0.750

+14817-09-5 NC(=O)c1cc(OC)c(OCCCCCCCCCC)c(c1)OC 4.670

#18507-89-6 O=C(OCC)c1cnc2cc(OCC)c(cc2c1O)OCCCCCCCCCC 7.800

\*14484-47-0 CC(=O)OCC(=O)[C@]45N=C(C)O[C@@H]5C[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3CCC1=CC(=O)C=C[C@@]12C 1.310

+4914-30-1 COc4cc5CCN[C@H](CC=1C[C@H]2c3cc(OC)c(OC)cc3CCN2CC=1CC)c5cc4OC 5.240

+477-30-5 COc2c3C1=CC=C(OC)C(=O)C=C1[C@@H](CCc3cc(OC)c2OC)NC 1.370

+83-44-3 O=C(O)CC[C@@H](C)[C@H]2CC[C@H]1[C@@H]3CC[C@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@@]12C 3.500

+64-85-7 OCC(=O)[C@H]3CC[C@H]2[C@@H]4CCC1=CC(=O)CC[C@]1(C)[C@H]4CC[C@]23C 2.880

+131-01-1 COc1cc(cc(OC)c1OC)C(=O)O[C@@H]3C[C@@H]4CN5CCc2c6ccccc6nc2[C@H]5C[C@H]4[C@H](C(=O)OC)[C@H]3OC 3.240

+50-47-5 CNCCCN2c3ccccc3CCc1ccccc12 4.900

+382-67-2 OCC(=O)[C@@H]3[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C 2.350

+50-02-2 OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C 1.830

\*475-26-3 Fc1ccc(cc1)C(c2ccc(F)cc2)C(Cl)(Cl)Cl 5.910

-13739-02-1 CC(=O)Oc3cccc2C(=O)c1cc(cc(OC(C)=O)c1C(=O)c23)C(=O)O 2.420

+83-63-6 O=C(C)N(C(C)=O)c1ccc(cc1C)/N=N/c2ccccc2C 2.670

#124-02-7 C=CCNCC=C 1.110

\*36141-82-9 CC(=O)Nc1ccc(cc1)OCCOCCOc2ccc(cc2)NC(C)=O 1.750

\*552-25-0 CCC(=O)N(C[C@H](C)N(C)CCc1ccccc1)c2ccccc2 3.510

#333-41-5 Cc1cc(OP(=S)(OCC)OCC)nc(n1)C(C)C 3.810

#57998-68-2 O=C(OCC)NC=1C(=O)C(=C(NC(=O)OCC)C(=O)C=1N2CC2)N3CC3 -0.020

\*364-98-7 Clc1ccc2N=C(C)NS(=O)(=O)c2c1 1.200

-120-46-7 O=C(CC(=O)c1ccccc1)c2ccccc2 2.510

#103-49-1 C(NCc1ccccc1)c2ccccc2 2.670

+1918-00-9 COc1c(c(Cl)ccc1Cl)C(=O)O 2.210

#2463-84-5 Clc1cc(ccc1OP(=S)(OC)OC)[N+]([O-])=O 3.580

+97-17-6 Clc1cc(Cl)ccc1OP(=S)(OCC)OCC 5.140

\*7008-26-6 OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](Cl)[C@@]2(Cl)[C@H]3CCC1=CC(=O)C=C[C@@]12C 3.340

\*75-71-8 ClC(Cl)(F)F 2.160

#133-53-9 Cc1cc(O)c(Cl)c(C)c1Cl 3.900

+120-97-8 Clc1c(cc(cc1Cl)S(N)(=O)=O)S(N)(=O)=O 1.060

+2164-09-2 Clc1ccc(NC(=O)C(=C)C)cc1Cl 3.290

#66-76-2 OC=3c4ccccc4OC(=O)C=3CC1=C(O)c2ccccc2OC1=O 2.070

+84-17-3 Oc1ccc(cc1)C(=C\C)\C(=C\C)c2ccc(O)cc2 5.320

\*702-54-5 CCC1(CC)COC(=O)NC1=O 1.170

+111-42-2 OCCNCCO -1.430

+60-91-3 CCN(CC)CCN1c3ccccc3Sc2ccccc12 5.940

\*109-89-7 CCNCC 0.580

\*90-89-1 O=C(N1CCN(C)CC1)N(CC)CC 0.370

+56-53-1 Oc1ccc(cc1)C(\CC)=C(\CC)c2ccc(O)cc2 5.070

+28782-42-5 O=C(O)C3(CCN(CCC(C#N)(c1ccccc1)c2ccccc2)CC3)c4ccccc4 1.990

+2557-49-5 OCC(=O)[C@@]3(O)[C@]4(C)C[C@H](O)[C@@]2(F)[C@@H](C[C@H](F)C1=CC(=O)C=C[C@]12C)[C@@H]4C[C@@H]3C 1.590

+35367-38-5 Clc2ccc(NC(=O)NC(=O)c1c(F)cccc1F)cc2 3.880

+22494-42-4 OC(=O)c1cc(ccc1O)c2ccc(F)cc2F 4.440

+484-23-1 NNc2nnc(NN)c1ccccc12 -0.750

+125-28-0 COc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)CC[C@@H]23 1.490

+67-96-9 C[C@@H]3CC[C@H](O)C\C3=C\C=C1/CCC[C@@]2(C)[C@H](CC[C@H]12)[C@H](C)/C=C/[C@H](C)C(C)C 10.450

+5966-41-6 CC(C)N(CCC(c1ccccc1)c2ccccc2)C(C)C 5.660

#579-38-4 CN(c1ccc(O)cc1)C(=O)C(Cl)Cl 1.780

+42399-41-7 CN(C)CCN2c3ccccc3S[C@@H](c1ccc(OC)cc1)[C@@H](OC(C)=O)C2=O 2.790

\*545-90-4 OC(CC)C(CC(C)N(C)C)(c1ccccc1)c2ccccc2 4.160

\*59-52-9 OC[C@H](S)CS 0.160

#519-30-2 CN(C)CCn2cnc1c2C(=O)N(C)C(=O)N1C -0.150

+60-51-5 COP(=S)(OC)SCC(=O)NC 0.780

#477-93-0 CN(C)CCOCCOC(=O)N1c3ccccc3Sc2ccccc12 4.120

\*131-11-3 COC(=O)c1ccccc1C(=O)OC 1.600

\*124-40-3 CNC -0.380

+22950-29-4 COc1cc(cc(OC)c1O)[C@H](O)CNC -0.560

+551-92-8 O=[N+]([O-])c1cnc(C)n1C 0.310

\*148-01-6 Cc1c(cc(cc1[N+](=O)[O-])[N+]([O-])=O)C(N)=O 0.190

#88-85-7 O=[N+]([O-])c1cc(cc(c1O)[C@H](C)CC)[N+]([O-])=O 3.560

+520-27-4 COc1ccc(cc1O)C2=CC(=O)c3c(O)cc(cc3O2)O[C@@H]5O[C@H](CO[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O)[C@@H](O)[C@H](O)[C@H]5O 0.140

+537-12-2 Cl.O=C(Nc1ccccc1)OC[C@H](OC(=O)Nc2ccccc2)CN3CCCCC3 2.630

#82-66-6 O=C2c1ccccc1C(=O)C2C(=O)C(c3ccccc3)c4ccccc4 4.850

\*58-73-1 CN(C)CCOC(c1ccccc1)c2ccccc2 3.270

+972-02-1 OC(CCCN1CCCCC1)(c2ccccc2)c3ccccc3 4.710

+915-30-0 O=C(OCC)C3(CCN(CCC(C#N)(c1ccccc1)c2ccccc2)CC3)c4ccccc4 6.340

\*117-34-0 OC(=O)C(c1ccccc1)c2ccccc2 3.090

\*122-39-4 c1ccccc1Nc2ccccc2 3.500

+538-62-5 O=C(NNc1ccccc1)/N=N/c2ccccc2 0.980

#101-81-5 c1ccccc1Cc2ccccc2 4.140

\*4147-51-7 CCSc1nc(nc(NC(C)C)n1)NC(C)C 3.810

\*58-32-2 OCCN(CCO)c2nc1c(nc(nc1c(n2)N3CCCCC3)N(CCO)CCO)N4CCCCC4 2.740

+3737-09-5 CC(C)N(CC[C@](c1ccccn1)(c2ccccc2)C(N)=O)C(C)C 2.580

+330-54-1 Clc1ccc(NC(=O)N(C)C)cc1Cl 2.680

+502-55-6 CCOC(=S)SSC(=S)OCC 2.060

+57808-66-9 Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4 3.900

+51-61-6 Oc1ccc(CCN)cc1O -0.980

+86197-47-9 Oc2ccc(CCNCCCCCCNCCc1ccccc1)cc2O 4.270

#309-29-5 O=C4N(CC)C[C@@H](CCN1CCOCC1)C4(c2ccccc2)c3ccccc3 3.420

#74191-85-8 COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)[C@H]4COc5ccccc5O4 2.090

+3254-93-1 O=C2NCNC2(c1ccccc1)c3ccccc3 1.400

#1668-19-5 CN(C)CC\C=C1/c3ccccc3OCc2ccccc12 4.290

+3094-09-5 FC1=CN(C(=O)NC1=O)[C@@H]2O[C@H](C)[C@@H](O)[C@H]2O -1.400

#564-25-0 NC(=O)C=4C(=O)[C@@]3(O)C(O)=C2C(=O)c1c(O)cccc1[C@H](C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C -0.020

\*58-19-5 O=C3C[C@H]4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)C[C@H]3C 3.990

#548-73-2 Fc1ccc(cc1)C(=O)CCCN2CC=C(CC2)N3c4ccccc4NC3=O 3.500

\*17692-31-8 O[C@@H](CN1CCN(CC1)c2ccccc2)CO 0.140

+527-18-4 Cc1c(O)c(C)c(C)c(O)c1C 3.220

+527-17-3 CC=1C(=O)C(C)=C(C)C(=O)C=1C 2.230

#124-28-7 CN(C)CCCCCCCCCCCCCCCCCC 8.390

\*479-18-5 OC[C@@H](O)Cn2cnc1c2C(=O)N(C)C(=O)N1C -1.460

+95-04-5 CC\C(=C\C)C(=O)NC(N)=O 0.800

+483-18-1 COc4cc5CCN[C@H](C[C@H]1C[C@H]2c3cc(OC)c(OC)cc3CCN2C[C@@H]1CC)c5cc4OC 5.200

\*518-82-1 Cc3cc2C(=O)c1cc(O)cc(O)c1C(=O)c2c(O)c3 4.010

+75847-73-3 OC(=O)[C@@H]2CCCN2C(=O)[C@H](C)N[C@H](CCc1ccccc1)C(=O)OCC 2.450

#66778-36-7 CN3CCCC[C@@H]3CCc2ccccc2NC(=O)c1ccc(OC)cc1 4.240

+72-20-8 ClC1=C(Cl)[C@]2(Cl)C(Cl)(Cl)[C@]1(Cl)[C@@H]3[C@@H]2[C@H]4C[C@@H]3[C@H]5O[C@H]45 5.200

+74011-58-8 O=C(O)C2=CN(CC)c1nc(c(F)cc1C2=O)N3CCNCC3 -0.200

\*77671-31-9 O=C(C=1NC(=O)NC=1C)c2ccc(SC)cc2 1.860

+72301-79-2 CC(C)S(=O)(=O)n1c2cc(ccc2nc1N)\C(=N\O)c3ccccc3 3.100

\*86880-51-5 Oc1ccc(cc1)CC(=O)NCCNC[C@H](O)COc2ccccc2C#N 0.920

+299-42-3 O[C@H](c1ccccc1)[C@H](C)NC 1.130

\*481-29-8 O=C4CC[C@@H]3[C@]4(C)CC[C@H]1[C@H]3CC[C@H]2C[C@@H](O)CC[C@]12C 3.070

#7004-98-0 COc3cc4CC[C@@H]2[C@H](CC[C@]1(C)[C@@H]2C[C@H](O)[C@H]1O)c4cc3 3.370

+1764-85-8 NS(=O)(=O)c2cc1c(N[C@H](NS1(=O)=O)CSCC(F)(F)F)cc2Cl 0.790

+2363-58-8 O[C@H]2CC[C@H]1[C@@H]3CC[C@H]4C[C@@H]5S[C@@H]5C[C@]4(C)[C@H]3CC[C@@]12C 4.450

+10402-90-1 O=C(c1ccccc1)[C@@H](C)CN3CCN(C[C@@H](OCC)c2ccccc2)CC3 3.220

\*32665-36-4 O[C@@H](CCN2CCN(C[C@H](OC)c1ccccc1)CC2)c3ccccc3 2.140

+474-86-2 Oc3cc4CC=C1[C@H](CC[C@@]2(C)C(=O)CC[C@H]12)c4cc3 3.350

+57-87-4 CC(C)[C@@H](C)/C=C/[C@@H](C)[C@H]2CC[C@@H]3C4=CC=C1C[C@@H](O)CC[C@]1(C)[C@H]4CC[C@]23C 8.860

+149-32-6 OC[C@H](O)[C@H](O)CO -2.290

+305-01-1 Oc1cc2C=CC(=O)Oc2cc1O 0.550

+25573-43-7 CNC(=O)Oc1ccc2c(c1)[C@@]3(C)CCN(C)O[C@@H]3N2C 2.120

+50-28-2 Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@H]1O)c4cc3 4.010

#2998-57-4 ClCCN(CCCl)C(=O)Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@H]1O)c4cc3 5.500

#50-27-1 Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2C[C@@H](O)[C@@H]1O)c4cc3 2.450

\*53-16-7 Oc3cc4CC[C@@H]1[C@H](CC[C@]2(C)C(=O)CC[C@@H]12)c4cc3 3.130

\*90-54-0 CCC(=O)c1cccc(c1)c2ccccc2OCCN(CC)CC 4.690

+314-35-2 CCN(CC)CCn2cnc1c2C(=O)N(C)C(=O)N1C 0.840

+7432-25-9 CCc1ccccc1N3C(C)=Nc2ccccc2C3=O 4.820

+55283-68-6 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CC(=C)C)CC)C(F)(F)F 5.110

#304-84-7 Oc1ccc(cc1OC)C(=O)N(CC)CC 1.060

+75-08-1 CCS 1.270

#141-43-5 NCCO -1.310

\*486-47-5 CCOc1ccc(cc1OCC)Cc3nccc2cc(OCC)c(cc23)OCC 5.650

+563-12-2 S=P(SCSP(=S)(OCC)OCC)(OCC)OCC 5.070

#23947-60-6 CCNC1=NC(=O)C(CCCC)=C(C)N1 2.220

+434-03-7 O=C4CC[C@@]3(C)C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)=C4 3.110

+26225-79-6 CS(=O)(=O)Oc1cc2c(cc1)O[C@H](OCC)C2(C)C 2.700

+77-15-6 CN1CCC[C@@](CC1)(C(=O)OCC)c2ccccc2 3.520

\*77-67-8 C[C@@]1(CC)CC(=O)NC1=O 0.380

+86-35-1 O=C2N[C@H](c1ccccc1)C(=O)N2CC 1.050

+524-83-4 CCN4[C@H]1CC[C@@H]4CC(C1)OC(c2ccccc2)c3ccccc3 4.770

+93-89-0 O=C(OCC)c1ccccc1 2.640

+101-97-3 O=C(OCC)Cc1ccccc1 2.280

#118-61-6 Oc1ccccc1C(=O)OCC 2.950

\*75-04-7 CCN -0.130

\*100-41-4 CCc1ccccc1 3.150

\*107-15-3 NCCN -2.040

+965-90-2 C[C@]32CC[C@@H]1[C@H]4CCCC=C4CC[C@H]1[C@@H]3CC[C@@]2(O)CC 5.520

+76-58-4 CCOc5ccc1C[C@H]2N(C)CC[C@]34c1c5O[C@@H]4[C@@H](O)C=C[C@@H]23 1.770

+41340-25-4 O=C(O)C[C@]3(CC)OCCc2c3nc1c(cccc12)CC 3.930

#30544-47-9 FC(F)(F)c1cc(ccc1)Nc2ccccc2C(=O)OCCOCCO 4.200

+1954-28-5 C(OCCOC[C@H]1CO1)COCCOC[C@@H]2CO2 -1.680

\*33125-97-2 CC(c1ccccc1)n2cncc2C(=O)OCC 3.050

+38260-54-7 CCc1nc(OCC)cc(OP(=S)(OC)OC)n1 2.940

+2235-90-7 CC[C@@H](N)Cc2cnc1ccccc12 2.170

#470-82-6 CC2(C)OC1(C)CCC2CC1 2.740

\*100-91-4 C[C@@H]2C[C@@H](OC(=O)[C@H](O)c1ccccc1)CC(C)(C)N2C 1.870

\*97-53-0 Oc1ccc(cc1OC)CC=C 2.270

+1301-42-4 CC(C)CCOc1cc2c(cc1)nccc2[C@H](O)[C@H]4C[C@H]3CCN4C[C@H]3CC 5.320

#53370-90-4 NC(=O)c1ccccc1OCCCCCC 2.740

\*52479-85-3 Oc2ccc(C(=O)c1cc(O)c(O)c(O)c1)c(O)c2O 1.890

+76824-35-6 N/C(N)=N/c1nc(CSCCC(\N)=N/S(N)(=O)=O)cs1 -0.640

+52-85-7 O=S(=O)(N(C)C)c1ccc(OP(=S)(OC)OC)cc1 2.230

\*3102-00-9 CCCCOC[C@@H](O)COc1ccccc1 2.230

#25451-15-4 NC(=O)OCC(COC(N)=O)c1ccccc1 0.760

+5728-52-9 OC(=O)Cc1ccc(cc1)c2ccccc2 3.190

\*1008-65-7 Oc1ccccc1c2nnco2 0.220

+22224-92-6 Cc1cc(ccc1SC)OP(=O)(NC(C)C)OCC 3.230

+61019-78-1 N#C[C@@](CCCC)(Cn1ccnc1)c2ccccc2 2.940

#60168-88-9 O[C@@](c1ccccc1Cl)(c2cncnc2)c3ccc(Cl)cc3 3.600

+36330-85-5 O=C(CCC(=O)O)c1ccc(cc1)c2ccccc2 3.200

+4378-36-3 CC[C@H](c1ccccc1)C(=O)OCCN3CCO[C@H](c2ccccc2)[C@@H]3C 4.350

\*5977-10-6 OC1(CCC(CC1)c2ccccc2)[C@H](CC)C(=O)O 3.890

#458-24-2 FC(F)(F)c1cccc(C[C@H](C)NCC)c1 3.360

+49562-28-9 O=C(c1ccc(Cl)cc1)c2ccc(OC(C)(C)C(=O)OC(C)C)cc2 5.190

#67227-56-9 Oc1ccc(cc1)[C@H]3CNCCc2c3cc(O)c(O)c2Cl 2.390

#31879-05-7 O=C(O)[C@@H](C)c2cc(Oc1ccccc1)ccc2 3.900

#13392-18-2 Oc1cc(cc(O)c1)[C@H](O)CN[C@H](C)Cc2ccc(O)cc2 1.220

+37561-27-6 O=C(CN3CCN(Cc1ccc2OCOc2c1)CC3)N4c6ccccc6Sc5ccccc45 3.370

+4846-91-7 CC(C)c2ccccc2OCC1=NCCN1 3.330

#15302-16-6 CCNC1=NC(=O)[C@H](O1)c2ccccc2 0.050

+437-38-7 CCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3 4.050

+55-38-9 Cc1cc(ccc1SC)OP(=S)(OC)OC 4.090

+18046-21-4 O=C(O)Cc1sc(nc1c2ccc(Cl)cc2)c3ccccc3 5.190

+97-24-5 Oc2ccc(Cl)cc2Sc1cc(Cl)ccc1O 4.620

+51630-58-1 Clc1ccc(cc1)C(C(C)C)C(=O)OC(C#N)c3cccc(Oc2ccccc2)c3 6.200

+528-48-3 Oc1ccc(cc1O)C=3Oc2cc(O)ccc2C(=O)C=3O 1.180

+525-82-6 O=C2C=C(Oc1ccccc12)c3ccccc3 3.560

+15301-69-6 O=C(OCCN1CCCCC1)c4cccc2c4OC(=C(C)C2=O)c3ccccc3 4.950

#54143-55-4 FC(F)(F)COc2cc(C(=O)NC[C@@H]1CCCCN1)c(OCC(F)(F)F)cc2 3.780

+79660-72-3 CN1CCN(CC1)c2c(F)c3c(cc2F)C(=O)C(=CN3CCF)C(=O)O 0.240

+5250-39-5 OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1c(F)cccc1Cl)[C@H]4SC3(C)C 2.580

+1480-19-9 Fc1ccc(cc1)C(=O)CCCN2CCN(CC2)c3ccccc3OC 3.600

+31430-15-6 Fc1ccc(cc1)C(=O)c2cc3nc(NC(=O)OC)nc3cc2 2.910

#33245-39-5 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCCl)CCC)C(F)(F)F 5.070

#3693-39-8 OCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@H]3[C@]4(C)C[C@@H](Cl)[C@@]2(Cl)[C@@H]3C[C@H](F)C1=CC(=O)C=C[C@@]12C 4.180

+21679-14-1 Nc3nc(F)nc1c3ncn1[C@H]2O[C@H](CO)[C@@H](O)[C@@H]2O -1.180

\*78755-81-4 O=C(OCC)c3ncn2c3CN(C)C(=O)c1cc(F)ccc12 1.000

+56430-99-0 FC(F)(F)c1cccc(c1)[C@](O)(CC)c2ccccc2 4.620

+52468-60-7 Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4 5.780

\*3385-03-3 OCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3C[C@H](F)C1=CC(=O)C=C[C@]12C 2.660

+2321-07-5 Oc4cc5Oc1cc(O)ccc1C3(OC(=O)c2ccccc23)c5cc4 3.350

+462-06-6 Fc1ccccc1 2.270

\*426-13-1 CC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3C[C@H](C)C1=CC(=O)C=C[C@@]12C 2.000

\*54910-89-3 FC(F)(F)c2ccc(O[C@@H](CCNC)c1ccccc1)cc2 4.050

+76-43-7 C[C@]4(O)CC[C@@H]2[C@]4(C)C[C@H](O)[C@]1(F)[C@@]3(C)CCC(=O)C=C3CC[C@H]12 2.380

\*2709-56-0 FC(F)(F)c2cc3C(=C\CCN1CCN(CCO)CC1)/c4ccccc4Sc3cc2 4.510

+69-23-8 FC(F)(F)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2 4.360

#56995-20-1 Nc1nc(ccc1NC(=O)OCC)NCc2ccc(F)cc2 2.660

#53-34-9 OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3C[C@H](F)C1=CC(=O)C=C[C@@]12C 1.270

\*40666-16-8 O[C@@H]2C[C@H](O)[C@@H](/C=C/[C@H](O)COc1cc(ccc1)C(F)(F)F)[C@@H]2C\C=C/CCCC(=O)O 4.300

+17617-23-1 Fc3ccccc3C2=NCC(=O)N(CCN(CC)CC)c1ccc(Cl)cc12 3.020

+5104-49-4 Fc2cc(ccc2c1ccccc1)[C@H](C)C(=O)O 4.160

+1841-19-6 Fc1ccc(cc1)C(CCCN2CCC4(CC2)C(=O)NCN4c3ccccc3)c5ccc(F)cc5 5.860

+69409-94-5 Clc3cc(ccc3NC(C(=O)OC(C#N)c2cccc(Oc1ccccc1)c2)C(C)C)C(F)(F)F 6.810

+15687-22-6 Oc2cc3OC(=O)C=C(CN1CCOCC1)c3cc2O -0.080

+17692-39-6 C(CCN1CCOCC1)c3ccc(COc2ccccc2)cc3 4.130

\*2454-11-7 O=C2C=C3CC[C@H]1[C@@H]4CC[C@](C)(O)[C@@]4(C)C[C@@H](O)[C@@H]1[C@@]3(C)C=C2C=O 1.430

\*2825-60-7 CC(=O)OCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@H]3[C@]4(C)C[C@@H](O)[C@@]2(F)[C@@H]3CC(C=O)=C1C=C(OCCCl)CC[C@@]12C 3.760

+23155-02-4 O=P(O)(O)[C@H]1O[C@@H]1C -1.230

\*6064-83-1 OP(=O)(O)Oc1ccccc1C(=O)O 0.590

+5598-52-7 Clc1cc(Cl)c(Cl)nc1OP(=O)(OC)OC 1.910

+21548-32-3 CCOP(=O)(/N=C1\SCS1)OCC 0.680

\*23110-15-8 C[C@@]1(O[C@@H]1C\C=C(\C)C)[C@H]3[C@@]2(CO2)CC[C@@H](OC(=O)\C=C\C=C\C=C\C=C\C(=O)O)[C@H]3OC 4.790

+110-00-9 c1ccco1 1.340

+67-45-8 [O-][N+](=O)c2oc(/C=N/N1CCOC1=O)cc2 -0.040

+98-01-1 O=Cc1ccco1 0.410

+54-31-9 NS(=O)(=O)c2cc(c(NCc1ccco1)cc2Cl)C(=O)O 2.030

+60142-96-3 NCC1(CC(=O)O)CCCCC1 -1.100

\*106-24-1 C\C(C)=C\CCC(/C)=C\CO 3.560

#60282-87-3 O=C4CC[C@@]3(C)C(CC[C@@H]2[C@@H]3CC[C@@]1(CC)[C@H]2C=C[C@@]1(O)C#C)=C4 3.260

#545-26-6 O[C@H]5CC[C@@]3(C)[C@H](CC[C@@H]2[C@@]4(O)C[C@H](O)[C@H](C1=CC(=O)OC1)[C@]4(C)CC[C@@H]23)C5 1.600

+3820-67-5 OC[C@@H](O)COC(=O)c3ccccc3Nc1ccnc2cc(Cl)ccc12 3.660

+21187-98-4 Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2C[C@H]3CCC[C@@H]3C2 2.120

+29094-61-9 Cc1cnc(cn1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3 1.910

+33342-05-1 O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(cc2)CCN4C(=O)c3cc(ccc3C(C)(C)C4=O)OC 4.650

#52443-21-7 OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](C=O)NC(=O)Cc2c1cc(ccc1n(c2C)C(=O)c3ccc(Cl)cc3)OC 2.250

#50-99-7 O[C@H]([C@@H](O)C=O)[C@H](O)[C@H](O)CO -3.240

+77-21-4 CC[C@@]1(CCC(=O)NC1=O)c2ccccc2 1.900

+10238-21-8 O=C(NC1CCCCC1)NS(=O)(=O)c3ccc(CCNC(=O)c2cc(Cl)ccc2OC)cc3 4.790

#56-81-5 OCC(O)CO -1.760

-56-40-6 NCC(=O)O -3.210

#339-44-6 O=S(=O)(Nc1ncc(cn1)OCCOC)c2ccccc2 0.390

+87-52-5 CN(C)Cc2cnc1ccccc12 1.450

+126-07-8 O=C2c3c(O[C@@]21C(=CC(=O)C[C@H]1C)OC)c(Cl)c(OC)cc3OC 2.180

+90-05-1 Oc1ccccc1OC 1.320

+93-14-1 OCC(O)COc1ccccc1OC 1.390

#55-65-2 N=C(N)NCCN1CCCCCCC1 0.880

\*113-00-8 N=C(N)N -1.630

\*73-40-5 NC2=Nc1ncnc1C(=O)N2 -0.910

\*118-00-3 NC3=Nc1c(ncn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N3 -1.900

\*23092-17-3 FC(F)(F)CN2c1ccc(Cl)cc1C(=NCC2=O)c3ccccc3 3.970

#80-13-7 O=S(=O)(N(Cl)Cl)c1ccc(cc1)C(=O)O -0.170

\*3093-35-4 ClCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3CCC1=CC(=O)CC[C@@]12C 2.930

\*52-86-8 Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3 4.300

+777-11-7 Clc1cc(OCC#CI)c(Cl)cc1Cl 5.030

+442-51-3 COc1ccc3c(c1)nc2c3ccnc2C 3.560

\*509-86-4 O=C1NC(=O)NC(=O)C1(CC)C2=CCCCCC2 2.030

+76-44-8 ClC2=C(Cl)[C@]3(Cl)[C@@H]1C=C[C@H](Cl)[C@@H]1[C@@]2(Cl)C3(Cl)Cl 6.100

+372-66-7 CC(C)(O)CCC[C@H](N)C 1.150

+23560-59-0 ClC1=C(OP(=O)(OC)OC)C2CC=CC12 2.320

+3511-16-8 OC(=O)[C@@H]3N4C(=O)[C@H](N1C(=O)[C@H](NC1(C)C)c2ccccc2)[C@H]4SC3(C)C 2.350

+118-74-1 Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl 5.730

#67-72-1 ClC(Cl)(Cl)C(Cl)(Cl)Cl 4.140

+70-30-4 Clc2c(Cc1c(O)c(Cl)cc(Cl)c1Cl)c(O)c(Cl)cc2Cl 7.540

+51235-04-2 CN(C)C2=NC(=O)N(C1CCCCC1)C(=O)N2C 1.850

\*84-16-2 Oc1ccc(cc1)[C@@H](CC)[C@@H](CC)c2ccc(O)cc2 5.600

+141-94-6 CCC(CCCC)CN1CC(C)(N)CN(CC(CCCC)CC)C1 5.260

+56-29-1 C[C@@]1(C(=O)N=C(O)N(C)C1=O)C2=CCCCC2 1.980

#54-03-5 COc1c(cc(cc1OC)C(=O)OCCCN(C)CCN(C)CCCOC(=O)c2cc(OC)c(OC)c(OC)c2)OC 2.710

+495-69-2 O=C(NCC(=O)O)c1ccccc1 0.310

+51-45-6 NCCc1cncn1 -0.700

\*493-80-1 C(N(CCN1CCCC1)c2ccccc2)c3ccccc3 4.150

+71-00-1 N[C@@H](Cc1cncn1)C(=O)O -3.320

\*87-00-3 CN3[C@@H]1CC[C@@H]3C[C@H](C1)OC(=O)C(O)c2ccccc2 1.420

#848-53-3 Clc1ccc(cc1)[C@H](c2ccccc2)N3CCCN(C)CC3 4.100

+3833-99-6 FC(F)(F)c2cc3N(CCCN1CCCN(CCO)CC1)c4ccccc4Sc3cc2 4.630

\*118-56-9 O=C(O[C@H]1C[C@@H](C)CC(C)(C)C1)c2ccccc2O 6.160

+3105-97-3 CCN(CC)CCNc1ccc(CO)c2Sc3ccccc3C(=O)c12 4.580

+461-72-3 O=C1NC(=O)CN1 -1.690

#3614-47-9 O=C(N)C=1C=C/C(=N\N)NN=1 -1.010

+86-54-4 N\N=C1/NN=Cc2ccccc12 1.000

+118-08-1 CN2CCc1cc5OCOc5cc1[C@@H]2[C@H]4OC(=O)c3c(OC)c(ccc34)OC 1.890

+6592-85-4 CN2CCc1cc3OCOc3cc1[C@H]2O 1.890

+5103-42-4 O=C2c1ccccc1C(=O)C2(O)C4(O)C(=O)c3ccccc3C4=O -0.390

\*58-93-5 NS(=O)(=O)c2cc1c(NCNS1(=O)=O)cc2Cl -0.070

#76-47-1 CCN(CC)CC(=O)OCC(=O)[C@@]4(O)CC[C@@H]2[C@]4(C)C[C@H](O)[C@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 2.540

+50-23-7 OCC(=O)[C@@]4(O)CC[C@@H]2[C@]4(C)C[C@H](O)[C@@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 1.610

+123-31-9 Oc1ccc(O)cc1 0.590

+118-42-3 CCN(CCO)CCC[C@@H](C)Nc1ccnc2cc(Cl)ccc12 3.030

\*50-19-1 O[C@](COC(N)=O)(CC)c1ccccc1 1.090

\*495-99-8 Oc2cc(ccc2/C=C/c1ccc(cc1)C(=N)N)C(=N)N 1.560

+127-07-1 NC(=O)NO -1.800

#68-88-2 Clc1ccc(cc1)[C@@H](c2ccccc2)N3CCN(CC3)CCOCCO 2.360

\*68-94-0 O=C2NC=Nc1ncnc12 -1.110

+53648-05-8 C[C@@H](C(=O)NO)c1ccc(CC(C)C)cc1 2.790

\*288-32-4 c1cncn1 -0.080

+27885-92-3 O=C(Nc1cc(ccc1)C2=NCCN2)Nc3cccc(c3)C4=NCCN4 3.880

+318-23-0 CCN(CC)CCN2C(=N)ON=C2c1ccccc1 3.570

#496-11-7 c1cccc2CCCc12 3.180

\*26807-65-8 NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C 2.660

+74517-78-5 NC(=O)C3(CCCNC(C)C)c1ccccc1c2ccccc23 3.110

\*95-13-6 c1cccc2CC=Cc12 2.920

+60607-68-3 CC(C)NC[C@@H](O)COc2cccc1CC=Cc12 2.680

+60607-68-3 CC(C)NC[C@@H](O)COc2cccc1CC=Cc12 2.680

+482-89-3 O=C3c4ccccc4N\C3=C2/Nc1ccccc1C2=O 3.720

+120-72-9 c1cccc2nccc12 2.140

\*53-86-1 Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC 4.270

+26844-12-2 O=C(NC3CCN(CCc1cnc2ccccc12)CC3)c4ccccc4 3.600

+87-89-8 O[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O)[C@H]1O -2.080

+440-58-4 O=C(C)Nc1c(I)c(c(I)c(CNC(C)=O)c1I)C(=O)O 1.280

#606-17-7 O=C(Nc1c(I)c(c(I)cc1I)C(=O)O)CCCCC(=O)Nc2c(I)c(C(=O)O)c(I)cc2I 5.160

#18181-70-9 Clc1cc(I)c(Cl)cc1OP(=S)(OC)OC 5.510

+66108-95-0 OC[C@@H](O)CNC(=O)c1c(I)c(N(C[C@H](O)CO)C(C)=O)c(I)c(c1I)C(=O)NC[C@H](O)CO -3.050

+60166-93-0 O=C(Nc1c(I)c(c(I)c(c1I)C(=O)NC(CO)CO)C(=O)NC(CO)CO)[C@H](C)O -2.420

#73334-07-3 O=C(Nc1c(I)c(c(I)c(c1I)C(=O)N(C)C[C@H](O)CO)C(=O)NC[C@H](O)CO)COC -2.050

+5579-92-0 O[C@@H](CN1C=C(I)C(=O)C(I)=C1)CO 0.010

+5560-72-5 CN(C)CCCn3c1CCCCCCc1c2ccccc23 5.740

\*36734-19-7 O=C2CN(C(=O)NC(C)C)C(=O)N2c1cc(Cl)cc(Cl)c1 3.000

\*54-92-2 O=C(NNC(C)C)c1ccncc1 0.370

#91-56-5 O=C1c2ccccc2NC1=O 0.830

+58152-03-7 NC[C@@H](O)C(=O)N[C@@H]3C[C@@H](N)[C@H](O[C@H]1O[C@@H](CN)[C@@H](O)[C@@H](O)[C@H]1O)[C@H](O)[C@@H]3O[C@H]2OC[C@@](C)(O)[C@@H](NC)[C@H]2O -7.170

\*124-76-5 C[C@@]21CC[C@@H](C[C@H]1O)C2(C)C 3.240

+538-93-2 CC(C)Cc1ccccc1 4.680

+59-63-2 Cc1cc(no1)C(=O)NNCc2ccccc2 1.490

#530-08-5 Oc1ccc(cc1O)[C@H](O)[C@H](CC)NC(C)C 1.420

+97-54-1 Oc1ccc(cc1OC)\C=C\C 3.040

#25311-71-1 S=P(Oc1ccccc1C(=O)OC(C)C)(NC(C)C)OCC 4.120

\*50270-33-2 O=C(O)Cc2c(c(nn2c1ccccc1)c3ccccc3)c4ccccc4 4.790

\*338-95-4 OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3CCC1=CC(=O)C=C[C@@]12C 1.510

#26675-46-7 FC(F)(F)[C@H](Cl)OC(F)F 2.060

\*466-40-0 CCC(=O)C(C(C)CN(C)C)(c1ccccc1)c2ccccc2 4.170

\*503-01-5 C[C@H](CC\C=C(\C)C)NC 3.030

+54-85-3 O=C(NN)c1ccncc1 -0.700

#55-22-1 O=C(O)c1ccncc1 0.320

+498-94-2 O=C(O)C1CCNCC1 -3.050

+57021-61-1 O=C(Nc1c(C)cccc1C)C2=CC=CNC2=O 1.010

\*78-59-1 O=C1C=C(C)CC(C)(C)C1 1.700

#121-91-5 OC(=O)c1cccc(c1)C(=O)O 1.660

\*33820-53-0 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)C(C)C 5.800

\*119-65-3 c1cccc2ccncc12 2.080

#482-15-5 CN(C)[C@@H](C)CN1c3ccccc3Sc2cccnc12 3.940

#395-28-8 Oc1ccc(cc1)[C@H](O)[C@H](C)N[C@H](C)COc2ccccc2 2.350

#520-18-3 Oc1ccc(cc1)C=3Oc2cc(O)cc(O)c2C(=O)C=3O 1.960

+59-01-8 O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CN)O[C@@H]3O[C@H]2[C@H](O)[C@@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](N)[C@H]1O)[C@H](N)C[C@@H]2N -6.700

+853-34-9 CC(=O)CCC2C(=O)N(c1ccccc1)N(C2=O)c3ccccc3 1.470

\*27762-78-3 OC(O)C(=O)[C@H](C)OCC 0.600

+469-79-4 O=C(CC)C1(CCN(C)CC1)c2cccc(O)c2 1.940

+22071-15-4 C[C@H](C(=O)O)c1cccc(c1)C(=O)c2ccccc2 3.120

#74103-06-3 O=C(O)[C@H]2CCn1c(ccc12)C(=O)c3ccccc3 2.320

\*82-02-0 COc3c1c(OC(C)=CC1=O)c(OC)c2occc23 3.000

+525-79-1 n1cnc3ncnc3c1NCc2ccco2 0.600

+501-30-4 O=C1C=C(CO)OC=C1O -0.640

+36894-69-6 O=C(N)c1cc(ccc1O)[C@@H](O)CN[C@@H](C)CCc2ccccc2 3.090

+103890-78-4 CC=1NC(C)=C(C(C=1C(=O)OCC)c2ccccc2/C=C/C(=O)OC(C)(C)C)C(=O)OCC 5.200

#4618-18-2 O[C@H]2[C@H](O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O)[C@@H](CO)O[C@]2(O)CO -4.670

\*84-79-7 C/C(C)=C\CC=2C(=O)c1ccccc1C(=O)C=2O 3.130

\*2688-77-9 COc1ccc(cc1OC)C[C@H]2c3cc(OC)c(cc3CCN2C)OC 3.370

+53943-88-7 OC(=O)[C@@H]1N[C@@H](CCSCC(=O)OCC)SC1 -2.010

+61-90-5 CC(C)C[C@H](N)C(=O)O -1.520

+14769-73-4 N1=C3SCCN3C[C@@H]1c2ccccc2 1.840

+47141-42-4 CC(C)(C)NC[C@H](O)COc2cccc1c2CCCC1=O 2.400

\*137-58-6 O=C(Nc1c(C)cccc1C)CN(CC)CC 2.440

+59160-29-1 O=C(Nc1c(C)cccc1C)CN(CC(=O)O)CC(=O)O -2.430

+154-21-2 O[C@@H]1[C@@H](O)[C@@H](O)[C@@H](O[C@@H]1SC)[C@@H](NC(=O)[C@@H]2C[C@@H](CCC)CN2C)[C@@H](C)O 0.560

+330-55-2 Clc1ccc(NC(=O)N(C)OC)cc1Cl 3.200

#90-69-7 CN2[C@H](CCC[C@H]2C[C@@H](O)c1ccccc1)CC(=O)c3ccccc3 3.740

+31036-80-3 Clc2cccc(Cl)c2O[C@H](C)C1=NCCN1 3.580

+790-69-2 Clc2cc(NC(=S)Nc1ccc(F)cc1)cc(Cl)c2 4.700

#98079-51-7 O=C(O)C2=CN(CC)c1c(F)c(c(F)cc1C2=O)N3C[C@H](C)NCC3 -0.300

+13010-47-4 O=C(NC1CCCCC1)N(CCCl)N=O 2.830

+91431-42-4 CC(=O)Oc2c1cc(Cl)ccc1c(OC(C)=O)c(OC)c2OC 3.260

\*53808-88-1 O=C(O)Cc1cn(nc1c2ccc(Cl)cc2)c3ccccc3 3.670

+50264-69-2 O=C(O)c3nn(Cc1ccc(Cl)cc1Cl)c2ccccc23 4.660

#53179-11-6 CN(C)C(=O)C(CCN1CCC(O)(CC1)c2ccc(Cl)cc2)(c3ccccc3)c4ccccc4 5.150

+846-49-1 Clc3ccccc3C2=NC(O)C(=O)Nc1ccc(Cl)cc12 2.390

+59729-31-6 CC(C)N1CCC(CC1)N(c2ccc(Cl)cc2)C(=O)Cc3ccccc3 4.850

\*848-75-9 Clc3ccccc3C2=N[C@@H](O)C(=O)N(C)c1ccc(Cl)cc12 2.230

\*75330-75-5 C[C@@H](CC)C(=O)O[C@H]3C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@H]23 4.260

+1977-10-2 CN1CCN(CC1)C3=Nc4ccccc4Oc2ccc(Cl)cc23 3.600

+73-22-3 O=C(O)[C@@H](N)Cc2cnc1ccccc12 -1.060

+487-21-8 Oc2nc(O)nc1nccnc12 -0.410

+1086-80-2 Cc1cc2nc3NC(=O)NC(=O)c3nc2cc1C 1.860

+52-76-6 C[C@]32CC[C@@H]1[C@H]4CCCC=C4CC[C@H]1[C@@H]3CC[C@@]2(O)C#C 4.750

+59937-28-9 CC(C)OC(=O)C(/C(=O)OC(C)C)=C1/SC=CS1 3.750

+69-79-4 O[C@H]2[C@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)[C@@H](CO)O[C@@H](O)[C@@H]2O -5.030

\*591-27-5 Nc1cccc(O)c1 0.210

#532-28-5 O[C@H](C#N)c1ccccc1 0.020

+10262-69-8 CNCCCC24CCC(c1ccccc12)c3ccccc34 4.520

+22232-71-9 Clc1ccc(cc1)[C@]4(O)c2ccccc2C3=NCCN34 4.090

\*31431-39-7 O=C(OC)Nc1nc2cc(ccc2n1)C(=O)c3ccccc3 2.830

+78266-06-5 Cc1cc(C)c(Br)c(C)c1NC(=O)CN(CC(=O)O)CC(=O)O 0.110

\*569-65-3 Cc1cccc(c1)CN2CCN(CC2)[C@@H](c3ccc(Cl)cc3)c4ccccc4 5.870

+51-68-3 Clc1ccc(OCC(=O)OCCN(C)C)cc1 1.960

+137-05-3 N#CC(=C)C(=O)OC 0.930

+2898-12-6 Clc1ccc2c(c1)C(=NCCN2C)c3ccccc3 4.410

+53-31-6 c1cc(cc2OCOc12)CN3CCN(CC3)C(c4ccccc4)c5ccccc5 4.610

#977-79-7 CC(=O)[C@@]3(C)CC[C@H]2[C@@H]4C=C(C)C1=CC(=O)CC[C@]1(C)[C@H]4CC[C@@]23C 4.450

+520-85-4 CC(=O)[C@@]3(O)CC[C@H]2[C@@H]4C[C@H](C)C1=CC(=O)CC[C@]1(C)[C@H]4CC[C@@]23C 3.500

+7195-27-9 C[C@@]2(CN(C)S(=O)(=O)c1ccc(Cl)c(c1)S(N)(=O)=O)CCCO2 1.540

\*5633-18-1 CC(=O)[C@@]3(O)C(=C)C[C@H]2[C@@H]4C=C(C)C1=CC(=O)CC[C@]1(C)[C@H]4CC[C@@]23C 3.830

#5118-29-6 CN(C)CC\C=C2/c1ccccc1C(C)(C)c3ccccc23 4.810

+517-60-2 OC(=O)c1c(c(c(c(c1C(=O)O)C(=O)O)C(=O)O)C(=O)O)C(=O)O 1.500

+71125-38-7 Cc3cnc(NC(=O)C2=C(O)c1ccccc1S(=O)(=O)N2C)s3 3.430

+481-85-6 Oc1cc(C)c(O)c2ccccc12 2.760

\*58-27-5 O=C2C=C(C)C(=O)c1ccccc12 2.200

+1490-04-6 CC(C)[C@H]1CC[C@H](C)C[C@H]1O 3.380

\*60-89-9 CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23 5.360

#57-42-1 CN1CCC(CC1)(C(=O)OCC)c2ccccc2 2.720

+70-07-5 COc2ccccc2OC[C@@H]1CNC(=O)O1 3.220

\*100-92-5 CC(C)(NC)Cc1ccccc1 2.670

+17854-59-0 O=C3c4ccccc4Oc2c3ccc(OC)c2CN1CCCCC1 5.040

+1247-42-3 OCC(=O)[C@@]3(O)C(C)C[C@H]2[C@@H]4CCC1=CC(=O)C=C[C@]1(C)[C@H]4C(=O)C[C@@]23C 2.010

+57-53-4 O=C(N)OCC(C)(COC(=O)N)CCC 0.700

+89-57-6 OC(=O)c1cc(N)ccc1O 0.980

+54-04-6 COc1c(cc(cc1OC)CCN)OC 0.780

+1424-00-6 O=C4C[C@H]3CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]3(C)[C@@H](C)C4 3.480

#72-33-3 COc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)c4cc3 4.680

+135-58-0 Cc1ccc2Sc3ccc(C)cc3Sc2c1 5.920

+57837-19-1 C[C@@H](N(C(=O)COC)c1c(C)cccc1C)C(=O)OC 1.650

+15351-09-4 O=C(c1ccccc1)[C@H](C)N(C)C 2.060

\*5001-33-2 Oc1ccc(cc1OC)[C@H](O)CNC -0.640

+586-06-1 Oc1cc(cc(O)c1)[C@H](O)CNC(C)C 0.210

+914-00-1 NC(=O)C=4C(=O)[C@@]3(O)C(O)=C2C(=O)c1c(O)cccc1C(=C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C -1.370

\*517-18-0 O=C(O)C(C)(C)[C@H](CC)c1ccc2cc(ccc2c1)OC 5.320

\*926-93-2 C[C@@H](NC(=S)NNC(=S)NC)C=C 0.320

#521-10-8 C[C@]4(O)CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C 4.350

+67-56-1 CO -0.770

+91-80-5 CN(C)CCN(Cc1cccs1)c2ccccn2 2.870

+72-44-6 Cc1ccccc1N3C(C)=Nc2ccccc2C3=O 4.330

+554-57-4 CN1N=C(S/C1=N/C(C)=O)S(=O)(N)=O 0.130

+100-97-0 C1N3CN2CN(CN1C2)C3 -4.150

+153-00-4 O=C3C[C@@H]4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)C(C)=C3 3.690

+950-37-8 O=C1SC(=NN1CSP(=S)(OC)OC)OC 2.200

#63-68-3 O=C(O)[C@@H](N)CCSC -1.870

+4969-02-2 CN1CCC[C@@H](C1)CC2c4ccccc4Sc3ccccc23 5.670

#16752-77-5 C\C(=N\OC(=O)NC)SC 0.600

#59-05-2 O=C(O)[C@H](CCC(=O)O)NC(=O)c1ccc(cc1)N(C)Cc2nc3c(nc2)nc(N)nc3N -1.850

\*298-81-7 COc1c3occc3cc2C=CC(=O)Oc12 2.140

+76-38-0 ClC(Cl)C(F)(F)OC 2.210

+93-30-1 COc1ccccc1C[C@H](C)NC 2.300

\*77-41-8 C[C@@]1(CC(=O)N(C)C1=O)c2ccccc2 1.450

#134-20-3 Nc1ccccc1C(=O)OC 1.880

+93-58-3 COC(=O)c1ccccc1 2.120

+93-60-7 COC(=O)c1cccnc1 0.830

#502-02-3 OS(=O)(=O)c2ccc(/N=N/c1ccc(cc1)N(C)C)cc2 1.130

+493-52-7 CN(C)c2ccc(/N=N/c1ccccc1C(=O)O)cc2 3.830

+74-89-5 CN -0.570

+60-34-4 CNN -1.050

+113-45-1 O=C(OC)[C@@H](c1ccccc1)[C@@H]2CCCCN2 0.200

\*1084-65-7 NS(=O)(=O)c2cc1c(CCCS1(=O)=O)cc2C 1.260

\*364-62-5 Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC 2.620

#51218-45-2 ClCC(=O)N(c1c(C)cccc1CC)[C@H](C)COC 3.130

#17560-51-9 NS(=O)(=O)c2cc3C(=O)N(c1ccccc1C)[C@H](C)Nc3cc2Cl 1.840

\*5377-20-8 C[C@H](c1ccccc1)n2cncc2C(=O)OC 2.570

+21087-64-9 O=C1C(=NN=C(SC)N1N)C(C)(C)C 1.700

+31112-62-6 O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]2NC(=O)c1c(I)c(NC(C)=O)c(I)c(N(C)C(C)=O)c1I -1.890

+114-91-0 COCCc1ccccn1 1.080

+73573-88-3 C[C@@H](CC)C(=O)O[C@H]3CCC=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@@H]23 3.950

+7786-34-7 O=P(OC)(OC)OC(/C)=C/C(=O)OC 0.130

+3704-09-4 C[C@@H]4CC1=CC(=O)CC[C@@H]1[C@H]3CC[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@@H]34 3.190

+22916-47-8 Clc1ccc(c(Cl)c1)[C@H](OCc2ccc(Cl)cc2Cl)Cn3ccnc3 6.250

+59467-70-8 Fc4ccccc4C2=NCc1cnc(C)n1c3ccc(Cl)cc23 4.330

+78415-72-2 N#CC1=CC(=C(C)NC1=O)c2ccncc2 1.170

+25905-77-5 Cc2cc(nnc2NCCN1CCOCC1)c3ccccc3 2.030

+10118-90-8 CN(C)c2ccc(O)c1C(=O)C3=C(O)[C@]4(O)C(=O)C(=C(O)[C@@H](N(C)C)[C@@H]4C[C@@H]3Cc12)C(N)=O 0.050

+2385-85-5 ClC53C1(Cl)C4(Cl)C2(Cl)C1(Cl)C(Cl)(Cl)C5(Cl)C2(Cl)C3(Cl)C4(Cl)Cl 6.890

\*99-09-2 O=[N+]([O-])c1cccc(N)c1 1.370

\*554-84-7 O=[N+]([O-])c1cccc(O)c1 2.000

\*2210-63-1 O=C2NN(c1ccccc1)C(=O)[C@H]2CCCC 1.900

+7416-34-4 O=C2c3c(CC)c(C)nc3CC[C@H]2CN1CCOCC1 2.310

+103-16-2 Oc2ccc(OCc1ccccc1)cc2 3.300

\*5741-22-0 CC(C)NC[C@H](O)COc1ccccc1OC 1.690

\*20574-50-9 Cc2ccsc2/C=C/C1=NCCCN1C 3.690

+6536-18-1 CC4=C(CN2CCO[C@H](c1ccccc1)[C@@H]2C)C(=O)N(c3ccccc3)N4C 2.010

+480-16-0 Oc3ccc(C=2Oc1cc(O)cc(O)c1C(=O)C=2O)c(O)c3 1.540

+3731-59-7 N=C(N)NC(=N)N1CCOCC1 -3.030

#57-27-2 Oc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 0.890

#110-91-8 C1CNCCO1 -0.860

+56281-36-8 Cc1c(C)c(/C=CC(\C)=C\C=C\C(\C)=C\C(=O)NCC)c(C)cc1OC 6.900

\*54-32-0 CC(=O)Oc1cc(C(C)C)c(OCCN(C)C)cc1C 3.170

+108-45-2 Nc1cccc(N)c1 -0.330

+3051-09-0 [NH4+].O=C2NC(=O)NC(=O)/C2=N/C1=C([O-])NC(=O)NC1=O -3.970

#529-44-2 Oc1cc(cc(O)c1O)C=3Oc2cc(O)cc(O)c2C(=O)C=3O 1.420

\*127-19-5 CN(C)C(C)=O -0.770

+42924-53-8 CC(=O)CCc1ccc2cc(ccc2c1)OC 3.080

+42200-33-9 CC(C)(C)NC[C@@H](O)COc2cccc1C[C@@H](O)[C@@H](O)Cc12 0.810

+62-67-9 Oc5ccc1C[C@H]2N(CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23)CC=C 1.860

+465-65-6 O=C1CC[C@@]5(O)[C@H]2Cc4ccc(O)c3O[C@@H]1[C@]5(CCN2CC=C)c34 2.090

\*434-22-0 O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@H]1O)=C4 2.620

+835-31-4 c2cc(CC1=NCCN1)c3ccccc3c2 3.520

#91-20-3 c1cccc2ccccc12 3.300

+15299-99-7 CCN(CC)C(=O)C(C)Oc2cccc1ccccc12 3.360

\*132-66-1 O=C(O)c1ccccc1C(=O)Nc3cccc2ccccc23 3.410

+131-28-2 O=C(O)c1c(OC)c(OC)ccc1C(=O)Cc2c(cc3OCOc3c2OC)CCN(C)C 1.970

+83366-66-9 Clc1cccc(c1)N4CCN(CCCN3N=C(CC)N(CCOc2ccccc2)C3=O)CC4 5.000

+463-82-1 CC(C)(C)C 3.110

+13997-19-8 O=C(OC)C3=CNc2cc(OCc1ccccc1)c(CCCC)cc2C3=O 6.560

#466-07-9 O=C1C=C(CO1)[C@@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CC[C@@H]2C[C@H](CC[C@@]23C)O[C@@H]4O[C@@H](C)[C@@H](O)[C@H](OC)[C@H]4O 2.100

#128-53-0 O=C1C=CC(=O)N1CC 0.580

\*5868-05-3 O=C(OCC(COC(=O)c1cccnc1)(COC(=O)c2cccnc2)COC(=O)c3cccnc3)c4cccnc4 1.910

+10571-59-2 Clc1ccc(cc1)[C@H](OC(=O)c2cccnc2)C(C)C 4.320

#31980-29-7 Clc1ccc(cc1)OC(C)(C)C(=O)OCc2cccnc2 3.650

+54-11-5 CN2CCC[C@H]2c1cnccc1 1.170

#59-67-6 O=C(O)c1cccnc1 0.360

\*405-22-1 O=[N+]([O-])c1ccc(/C=N/N(CCO)C(N)=O)o1 -0.540

#555-84-0 O=[N+]([O-])c2ccc(/C=N/N1CCNC1=O)o2 0.240

+4936-47-4 CSC[C@@H]2CN(/N=C\c1ccc(o1)[N+]([O-])=O)C(=O)O2 1.530

#3363-58-4 [O-][N+](=O)c1ccc(o1)/C=N/N3CC(=O)N(CN2CCOCC2)C3=O -1.140

+57474-29-0 O=[N+]([O-])c1ccc(o1)c2cc(C(=O)O)[n+]([O-])c3ccccc23 1.230

+6236-05-1 O=[N+]([O-])c1ccc(\C=N\O)o1 0.300

+13411-16-0 O=[N+]([O-])c2ccc(/C=C/c1cccc(CO)n1)o2 1.370

-1614-20-6 O=[N+]([O-])c2ccc(/C=C/c1ccc(N)nn1)o2 1.600

+23256-30-6 O=S2(=O)C[C@H](C)N(/N=C/c1ccc(o1)[N+]([O-])=O)CC2 -0.340

\*1088-92-2 O=[N+]([O-])c2ccc(/C=N/N1CC(=O)N(CO)C1=O)o2 -1.420

+2011-67-8 [O-][N+](=O)c1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3 2.160

#66085-59-4 CC=1NC(C)=C(C(C=1C(=O)OC(C)C)c2cccc(c2)[N+]([O-])=O)C(=O)OCCOC 3.050

+63675-72-9 CC=1NC(C)=C(C(C=1C(=O)OCC(C)C)c2ccccc2[N+]([O-])=O)C(=O)OC 3.260

+98-95-3 [O-][N+](=O)c1ccccc1 1.850

\*79-24-3 [O-][N+](=O)CC 0.180

\*75-52-5 [O-][N+](C)=O -0.350

\*19881-18-6 [O-][N+](=O)c1ccc(cc1)Oc2ccc(cc2)\N=C=S 5.200

+76963-41-2 CN(C)Cc1nc(CSCCNC(=C\[N+]([O-])=O)\NC)cs1 -0.430

\*579-10-2 CN(C(C)=O)c1ccccc1 1.120

+62-75-9 CN(C)N=O -0.570

#59-89-2 O=NN1CCOCC1 -0.440

\*24526-64-5 Nc3cccc1c3CN(C)C[C@@H]1c2ccccc2 2.380

+1477-39-0 C[C@H](NC)CC(c1ccccc1)(c2ccccc2)[C@@H](OC(C)=O)CC 5.470

+1088-11-5 Clc1ccc2NC(=O)CN=C(c2c1)c3ccccc3 2.930

#52-78-8 O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@]1(O)CC)=C4 3.760

#68-22-4 O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)=C4 2.970

+68-23-5 O=C1CCC4=C(C1)CC[C@@H]3[C@@H]4CC[C@@]2(C)[C@H]3CC[C@@]2(O)C#C 3.510

+27314-13-2 FC(F)(F)c1cc(ccc1)N2N=CC(NC)=C(Cl)C2=O 2.300

#6533-00-2 O=C4CC[C@H]3C(CC[C@@H]2[C@H]3CC[C@]1(CC)[C@H]2CC[C@@]1(O)C#C)=C4 3.480

\*848-21-5 O=C3C=C4CC[C@@H]2C(C=C[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)=C4CC3 2.590

#1531-12-0 Oc3ccc4C[C@H]1NCC[C@@]2(CCCC[C@@H]12)c4c3 3.200

+467-85-6 CCC(=O)C(CCN(C)C)(c1ccccc1)c2ccccc2 3.750

+466-97-7 Oc5ccc1C[C@H]2NCC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 -0.170

\*561-48-8 CCC(=O)C(CCN1CCCCC1)(c2ccccc2)c3ccccc3 5.110

#941-69-5 O=C2C=CC(=O)N2c1ccccc1 1.090

+120-34-3 Nc1ccc(cc1)S(=O)(=O)NC(=O)c2ccc(C)c(C)c2 2.390

\*1843-05-6 O=C(c1ccc(cc1O)OCCCCCCCC)c2ccccc2 6.960

+95-50-1 Clc1ccccc1Cl 3.430

+88-74-4 O=[N+]([O-])c1ccccc1N 1.850

+94-70-2 CCOc1ccccc1N 1.650

+90-43-7 Oc2ccccc2c1ccccc1 3.090

+16773-42-5 Cc1ncc([N+]([O-])=O)n1C[C@H](O)CCl 0.600

+70-26-8 NCCC[C@H](N)C(=O)O -4.220

+119-93-7 Cc1cc(ccc1N)c2ccc(N)c(C)c2 2.340

+529-20-4 Cc1ccccc1C=O 2.260

#529-19-1 N#Cc1ccccc1C 2.210

+508-52-1 O[C@@H]3C[C@@]4(O)CC[C@@H]2[C@@]5(O)CC[C@H](C1=CC(=O)OC1)[C@@]5(C)C[C@@H](O)[C@@H]2[C@@]4(CO)[C@H](O)C3 -0.020

\*33996-33-7 O[C@@H]1C[C@@H](C(=O)O)N(C1)C(=O)C -1.550

#66-79-5 OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1ccccc1)[C@H]4SC3(C)C 2.380

\*19666-30-9 O=C2OC(=NN2c1cc(OC(C)C)c(Cl)cc1Cl)C(C)(C)C 4.800

\*21738-42-1 [O-][N+](=O)c1cc2N[C@H](CCc2cc1CO)CNC(C)C 2.240

\*23135-22-0 O=C(C(=N\OC(=O)NC)\SC)N(C)C -0.480

+126-93-2 O=C(N)[C@@]1(CC)O[C@H]1CCC 1.720

\*53-39-4 O=C2C[C@H]3CC[C@H]1[C@@H]4CC[C@](C)(O)[C@]4(C)CC[C@@H]1[C@@]3(C)CO2 2.580

\*21256-18-8 OC(=O)CCc1nc(c(o1)c2ccccc2)c3ccccc3 4.190

+60607-34-3 O=C5Nc1ccccc1N5CCCN2CCN(CC2)C(c3ccccc3)c4ccccc4 4.150

\*604-75-1 Clc1ccc2NC(=O)[C@H](O)N=C(c2c1)c3ccccc3 2.240

#27591-42-0 O=C3c4ccccc4C(=O)C3(CN1CCOCC1)c2ccccc2 2.090

#468-61-1 CCC(CC)(C(=O)OCCOCCN(CC)CC)c1ccccc1 4.340

+53716-50-0 O=C(OC)Nc1nc2ccc(cc2n1)S(=O)c3ccccc3 1.630

+959-14-8 CCN(CC)CCc1nc(no1)c2ccccc2 2.360

\*131-57-7 O=C(c1ccc(cc1O)OC)c2ccccc2 3.790

\*485-89-2 O=C(O)c1c3ccccc3nc(c1O)c2ccccc2 4.160

+2277-92-1 Clc2c(C(=O)Nc1cc(Cl)cc(Cl)c1O)c(O)c(Cl)cc2Cl 6.040

#145-12-0 OC=4C(=O)CC[C@@]3(C)C=4CC[C@@H]2[C@@H]3CC[C@]1(C)[C@H]2CC[C@]1(C)O 4.160

+1491-59-4 CC(C)(C)c2cc(C)c(CC1=NCCN1)c(C)c2O 4.870

+434-07-1 O=C3C[C@@H]4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@]1(C)O)[C@@]4(C)C/C3=C\O 3.610

+76-41-5 O=C1CC[C@@]5(O)[C@H]2Cc4ccc(O)c3O[C@@H]1[C@]5(CCN2C)c34 0.830

+153-87-7 COc3cc4nc(C)c(CCN1CCN(CC1)c2ccccc2)c4cc3OC 3.850

+129-20-4 Oc1ccc(cc1)N3C(=O)[C@@H](CCCC)C(=O)N3c2ccccc2 2.720

+125-53-1 CN3CCCN=C3COC(=O)[C@@](O)(c1ccccc1)C2CCCCC2 3.520

+2439-01-2 Cc1ccc2nc3SC(=O)Sc3nc2c1 3.780

+491-92-9 CCN(CC)CCC[C@@H](C)Nc1cc(cc2cccnc12)OC 4.730

#123-30-8 Nc1ccc(O)cc1 0.040

+130-85-8 O=C(O)c4cc1ccccc1c(Cc2c3ccccc3cc(C(=O)O)c2O)c4O 6.870

+100-09-4 COc1ccc(cc1)C(=O)O 1.960

+123-63-7 CC1OC(C)OC(C)O1 0.670

#53-33-8 OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@H]2[C@@H](C[C@H](F)C1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C 1.680

+14255-87-9 O=C(OC)Nc1nc2ccc(cc2n1)CCCC 3.570

+7542-37-2 N[C@@H]4[C@@H](O)[C@H](O)[C@@H](CO)O[C@@H]4O[C@@H]3[C@@H](N)C[C@H](N)[C@H](O)[C@H]3O[C@H]2O[C@H](CO)[C@@H](O[C@H]1O[C@@H](CN)[C@@H](O)[C@H](O)[C@H]1N)[C@H]2O -6.920

+61869-08-7 Fc1ccc(cc1)[C@@H]4CCNC[C@H]4COc2ccc3OCOc3c2 3.950

+70-70-2 O=C(CC)c1ccc(O)cc1 2.030

#508-59-8 O=C2C=C[C@@]3(O)[C@@H](C)CC[C@H]1C(=C)C(=O)O[C@H]1[C@@]23C 0.770

#4042-30-2 OC2=C(C(=O)c1ccccc1C2=O)C3CCCCC3 3.590

\*103-88-8 Brc1ccc(NC(C)=O)cc1 2.290

+99-91-2 O=C(C)c1ccc(Cl)cc1 2.320

+106-37-6 Brc1ccc(Br)cc1 3.790

#540-36-3 Fc1ccc(F)cc1 2.130

-70458-92-3 CN1CCN(CC1)c2cc3N(CC)C=C(C(=O)O)C(=O)c3cc2F 0.270

\*2152-34-3 NC1=NC(=O)[C@@H](O1)c2ccccc2 0.540

+79-55-0 CC1(C)CCCC(C)(C)N1C 2.690

+983-85-7 CC(=O)OCOC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)Cc1ccccc1)[C@H]3SC2(C)C 0.620

\*40487-42-1 [O-][N+](=O)c1c(C)c(C)cc([N+]([O-])=O)c1NC(CC)CC 5.180

\*135-48-8 c1c3cc4cc5ccccc5cc4cc3cc2ccccc12 7.110

#87-86-5 Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl 5.120

\*115-77-5 OCC(CO)(CO)CO -1.690

+100-33-4 N=C(N)c1ccc(cc1)OCCCCCOc2ccc(cc2)C(=N)N 2.790

#109-66-0 CCCCC 3.390

+76-74-4 O=C1NC(=O)NC(=O)C1(CC)C(C)CCC 2.100

+53910-25-1 O[C@@H]3CNC=Nc1c3ncn1[C@H]2C[C@@H](O)[C@H](CO)O2 -2.540

#84-97-9 CN1CCN(CC1)CCCN2c4ccccc4Sc3ccccc23 4.000

+37924-13-3 O=S(=O)(c1ccccc1)c2cc(C)c(NS(=O)(=O)C(F)(F)F)cc2 4.240

#6621-47-2 C(C(C1CCCCC1)C2CCCCC2)[C@@H]3CCCCN3 7.540

#52645-53-1 Cl/C(Cl)=C/[C@H]3[C@@H](C(=O)OCc2cccc(Oc1ccccc1)c2)C3(C)C 6.500

+58-39-9 OCCN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 4.200

#1182-87-2 O=C1C=C(CO1)[C@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CC[C@@H]2C[C@@H](CC[C@@]23C=O)O[C@H]4O[C@@H](C)[C@@H](O)[C@H](OC)[C@H]4O 1.050

\*371-40-4 Fc1ccc(N)cc1 1.150

#85-01-8 c2cc3ccc1ccccc1c3cc2 4.460

+84-11-7 O=C2c3ccccc3c1ccccc1C2=O 2.520

#92-82-0 n1c3ccccc3nc2ccccc12 2.840

#3735-90-8 CCN(CC)CCSC(=O)N(c1ccccc1)c2ccccc2 3.600

#77-10-1 C1CC(CCC1)(c2ccccc2)N3CCCCC3 4.690

#51-71-8 NNCCc1ccccc1 0.970

+60-12-8 OCCc1ccccc1 1.360

\*103-73-1 CCOc1ccccc1 2.510

+103-03-7 NC(=O)NNc1ccccc1 0.130

\*82-88-2 CN1CC3=C(CC1)c2ccccc2[C@H]3c4ccccc4 4.220

+86-21-5 CN(C)CC[C@H](c1ccccn1)c2ccccc2 3.170

+554-24-5 O=C(O)[C@@H](CC)Oc1c(I)cc(I)cc1I 5.740

#108-95-2 Oc1ccccc1 1.460

+77-09-8 Oc1ccc(cc1)C3(OC(=O)c2ccccc23)c4ccc(O)cc4 2.410

#143-74-8 Oc1ccc(cc1)C3(OS(=O)(=O)c2ccccc23)c4ccc(O)cc4 3.020

+92-84-2 c1ccc2Sc3ccccc3Nc2c1 4.150

#26002-80-2 C/C(C)=C/[C@@H]3[C@H](C(=O)OCc2cccc(Oc1ccccc1)c2)C3(C)C 7.540

+135-67-1 c1ccc2Oc3ccccc3Nc2c1 3.850

+59-96-1 C[C@H](COc1ccccc1)N(Cc2ccccc2)CCCl 4.640

+3818-37-9 C[C@@H](COc1ccccc1)NN 1.200

+673-31-4 NC(=O)OCCCc1ccccc1 1.960

+435-97-2 OC=1c3ccccc3OC(=O)C=1[C@H](CC)c2ccccc2 3.620

+86-34-0 O=C2N(C)C(=O)C[C@@H]2c1ccccc1 0.990

+122-09-8 NC(C)(C)Cc1ccccc1 1.900

+122-79-2 O=C(C)Oc1ccccc1 1.490

+101-84-8 c1ccccc1Oc2ccccc2 4.210

\*139-66-2 c1ccccc1Sc2ccccc2 4.450

\*122-78-1 O=CCc1ccccc1 1.780

+103-82-2 OC(=O)Cc1ccccc1 1.410

+63-91-2 N[C@@H](Cc1ccccc1)C(=O)O -1.380

+50-33-9 O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2 3.160

\*100-63-0 NNc1ccccc1 1.250

\*92-12-6 CN(C)CCOc2ccccc2Cc1ccccc1 3.790

+64-10-8 O=C(N)Nc1ccccc1 0.830

+553-69-5 O[C@H](CNc1ccccn1)c2ccccc2 1.740

\*509-67-1 CN5CC[C@@]32c6c4ccc(OCCN1CCOCC1)c6O[C@H]2[C@@H](O)C=C[C@H]3[C@H]5C4 0.590

+2310-17-0 CCOP(=S)(OCC)SCN1c2ccc(Cl)cc2OC1=O 4.380

+732-11-6 COP(=S)(OC)SCN2C(=O)c1ccccc1C2=O 2.780

+13171-21-6 O=P(OC)(OC)OC(\C)=C(/Cl)C(=O)N(CC)CC 0.790

+253-52-1 c1cccc2cnncc12 0.570

+85-41-6 O=C1NC(=O)c2ccccc12 1.150

+131-69-1 O=S(=O)(NC(C)=O)c2ccc(NC(=O)c1ccccc1C(=O)O)cc2 1.260

\*57-47-6 CNC(=O)Oc1cc2c(cc1)N(C)[C@H]3N(C)CC[C@]23C 1.580

+98-98-6 O=C(O)c1ccccn1 0.720

+32828-81-2 O=C(NCc1cccnc1)c3cc(C(=O)NCc2cccnc2)c(OC)cc3 1.530

#13495-09-5 O=C(OCC)C2(CCN(CCCNc1ccccc1)CC2)c3ccccc3 4.800

#75-97-8 CC(C)(C)C(C)=O 1.200

+52463-83-9 Clc1ccc2c(c1)C(=NCC(=O)N2CC#C)c3ccccc3 2.910

+13523-86-9 CC(C)NCC(O)COc2cccc1nccc12 1.750

+540-38-5 Ic1ccc(O)cc1 2.910

\*84-04-8 NC(=O)C1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 4.440

+1893-33-0 Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)(C(N)=O)N3CCCCC3 2.020

+2167-85-3 O=C(OCCOCCN1CCCCC1)N2c4ccccc4Sc3cccnc23 4.940

#3819-00-9 CC(=O)c2cc3N(CCCN1CCC(CCO)CC1)c4ccccc4Sc3cc2 5.050

+110-85-0 C1CNCCN1 -1.500

\*110-89-4 C1CCCCN1 0.840

\*94-62-2 O=C(/C=C/C=C/c1ccc2OCOc2c1)N3CCCCC3 3.690

\*120-57-0 O=Cc1ccc2OCOc2c1 1.050

#94-53-1 O=C(O)c1ccc2OCOc2c1 1.940

+2531-04-6 CN1CCC(CC1)N2NC(=C(CC)C2=O)c3ccccc3 1.720

+54-91-1 O=C(CCBr)N1CCN(CC1)C(=O)CCBr 0.420

+467-60-7 OC(c1ccccc1)(c2ccccc2)[C@@H]3CCCCN3 3.450

+17243-64-0 O=C(OCC)/C=C2/S[C@H](N1CCCCC1)C(=O)N2CC 2.850

\*7491-74-9 O=C1CCCN1CC(=O)N -1.540

+1043-21-6 O=C(O)c1cc(O)c2C3=Nc4ccccc4OC3=CC(=O)c2n1 1.430

+55837-27-9 O=C(O)c2cc(c(Oc1ccccc1)c(c2)N3CCCC3)S(N)(=O)=O 3.920

\*87-21-8 Nc1ccccc1C(=O)OCC[C@@H]2CCCCN2 3.530

+302-41-0 N#CC(CCN1CCC(CC1)(C(N)=O)N2CCCCC2)(c3ccccc3)c4ccccc4 3.910

+72732-56-0 COc3cc(Cc1cnc2nc(N)nc(N)c2c1C)c(OC)cc3 2.130

+50650-76-5 CC=1C=C(C[C@H](C)CC(C)(C)C)N(O)C(=O)C=1 3.710

+36322-90-4 OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 3.060

+31793-07-4 O=C(O)[C@@H](C)c1cc(Cl)c(cc1)N2CC=CC2 3.320

+100-01-6 O=[N+]([O-])c1ccc(N)cc1 1.390

+100-02-7 O=[N+]([O-])c1ccc(O)cc1 1.910

#5947-49-9 O=C(O)[C@@]2(C)CCC[C@]1(C)c3cc(O)ccc3CC[C@H]12 4.590

+801-52-5 NC(=O)OC[C@@H]3C=1C(=O)C(N)=C(C)C(=O)C=1N2C[C@@H]4N(C)[C@@H]4[C@]23OC -0.960

#156-43-4 CCOc1ccc(N)cc1 1.240

\*106-50-3 Nc1ccc(N)cc1 -0.300

+92-69-3 Oc1ccc(cc1)c2ccccc2 3.200

+140-65-8 CCCCOc1ccc(cc1)OCCCN2CCOCC2 3.430

#55268-74-1 O=C1CN(C[C@@H]2c3ccccc3CCN12)C(=O)C4CCCCC4 2.420

#19216-56-9 O=C(N1CCN(CC1)c3nc2cc(OC)c(OC)cc2c(N)n3)c4ccco4 1.280

+53-03-2 OCC(=O)[C@@]3(O)CC[C@H]2[C@@H]4CCC1=CC(=O)C=C[C@]1(C)[C@H]4C(=O)C[C@@]23C 1.460

\*599-33-7 OCC(=O)[C@@]4(O)C(=C)C[C@@H]3[C@]4(C)C[C@H](O)[C@H]2[C@H]3CCC1=CC(=O)C=C[C@@]12C 1.810

+145-13-1 CC(=O)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C 4.220

\*57526-81-5 CC(C)NC[C@H](O)COc1ccc(O)cc1 0.940

#511-45-5 OC(CCN1CCCCC1)(c2ccccc2)c3ccccc3 4.220

+90-34-6 CC(CCCN)Nc1cc(cc2cccnc12)OC 3.150

+23288-49-5 CC(C)(C)c2cc(SC(C)(C)Sc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C)cc(c2O)C(C)(C)C 10.910

\*59-46-1 Nc1ccc(cc1)C(=O)OCCN(CC)CC 2.140

#671-16-9 CC(C)NC(=O)c1ccc(CNNC)cc1 0.080

#67747-09-5 O=C(N(CCOc1c(Cl)cc(Cl)cc1Cl)CCC)n2ccnc2 4.100

+58-38-8 CN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 4.880

+77-37-2 O[C@](CCN1CCCC1)(c2ccccc2)C3CCCCC3 4.780

+13931-64-1 NC(=O)O[C@@H](CC)C1CCCCC1 3.160

+32809-16-8 Clc1cc(cc(Cl)c1)N2C(=O)[C@]3(C)C[C@@]3(C)C2=O 3.080

#31314-38-2 CC(C)N1CCC(CC1)(c2ccccc2)c3ccccc3 5.100

+26399-36-0 CCCN(CC1CC1)c2c(cc(cc2[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O 5.580

+62666-20-0 Clc1ccc(cc1)/C(=N\CCCC(N)=O)c2cc(F)ccc2O 3.060

+57-83-0 CC(=O)[C@H]3CC[C@H]2[C@@H]4CCC1=CC(=O)CC[C@]1(C)[C@H]4CC[C@]23C 3.870

#77-14-5 C[C@@H]2CN(C)CCC[C@]2(OC(=O)CC)c1ccccc1 3.940

+147-85-3 O=C(O)[C@@H]1CCCN1 -2.540

#1918-16-7 CC(C)N(C(=O)CCl)c1ccccc1 2.180

+54063-53-5 CCCNC[C@@H](O)COc2ccccc2C(=O)CCc1ccccc1 3.370

+493-76-5 CCN(CC)CCC(OC(=O)c1ccccc1)c2ccccc2 4.630

+499-67-2 CCN(CC)CCOC(=O)c1ccc(OCCC)c(N)c1 3.050

+4354-45-4 CN3CCC[C@H](OC(=O)[C@@](O)(c1ccccc1)C2CCCCC2)C3 3.510

\*551-27-9 OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)C(CC)Oc1ccccc1)[C@H]3SC2(C)C 2.650

#362-29-8 CCC(=O)c1cc2N(CC(C)N(C)C)c3ccccc3Sc2cc1 4.790

+123-38-6 CCC=O 0.590

+79-05-0 CCC(N)=O -0.660

\*107-12-0 CCC#N 0.160

\*93-55-0 O=C(CC)c1ccccc1 2.190

#2078-54-8 CC(C)c1cccc(C(C)C)c1O 3.790

+525-66-6 CC(C)NC[C@@H](O)COc2cccc1ccccc12 3.480

\*121-79-9 Oc1cc(cc(O)c1O)C(=O)OCCC 1.800

\*107-10-8 CCCN 0.480

+115-07-1 C=CC 1.770

\*101-40-6 C[C@H](NC)CC1CCCCC1 3.500

+22760-18-5 CC(C)N2c1cc(C)ccc1C(=NC2=O)c3ccccc3 3.020

+466-06-8 O=C1C=CC(=CO1)[C@@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CCC2=C[C@H](CC[C@@]23C)O[C@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O 2.480

+59-58-5 Nc1nc(C)ncc1CN(C=O)C(/C)=C(/CCO)SSCCC 1.850

\*303-69-5 CN(C)CCCN1c3ccccc3Sc2cccnc12 4.010

#136-70-9 Oc1ccc(cc1O)[C@@H](O)CN[C@@H](C)Cc2ccc3OCOc3c2 1.760

#438-60-8 CNCCCC2c3ccccc3C=Cc1ccccc12 4.890

+2537-29-3 O=C1NC(=O)NC(=O)C1(C[C@@H](C)O)CC=C -0.050

+603-00-9 C[C@@H](O)Cn2cnc1c2C(=O)N(C)C(=O)N1C -0.770

\*3426-08-2 C(CN1CCCCCC1)C(c2ccccc2)c3ccccc3 5.700

#66-97-7 O=C1C=Cc2cc3ccoc3cc2O1 1.670

+91-18-9 n1ccnc2ncncc12 -0.580

+53-79-2 COc1ccc(cc1)C[C@@H](N)C(=O)N[C@H]4[C@@H](CO)O[C@@H](n3cnc2c3ncnc2N(C)C)[C@@H]4O 0.030

#81-54-9 O=C2c1ccccc1C(=O)c3c2c(O)cc(O)c3O 3.460

+569-77-7 Oc1cccc2C=C(O)C(O)=C(O)C(=O)c12 1.850

\*24691-76-7 CC=2OCCCC=2C(=O)Nc1ccccc1 2.080

+15686-83-6 CN2CCCN=C2/C=C/c1cccs1 3.140

+290-37-9 c1cnccn1 -0.260

#13457-18-6 O=C(OCC)c1cn2nc(cc2nc1C)OP(=S)(OCC)OCC 3.800

+129-00-0 c1ccc2ccc3cccc4ccc1c2c34 4.880

#289-80-5 c1cccnn1 -0.720

+110-86-1 c1ccccn1 0.650

#58-14-0 CCc1nc(N)nc(N)c1c2ccc(Cl)cc2 2.690

+1740-22-3 OC(C=1C=C/C(C=1)=C(/c2ccccn2)c3ccccn3)(c4ccccn4)c5ccccn5 2.890

+77-04-3 CCC1(CC)C(=O)C=CNC1=O 1.030

\*91-82-7 Clc3ccc(C/C(=C\CN1CCCC1)c2ccccc2)cc3 6.280

+123-75-1 C1CCCN1 0.460

+1018-71-9 Clc2cncc2c1cccc(Cl)c1[N+]([O-])=O 3.750

+36735-22-5 Fc3ccccc3C2=NCC(=S)N(CC(F)(F)F)c1ccc(Cl)cc12 4.030

#1596-63-0 OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c1nc2ccccc2nc1C(=O)O)[C@H]4SC3(C)C 1.490

+91-63-4 Cc1ccc2ccccc2n1 2.590

\*85441-61-8 O=C(OCC)[C@H](CCc1ccccc1)N[C@@H](C)C(=O)N2Cc3ccccc3C[C@H]2C(=O)O 3.720

\*152-43-2 C#C[C@]5(O)CC[C@@H]2[C@]5(C)CC[C@@H]3c4ccc(OC1CCCC1)cc4CC[C@@H]23 6.460

\*73-49-4 NS(=O)(=O)c1cc2C(=O)N[C@@H](Nc2cc1Cl)CC 0.160

+130-95-0 COc1cc2c(cc1)nccc2[C@@H](O)[C@@H]4C[C@@H]3CCN4C[C@@H]3C=C 3.440

+81-64-1 O=C2c1ccccc1C(=O)c3c2c(O)ccc3O 3.940

\*91-22-5 c1cccc2cccnc12 2.030

+91-19-0 c1cccc2nccnc12 1.320

#100-76-5 C1CN2CCC1CC2 1.380

+22662-39-1 Clc2cc(ccc2Oc1ccc(Cl)cc1)NC(=O)c3cc(I)cc(I)c3O 8.140

+3615-24-5 CC(C)NC=2C(=O)N(c1ccccc1)N(C)C=2C 1.300

\*58994-96-0 O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CNC(=O)N(CCCl)N=O)O[C@@H]1OC -1.290

\*66357-35-5 [O-][N+](=O)\C=C(/NC)NCCSCc1ccc(CN(C)C)o1 0.270

+80125-14-0 CCN2CCC[C@H]2CNC(=O)c1c(OC)ccc(Br)c1OC 2.100

+20788-07-2 Brc2ccc(NC(=O)c1c(O)cccc1O)cc2 4.480

#480-85-3 O[C@@H]2CCN1CC=C(CO)[C@@H]12 -0.560

\*3615-41-6 O[C@@H](C)[C@H](O)[C@@H](O)[C@@H](O)C=O -1.560

+81-88-9 [Cl-].O=C(O)c4ccccc4C=1c3ccc(cc3OC2=CC(\C=CC=12)=[N+](/CC)CC)N(CC)CC 1.950

+36791-04-5 NC(=O)c1ncn(n1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -1.850

+25546-65-0 N[C@@H]3[C@@H](O)[C@H](O)[C@@H](CN)O[C@@H]3O[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O)[C@H]2O[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O -8.050

\*106266-06-2 CC=5N=C1CCCCN1C(=O)C=5CCN2CCC(CC2)c4noc3cc(F)ccc34 3.490

+53716-44-2 O[C@@]1(CCCC[C@H]1C(=O)O[C@@H](C)CN(CC)CC)C2CCCCC2 4.920

+84057-95-4 CCCN2CCCC[C@@H]2C(=O)Nc1c(C)cccc1C 2.900

+35834-26-5 CN(C)[C@H]3C[C@@H](C)O[C@@H](O[C@@H]1[C@@H](C)[C@H](O)CC(=O)O[C@H](CC)[C@@H](C)[C@@H]2O[C@@]2(C)C=CC(=O)[C@H](C)C[C@@H]1CC=O)[C@H]3O 2.190

+40034-42-2 O=C(O)C2=CN(CC)c1cc(ccc1C2=O)c3ccncc3 2.220

+83-79-4 C=C(C)[C@@H]2Oc3ccc1C(=O)[C@H]4c5cc(OC)c(OC)cc5OC[C@H]4Oc1c3C2 4.100

+104383-17-7 Fc1ccc(cc1)OC[C@H](O)CN2CCC(CC2)N(C)c3nc4ccccc4s3 4.610

#81-07-2 O=C2NS(=O)(=O)c1ccccc12 0.910

+94-59-7 C=CCc1ccc2OCOc2c1 3.450

+138-52-3 OCc2ccccc2O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O -1.220

+90-02-8 O=Cc1ccccc1O 1.810

\*94-67-7 Oc1ccccc1\C=N\O 1.390

+87-17-2 O=C(Nc1ccccc1)c2ccccc2O 3.270

+89-73-6 O=C(NO)c1ccccc1O 0.910

+69-72-7 OC(=O)c1ccccc1O 2.260

+552-94-3 O=C(Oc1ccccc1C(=O)O)c2ccccc2O 3.360

\*89-31-6 COc1cc2C(C)NCCc2cc1O 1.510

\*6376-26-7 CCN(CCOc2ccccc2C(=O)Nc1ccccc1)CC 3.460

\*107-97-1 CNCC(=O)O -2.780

+92-61-5 COc1cc2C=CC(=O)Oc2cc1O 0.860

\*3366-95-8 Cc1ncc([N+]([O-])=O)n1CC(O)C 0.220

+50-67-9 Oc1cc2c(cc1)ncc2CCN 0.210

+28523-86-6 FC(F)(F)C(OCF)C(F)(F)F 1.750

#138-59-0 O[C@@H]1CC(=C[C@@H](O)[C@H]1O)C(=O)O -1.340

\*93-72-1 Clc1cc(OC(C)C(=O)O)c(Cl)cc1Cl 3.800

+79902-63-9 CC(C)(CC)C(=O)O[C@H]3C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@H]23 4.680

+532-32-1 [Na+].[O-]C(=O)c1ccccc1 -2.270

+3930-20-9 O=S(C)(=O)Nc1ccc(cc1)[C@H](O)CNC(C)C 0.240

+1404-64-4 CC=1NC(=O)NC(=O)C=1/C=C/C(=O)N[C@H](CO)CS(=O)CSC -1.710

+90-39-1 C3CCCN4C[C@H]2C[C@H](CN1CCCC[C@@H]12)[C@H]34 2.730

+52-01-7 CC(=O)S[C@@H]4CC1=CC(=O)CC[C@]1(C)[C@H]5CC[C@@]3(C)[C@@H](CC[C@]23CCC(=O)O2)[C@H]45 2.780

+111-01-3 CC(C)CCC[C@@H](C)CCC[C@@H](C)CCCC[C@@H](C)CCC[C@H](C)CCCC(C)C 14.630

+111-02-4 C\C(C)=C\CCC(\C)=C\CCC(\C)=C\CC\C=C(/C)CC\C=C(\C)CC\C=C(/C)C 14.120

+521-18-6 O=C3C[C@H]4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)CC3 3.550

+83-48-7 CC(C)[C@H](CC)/C=C/[C@@H](C)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C 9.430

+3930-19-6 O=C(O)c3nc(c1nc2c(cc1)C(=O)C(OC)=C(N)C2=O)c(N)c(c3C)c4ccc(OC)c(OC)c4O -0.560

+18883-66-4 O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1NC(=O)N(C)N=O -1.450

#57-24-9 O=C2C[C@H]7OCC=C6CN4CC[C@@]53c1ccccc1N2[C@@H]3[C@H]7[C@H]6C[C@@H]45 1.930

\*94-35-9 O[C@H](COC(N)=O)c1ccccc1 0.150

\*100-42-5 C=Cc1ccccc1 2.950

+121-55-1 O=S(=O)(CC)c1ccc(/C=N/NC(N)=S)cc1 1.040

+30279-49-3 NS(=O)(=O)c1cc(Cl)c(cc1)N2C(=O)C[C@@H](C2=O)c3ccccc3 0.690

+56030-54-7 CCC(=O)N(c1ccccc1)C2(COC)CCN(CC2)CCc3cccs3 3.950

+41744-40-5 OC(=O)[C@@H]2N3C(=O)[C@H](NC(=O)[C@@H](c1ccccc1)S(=O)(=O)O)[C@H]3SC2(C)C 0.590

+350-12-9 S=C3SCN(Cc1ccccc1)CN3Cc2ccccc2 4.350

+485-41-6 O=S(N)(=O)c2ccc(/N=N/c1c(cc(N)cc1N)C(=O)O)cc2 0.040

+17784-12-2 O=C1N=C(C=CN1CC)NS(=O)(=O)c2ccc(N)cc2 -0.730

+115-68-4 Nc1ccc(cc1)S(=O)(=O)NC(=O)/C=C(\C)C 0.710

\*2447-57-6 O=S(=O)(Nc1ncnc(OC)c1OC)c2ccc(N)cc2 0.700

\*94-19-9 O=S(=O)(Nc1nnc(CC)s1)c2ccc(N)cc2 1.010

\*57-67-0 Nc1ccc(cc1)S(=O)(=O)/N=C(\N)N -1.220

+95-06-7 C=C(Cl)CSC(=S)N(CC)CC 3.150

\*57-68-1 O=S(=O)(Nc1nc(C)cc(C)n1)c2ccc(N)cc2 0.890

+723-46-6 Cc2cc(NS(=O)(=O)c1ccc(N)cc1)no2 0.890

+80-35-3 O=S(=O)(Nc1ccc(OC)nn1)c2ccc(N)cc2 0.320

+32909-92-5 COc2nsnc2NS(=O)(=O)c1ccc(N)cc1 1.880

#63-74-1 Nc1ccc(cc1)S(=O)(N)=O -0.620

+121-57-3 Nc1ccc(cc1)S(O)(=O)=O -2.160

#98-62-4 Nc1ccc(cc1)S(=O)(F)=O 1.710

\*116-42-7 Nc1ccc(cc1)S(=O)(=O)NC(=O)c2ccc(OC(C)C)cc2 2.290

+144-83-2 O=S(=O)(Nc1ccccn1)c2ccc(N)cc2 0.350

\*59-40-5 Nc1ccc(cc1)S(=O)(=O)Nc2cnc3ccccc3n2 1.680

+599-79-1 O=S(=O)(Nc1ccccn1)c3ccc(/N=N/c2cc(C(=O)O)c(O)cc2)cc3 3.810

+72-14-0 O=S(=O)(Nc1nccs1)c2ccc(N)cc2 0.050

\*515-49-1 Nc1ccc(cc1)S(=O)(=O)NC(N)=S -1.280

+852-19-7 Nc1ccc(cc1)S(=O)(=O)Nc3cc(C)nn3c2ccccc2 2.090

+57-96-5 O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3 2.300

+95-05-6 CCN(CC)C(=S)SC(=S)N(CC)CC 2.710

+515-64-0 Cc2cc(NS(=O)(=O)c1ccc(N)cc1)nc(C)n2 -0.330

+38194-50-2 CS(=O)c1ccc(cc1)/C=C3/c2ccc(F)cc2C(CC(=O)O)=C3C 3.420

+29334-07-4 O=S(=O)(O)Oc1cc2c(cc1OS(=O)(=O)O)OC(=O)C=C2C -3.870

#73384-60-8 CS(=O)c3ccc(c1nc2cccnc2n1)c(OC)c3 1.180

+60325-46-4 O[C@@H]2CC(=O)[C@@H](C/C=C\CCCC(=O)NS(C)(=O)=O)[C@H]2/C=C/[C@@H](O)COc1ccccc1 1.580

+53583-79-2 CCN2CCC[C@@H]2CNC(=O)c1cc(ccc1OC)S(=O)(=O)CC 1.060

#103628-46-2 CNS(=O)(=O)Cc1cc2c(cc1)ncc2CCN(C)C 0.930

+40828-46-4 O=C(c1ccc(cc1)[C@H](C)C(=O)O)c2cccs2 2.820

+53813-83-5 CN1CCN(CC1)C(=O)O[C@@H]5C=2SCCSC=2C(=O)N5c3ccc4ccc(Cl)nc4n3 2.180

+87-90-1 ClN1C(=O)N(Cl)C(=O)N(Cl)C1=O 0.940

#134-96-3 COc1cc(cc(OC)c1O)C=O 0.880

+321-64-2 Nc1c3ccccc3nc2CCCCc12 2.710

+47747-56-8 N[C@H](c1ccccc1)C(=O)N[C@@H]5C(=O)N4[C@@H](C(=O)OC3OC(=O)c2ccccc23)C(C)(C)S[C@@H]45 1.700

+4267-05-4 NS(=O)(=O)c2cc1c(N[C@@H](NS1(=O)=O)C(Cl)(Cl)Cl)cc2Cl 0.820

+5560-78-1 ClC(Cl)C(=O)N(CCOCC)Cc1ccc(CN(CCOCC)C(=O)C(Cl)Cl)cc1 3.030

+124-72-1 FC(F)(F)[C@H](Br)F 1.950

#3810-35-3 O=C(Nc1ncc(s1)[N+]([O-])=O)c2cccs2 2.090

\*59804-37-4 OC=2c1sccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 2.400

+63590-64-7 O=C(N1CCN(CC1)c3nc2cc(OC)c(OC)cc2c(N)n3)C4CCCO4 1.470

#5902-51-2 O=C1NC(C)=C(Cl)C(=O)N1C(C)(C)C 1.890

#23031-25-6 Oc1cc(cc(O)c1)[C@@H](O)CNC(C)(C)C 0.900

#15793-40-5 CC(C)(C)N[C@@H](C)CC(c1ccccc1)c2ccccc2 5.420

#968-93-4 O=C3C=C4CC[C@@H]1[C@H](CC[C@]2(C)OC(=O)CC[C@@H]12)[C@@]4(C)C=C3 2.090

+58-22-0 O=C4CC[C@@]3(C)C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@H]1O)=C4 3.320

+76-23-3 O=C1NC(=O)NC(=O)C1(CC)[C@@H](CC)CCC 2.500

#58-46-8 CC(C)C[C@@H]2CN3CCc1cc(OC)c(OC)cc1[C@H]3CC2=O 2.660

+60-54-8 NC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@]2(O)C1=O)C(=O)c3c(O)cccc3[C@@]4(C)O -1.300

+116-29-0 Clc1cc(c(Cl)cc1Cl)S(=O)(=O)c2ccc(Cl)cc2 4.610

+109-99-9 C1CCCO1 0.460

#142-68-7 C1CCCCO1 0.950

+632-22-4 CN(C)C(=O)N(C)C 0.190

#10379-14-3 Clc1ccc2c(c1)C(=NCC(=O)N2C)C3=CCCCC3 3.200

+319-89-1 OC=1C(=O)C(O)=C(O)C(=O)C=1O 1.210

+50-35-1 O=C1NC(=O)CCC1N3C(=O)c2ccccc2C3=O 0.330

+115-37-7 COC1=CC=C3[C@H]2Cc4ccc(OC)c5O[C@@H]1[C@]3(CCN2C)c45 2.020

+467-98-1 O=C3C=CC4[C@H]2Cc1ccc(OC)c(O)c1[C@@]4(CCN2C)C3 1.260

+91-79-2 CN(C)CCN(Cc1ccsc1)c2ccccn2 2.550

+83-67-0 Cn1cnc2c1C(=O)NC(=O)N2C -0.780

+58-55-9 O=C2c1ncnc1N(C)C(=O)N2C -0.020

#148-79-8 n1c3ccccc3nc1c2cscn2 2.470

#5581-52-2 O=[N+]([O-])c3ncn(C)c3Sc2nc(N)nc1ncnc12 0.960

\*77-27-0 O=C1NC(=S)NC(=O)C1(CC=C)[C@H](C)CCC 3.230

+288-47-1 c1cncs1 0.440

#473-30-3 O=S(=O)(c1cnc(N)s1)c2ccc(N)cc2 0.520

\*59669-26-0 CN(SN(C)C(=O)O\N=C(\C)SC)C(=O)O\N=C(\C)SC 1.700

+154-42-7 NC2=Nc1ncnc1C(=S)N2 -0.070

+110-02-1 c1cccs1 1.810

\*108-98-5 Sc1ccccc1 2.520

#84-06-0 CC(=O)OCCN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 4.820

+316-81-4 CN(C)S(=O)(=O)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 2.950

\*50-52-2 CN4CCCCC4CCN1c3ccccc3Sc2ccc(SC)cc12 5.900

#5591-45-7 CN(C)S(=O)(=O)c2cc3C(=C\CCN1CCN(C)CC1)\c4ccccc4Sc3cc2 3.780

#62-56-6 NC(N)=S -1.080

+492-22-8 O=C1c3ccccc3Sc2ccccc12 3.990

\*137-26-8 CN(C)C(=S)SSC(=S)N(C)C 1.730

#655-05-0 CN(C)C1=NC(=O)[C@@H](O1)c2ccccc2 -0.230

+72-19-5 O=C(O)[C@@H](N)[C@@H](C)O -2.940

#50-89-5 CC1=CN(C(=O)NC1=O)[C@H]2C[C@H](O)[C@@H](CO)O2 -0.930

#65-71-4 CC1=CNC(=O)NC1=O -0.620

+89-83-8 CC(C)c1ccc(C)cc1O 3.300

+76-61-9 CC(C)c1cc(c(C)cc1O)C3(OS(=O)(=O)c2ccccc23)c4cc(C(C)C)c(O)cc4C 7.210

#125-20-2 CC(C)c1cc(c(C)cc1O)C3(OC(=O)c2ccccc23)c4cc(C(C)C)c(O)cc4C 7.060

+6964-20-1 OCCSCCCCCCCCCCSCCO 3.880

\*32527-55-2 OCCN1CCN(CC1)C(=O)CN2c3cc(Cl)ccc3SC2=O 1.040

+34787-01-4 OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)[C@@H](c1ccsc1)C(=O)O)[C@H]3SC2(C)C 1.010

#40180-04-9 O=C(c1ccc(OCC(=O)O)c(Cl)c1Cl)c2cccs2 3.590

+57648-21-2 Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)N3c4ccccc4NC3=S 4.510

+26839-75-8 O[C@H](COc1nsnc1N2CCOCC2)CNC(C)(C)C 1.830

+444-27-9 O=C(O)C1CSCN1 -3.040

\*22619-35-8 Clc1ccc(s1)[C@@H](C[C@H](O)c2ccc(Cl)cc2)C3=C(O)c4ccccc4OC3=O 5.480

+2205-73-4 CC(=O)S[C@@H]3CC1=CC(=O)C[C@H](SC(C)=O)[C@]1(C)[C@H]4CC[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@H]34 2.360

\*4991-65-5 Oc1cc2OC(=O)Sc2cc1 1.670

+51-24-1 O=C(O)Cc2cc(I)c(Oc1cc(I)c(O)cc1)c(I)c2 5.670

+15301-93-6 Cc1ccccc1[C@H](OCCNC)c2ccccc2 3.440

+22345-47-7 COc1ccc(cc1OC)C3=NN=C(C)[C@@H](CC)c2cc(OC)c(cc23)OC 5.390

\*1156-19-0 Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2CCCCCC2 2.690

+59-98-3 c2cc(CC1=NCCN1)ccc2 2.650

+64-77-7 Cc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC 2.340

+50838-36-3 Cc1cc(ccc1)N(C)C(=S)Oc2ccc4c(c2)[C@@H]3CC[C@@H]4C3 6.490

+2933-94-0 CC(C)NC[C@@H](O)COc1cc(C)ccc1 1.970

\*4201-22-3 Cc2cc(Cl)c(NC1=NCCN1)cc2 1.800

+29218-27-7 OC[C@@H]2CN(c1cccc(C)c1)C(=O)O2 1.880

+728-88-1 C[C@H](CN1CCCCC1)C(=O)c2ccc(C)cc2 3.650

+108-88-3 Cc1ccccc1 2.730

+3686-58-6 O=C(Nc1c(C)cccc1C(=O)OC)CN(CC)CC 2.300

+606-58-6 Nc3ncnc1c3c(cn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C#N -0.420

#27203-92-5 O[C@@]1(CCCC[C@@H]1CN(C)C)c2cc(OC)ccc2 3.010

\*1082-57-1 C2CCCc3cccc(NC1=NCCN1)c23 2.530

+53902-12-8 COc1cc(ccc1OC)/C=C/C(=O)Nc2ccccc2C(=O)O 3.620

+15421-84-8 CCN(CC)c1cc(C)nc2ncnn12 1.620

+19794-93-5 Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O 3.210

+5192-84-7 CC(=O)[C@H]2CC[C@H]3[C@@H]4C=C(Cl)C1=CC(=O)C=C[C@@]1(C)[C@@H]4CC[C@]23C 3.730

+68-76-8 O=C1C=C(C(=O)C(=C1N2CC2)N3CC3)N4CC4 -0.130

-24017-47-8 CCOP(=S)(OCC)Oc1ncn(n1)c2ccccc2 3.340

\*10310-32-4 O[C@H]2[C@@H](OCc1ccccc1)[C@H](O[C@H]2OCC)[C@H](COCc3ccccc3)OCc4ccccc4 4.940

+87-10-5 Oc1c(cc(Br)cc1Br)C(=O)Nc2ccc(Br)cc2 5.970

#133-67-5 NS(=O)(=O)c2cc1c(N[C@H](NS1(=O)=O)C(Cl)Cl)cc2Cl 0.620

+101-20-2 Clc2ccc(NC(=O)Nc1ccc(Cl)cc1)cc2Cl 4.900

#112-24-3 NCCNCCNCCN -2.650

+121-44-8 CCN(CC)CC 1.450

#280-57-9 C1CN2CCN1CC2 -0.490

+51-18-3 n1c(nc(nc1N2CC2)N3CC3)N4CC4 2.560

+1420-06-0 c1ccccc1C(N2CCOCC2)(c3ccccc3)c4ccccc4 4.210

\*117-89-5 FC(F)(F)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 5.030

+749-13-3 FC(F)(F)c1cccc(c1)C3(O)CCN(CCCC(=O)c2ccc(F)cc2)CC3 4.520

#146-54-3 FC(F)(F)c1cc2N(CCCN(C)C)c3ccccc3Sc2cc1 5.540

+1582-09-8 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)C(F)(F)F 5.340

#70-00-8 FC(F)(F)C1=CN(C(=O)NC1=O)[C@H]2C[C@H](O)[C@@H](CO)O2 -0.460

+322-79-2 O=C(C)Oc1cc(ccc1C(=O)O)C(F)(F)F 2.090

\*13647-35-3 N#C[C@@H]2C[C@]4(C)C5CC[C@@]1(C)C(CC[C@@H]1O)C5CC[C@]43O[C@@H]3C2=O 2.020

+616-68-2 O=C(Nc1c(C)cc(C)cc1C)CN(CC)CC 2.410

+552-30-7 O=C(O)c1ccc2C(=O)OC(=O)c2c1 1.950

+84-96-8 CN(C)CC(C)CN1c3ccccc3Sc2ccccc12 4.710

+5011-34-7 COc2ccc(CN1CCNCC1)c(OC)c2OC 0.630

+738-70-5 Nc2nc(N)ncc2Cc1cc(OC)c(OC)c(OC)c1 0.910

+635-41-6 O=C(c1cc(OC)c(OC)c(OC)c1)N2CCOCC2 -0.150

+52128-35-5 COc1cc(cc(OC)c1OC)NCc2ccc3nc(N)nc(N)c3c2C 2.550

+739-71-9 CN(C)C[C@@H](C)CN2c3ccccc3CCc1ccccc12 5.430

\*91-81-6 CN(C)CCN(Cc1ccccc1)c2ccccn2 2.730

\*217-59-4 c3cccc4c1ccccc1c2ccccc2c34 5.490

+519-73-3 c1ccccc1C(c2ccccc2)c3ccccc3 5.370

+486-12-4 Cc1ccc(cc1)C(=C\CN2CCCC2)\c3ccccn3 3.920

-477-75-8 c1ccc3c(c1)C4c2ccccc2C3c5ccccc45 4.870

+22089-22-1 O=P1(OCCCN1CCCl)N(CCCl)CCCl 2.270

\*53783-83-8 CN(C)CCOCC(=O)NC12CC3CC(C1)CC(C2)C3 1.790

+552-63-6 OC[C@@H](C(=O)O)c1ccccc1 0.380

\*61-54-1 NCCc2cnc1ccccc12 1.550

+526-55-6 OCCc2cnc1ccccc12 1.630

+69-33-0 Nc3ncnc1c3ccn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -0.800

+51-67-2 Oc1ccc(CCN)cc1 0.860

+60-18-4 Oc1ccc(C[C@H](N)C(=O)O)cc1 -2.260

+118-78-5 NC1C(=O)NC(=O)NC1=O -1.990

\*302-49-8 O=P(NC(=O)OCC)(N1CC1)N2CC2 -0.370

#58-96-8 O=C1NC(=O)N(C=C1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -1.980

#4171-13-5 CC[C@@H](C(N)=O)[C@H](C)CC 1.640

#93413-69-5 OC1(CCCCC1)[C@H](CN(C)C)c2ccc(OC)cc2 3.280

\*66644-81-3 C=CCN2CCC[C@@H]2CNC(=O)c1cc(cc(OC)c1OC)S(N)(=O)=O 1.470

+52-53-9 COc1cc(ccc1OC)[C@@](C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C 3.790

+1929-77-7 O=C(SCCC)N(CCC)CCC 3.840

+18542-37-5 O[C@H]3C[C@@]1(COC(=O)C(=C)[C@@H]1[C@H]2OC(=O)C(=C)[C@@H]23)C=C 0.310

+46817-91-8 CCOc2ccccc2OC[C@@H]1CNCCO1 1.750

+21363-18-8 C[C@@H](CC)N(C[C@H](O)c2cccn2Cc1ccccc1Cl)[C@@H](C)CC 5.280

#50471-44-8 O=C1N(C(=O)O[C@@]1(C)C=C)c2cc(Cl)cc(Cl)c2 3.100

#2430-49-1 O=C1NC(=O)NC(=O)C1(C=C)[C@H](C)CCC 1.870

#59-02-9 CC(C)CCC[C@H](C)CCC[C@H](C)CCC[C@@]1(C)CCc2c(O1)c(C)c(C)c(O)c2C 12.180

\*58-95-7 CC(=O)Oc2c(C)c(C)c1O[C@](C)(CCc1c2C)CCC[C@H](C)CCC[C@H](C)CCCC(C)C 12.260

+81-81-2 CC(=O)CC(C1=C(O)c2ccccc2OC1=O)c3ccccc3 2.600

+69-89-6 O=C1NC(=O)Nc2ncnc12 -0.730

+90-47-1 O=C1c3ccccc3Oc2ccccc12 3.390

+146-80-5 Oc3nc1c(ncn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)c(O)n3 -1.800

+56187-89-4 O=C(O)[C@H](C)c1ccc(cc1)[C@H]2C/C(CCC2)=N\O 2.400

#14293-44-8 O=S(N)(=O)c1cc(c(O)cc1Cl)C(=O)Nc2c(C)cccc2C 2.190

#7361-61-7 Cc2cccc(C)c2NC1=NCCCS1 4.520

+526-36-3 CC(C)(C)c2cc(C)c(CC1=NCCN1)c(C)c2 5.350

+146-48-5 O=C(OC)[C@H]2[C@@H](O)CC[C@H]3CN4CCc1c5ccccc5nc1[C@@H]4C[C@@H]23 2.730

+56775-88-3 Brc1ccc(cc1)C(=C\CN(C)C)/c2cccnc2 3.180

#1222-57-7 CS(=O)(=O)c1ccc(cc1)c2cn3ccccc3n2 2.090

+82626-48-0 CN(C)C(=O)Cc1c(nc2ccc(C)cn12)c3ccc(C)cc3 3.850

+43200-80-2 CN1CCN(CC1)C(=O)O[C@H]4c2nccnc2C(=O)N4c3ccc(Cl)cn3 1.540

**Table S3**

**The numerical data on water solubility (mg/L) for drug-like substances. Split 1**

\*79-00-5 ClCC(Cl)Cl -3.662

\*530-50-7 NN(c1ccccc1)c2ccccc2 -2.458

+87-61-6 Clc1cccc(Cl)c1Cl -1.255

#108-70-3 Clc1cc(Cl)cc(Cl)c1 -0.779

\*106-99-0 C=CC=C -2.866

\*534-07-6 ClCC(=O)CCl -4.742

+102-06-7 N=C(Nc1ccccc1)Nc2ccccc2 -3.000

+130-15-4 O=C2C=CC(=O)c1ccccc12 -2.825

+106-98-9 C=CCC -2.344

+112-53-8 CCCCCCCCCCCCO -0.602

+70-34-8 Fc1ccc(cc1[N+](=O)[O-])[N+]([O-])=O -2.602

\*288-88-0 c1nncn1 -5.627

#86-55-5 O=C(O)c2cccc1ccccc12 -1.934

\*90-15-3 Oc2cccc1ccccc12 -2.938

#108-03-2 [O-][N+](=O)CCC -4.176

+131-91-9 O=Nc1c2ccccc2ccc1O -3.000

\*109-67-1 CCCC=C -2.170

+92-43-3 O=C1CCN(N1)c2ccccc2 -4.064

+118-79-6 Brc1cc(Br)cc(Br)c1O -1.845

+87-40-1 COc1c(Cl)cc(Cl)cc1Cl -1.000

\*88-06-2 Clc1cc(Cl)cc(Cl)c1O -2.903

\*118-96-7 Cc1c(cc(cc1[N+](=O)[O-])[N+]([O-])=O)[N+]([O-])=O -2.114

#120-83-2 Clc1cc(Cl)c(O)cc1 -3.653

+367-25-9 Fc1ccc(N)c(F)c1 -3.652

+97-02-9 O=[N+]([O-])c1cc(ccc1N)[N+]([O-])=O -3.158

#51-28-5 O=[N+]([O-])c1cc(ccc1O)[N+]([O-])=O -3.446

+119-26-6 NNc1ccc(cc1[N+]([O-])=O)[N+]([O-])=O -3.394

+329-71-5 O=[N+]([O-])c1ccc(cc1O)[N+]([O-])=O -2.585

#1904-98-9 Nc1nc(N)nc2ncnc12 -3.377

\*87-65-0 Clc1cccc(Cl)c1O -3.279

+573-56-8 O=[N+]([O-])c1cccc([N+]([O-])=O)c1O -3.715

+108-48-5 Cc1cccc(C)n1 -5.477

+136-95-8 Nc1nc2ccccc2s1 -2.491

+96-50-4 Nc1nccs1 -4.743

#110-43-0 CC(=O)CCCCC -3.633

+149-30-4 Sc1nc2ccccc2s1 -2.079

#137-32-6 C[C@@H](CC)CO -4.473

+115-19-5 C#CC(C)(C)O -6.000

\*135-19-3 Oc1ccc2ccccc2c1 -2.878

#79-46-9 CC(C)[N+]([O-])=O -4.230

+123-96-6 CC(O)CCCCCC -3.049

#6032-29-7 C[C@@H](O)CCC -4.649

+109-68-2 C\C=C\CC -2.307

#122-99-6 OCCOc1ccccc1 -4.427

+141-90-2 O=C1C=CNC(=S)N1 -2.851

+95-76-1 Nc1cc(Cl)c(Cl)cc1 -1.964

+300-38-9 Brc1cc(cc(Br)c1O)C[C@H](N)C(=O)O -3.602

#13466-78-9 CC2(C)[C@H]1CC=C(C)C[C@@H]12 -0.464

+536-78-7 CCc1cccnc1 -5.568

\*598-75-4 CC(C)[C@@H](C)O -4.748

+56-49-5 Cc2ccc3cc1c5ccccc5ccc1c4CCc2c34 2.538

#584-02-1 CCC(O)CC -4.712

+536-75-4 CCc1ccncc1 -5.029

#104-91-6 O=Nc1ccc(O)cc1 -4.468

+537-47-3 O=C(Nc1ccccc1)NN -2.845

+51-20-7 BrC1=CNC(=O)NC1=O -2.911

#480-68-2 O=C1NC(=O)NC(=O)C1[N+]([O-])=O -2.954

+54-25-1 O=C1NC(=O)C=NN1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -4.918

+134-58-7 O=C1NC(N)=Nc2nnnc12 -4.167

+37517-30-9 CC(C)NCC(O)COc1ccc(cc1C(C)=O)NC(=O)CCC -2.413

+83-32-9 c1cc2cccc3CCc(c1)c23 -0.591

+152-72-7 [O-][N+](=O)c1ccc(cc1)[C@@H](CC(C)=O)C2=C(O)c3ccccc3OC2=O -1.691

+75-07-0 CC=O -6.000

#107-29-9 C\C=N\O -5.248

+60-35-5 CC(N)=O -6.352

\*103-84-4 O=C(C)Nc1ccccc1 -3.806

+59-66-5 O=S(N)(=O)c1nnc(NC(C)=O)s1 -2.991

+968-81-0 O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(cc2)C(C)=O -3.535

#75-05-8 CC#N -6.000

+2751-68-0 CC(=O)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2 -1.076

+98-86-2 CC(=O)c1ccccc1 -3.787

+74-86-2 C#C -3.079

+55079-83-9 Cc1c(C)c(/C=CC(\C)=C\C=C\C(\C)=C\C(=O)O)c(C)cc1OC 1.137

#79-06-1 C=CC(N)=O -5.806

+59277-89-3 NC2=Nc1c(ncn1COCCO)C(=O)N2 -3.210

+281-23-2 C1C3CC2CC1CC(C2)C3 -0.780

+73-24-5 NC=1NC=NC2=NC=NC=12 -3.013

+546-43-0 C[C@H]2CCC[C@]1(C)C[C@@H]3OC(=O)C(=C)[C@H]3C=C12 -1.584

#18559-94-9 OCc1cc(ccc1O)[C@@H](O)CNC(C)(C)C -4.155

#22131-79-9 Clc1cc(ccc1OCC=C)CC(=O)O -2.778

+116-06-3 CC(C)(\C=N\OC(=O)NC)SC -3.780

#52-39-1 OCC(=O)[C@H]4CC[C@@H]2[C@@]4(C=O)C[C@H](O)[C@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 -1.709

+309-00-2 ClC3=C(Cl)[C@@]4(Cl)[C@@H]2[C@@H]([C@@H]1C[C@H]2C=C1)[C@]3(Cl)C4(Cl)Cl 1.770

+59338-93-1 C=CCN3CCC[C@@H]3CNC(=O)c1cc2nnnc2cc1OC -2.470

+97-59-6 O=C1NC(=O)NC1NC(=O)N -3.721

+107-11-9 C=CCN -6.000

+1415-73-2 O[C@H]1[C@H](O)[C@@H](O)[C@@H](O[C@@H]1CO)[C@@H]4c2cccc(O)c2C(=O)c3c(O)cc(CO)cc34 -3.919

+77-20-3 C[C@@H]2CN(C)CC[C@]2(OC(=O)CC)c1ccccc1 -2.901

+768-94-5 NC12CC3CC(C1)CC(C2)C3 -3.799

+539-21-9 N=C(N)N\N=C1\C=C/C(=N\NC(N)=S)C=C1 -3.393

+834-12-8 CSc1nc(NCC)nc(NC(C)C)n1 -2.320

+37517-28-5 NCC[C@H](O)C(=O)N[C@@H]3C[C@H](N)[C@@H](O[C@H]1O[C@H](CN)[C@@H](O)[C@H](O)[C@H]1O)[C@H](O)[C@H]3O[C@H]2O[C@H](CO)[C@@H](O)[C@H](N)[C@H]2O -5.267

\*58-15-1 CN(C)C=2C(=O)N(c1ccccc1)N(C)C=2C -4.736

+1951-25-3 CCN(CC)CCOc1c(I)cc(cc1I)C(=O)c2c3ccccc3oc2CCCC 3.548

+50-48-6 CN(C)CC\C=C1\c3ccccc3CCc2ccccc12 -0.987

+88150-42-9 O=C(OC)C1=C(C)NC(COCCN)=C(C(=O)OCC)[C@@H]1c2ccccc2Cl -1.877

#300-62-9 NC(C)Cc1ccccc1 -4.447

+69-53-4 OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)[C@H](N)c1ccccc1)[C@H]3SC2(C)C -4.004

+538-68-1 CCCCCc1ccccc1 -0.528

+31698-14-3 N=C1N=C2O[C@H]3[C@H](O)[C@@H](CO)O[C@H]3N2C=C1 -6.000

#53-41-8 O=C4CC[C@@H]3[C@]4(C)CC[C@H]1[C@H]3CC[C@H]2C[C@H](O)CC[C@]12C -1.079

+62-53-3 Nc1ccccc1 -4.556

+117-37-3 COc1ccc(cc1)C3C(=O)c2ccccc2C3=O -1.902

#100-66-3 COc1ccccc1 -3.017

-91-75-8 C(c1ccccc1)N(CC2=NCCN2)c3ccccc3 -2.822

+120-12-7 c1ccc2cc3ccccc3cc2c1 1.363

+60-80-0 O=C2C=C(C)N(C)N2c1ccccc1 -4.715

+2835-06-5 N[C@H](C(=O)O)c1ccccc1 -5.061

+520-36-5 Oc1ccc(cc1)C3=CC(=O)c2c(cc(O)cc2O)O3 -2.262

+58-00-4 Oc3ccc2C[C@@H]1c4c(CCN1C)cccc4c2c3O -4.220

+147-81-9 O[C@H](C=O)[C@H](O)[C@H](O)CO -5.699

+74-79-3 N[C@@H](CCCNC(=N)N)C(=O)O -5.260

+63968-64-9 O=C4O[C@H]2O[C@@]1(C)CC[C@@H]3[C@]2(OO1)[C@@H](CC[C@H]3C)[C@H]4C -1.715

+466-49-9 CC(=O)N2c1c(cccc1OC)[C@]35CCN4CCC[C@@](CC[C@@H]23)(CC)[C@@H]45 -4.223

\*29122-68-7 CC(C)NCC(O)COc1ccc(cc1)CC(N)=O -4.124

\*51-55-8 CN3C1CCC3CC(C1)OC(=O)C(CO)c2ccccc2 -3.342

+320-67-2 NC1=NC(=O)N(C=N1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -4.949

#62973-76-6 Cn2c(cnc2/C=C/c1ccnc(N)n1)[N+]([O-])=O -3.279

+1649-18-9 Fc1ccc(cc1)C(=O)CCCN2CCN(CC2)c3ccccn3 -2.117

+1830-32-6 CCN(CC)C(=O)CSc1ccc(Cl)nn1 -3.699

#103-33-3 N(=N/c1ccccc1)\c2ccccc2 -0.806

#527-73-1 [O-][N+](=O)c1nccn1 -4.508

#275-51-4 c1cccc2cccc2c1 -1.701

+1134-47-0 Clc1ccc(cc1)C(CN)CC(=O)O -3.320

+101-27-9 Clc1cc(NC(=O)OCC#CCCl)ccc1 -1.041

+39552-01-7 CC(C)NC[C@@H](O)COc1cccc2cc(oc12)C(C)=O -3.422

\*22781-23-3 CNC(=O)Oc1cccc2OC(C)(C)Oc12 -2.415

+73-48-3 FC(F)(F)c1cc2N[C@H](NS(=O)(=O)c2cc1S(N)(=O)=O)Cc3ccccc3 -2.033

+17804-35-2 O=C(OC)Nc2nc1ccccc1n2C(=O)NCCCC -0.580

+51234-28-7 O=C(O)[C@@H](C)c1cc2nc(oc2cc1)c3ccc(Cl)cc3 -1.716

+2062-84-2 Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)N3c4ccccc4NC3=O -0.262

+100-52-7 O=Cc1ccccc1 -3.818

+55-21-0 NC(=O)c1ccccc1 -4.130

+93-98-1 O=C(Nc1ccccc1)c2ccccc2 -2.418

+71-43-2 c1ccccc1 -3.253

\*134-81-6 O=C(C(=O)c1ccccc1)c2ccccc2 -1.702

#51-17-2 c1cccc2ncnc12 -3.303

+22994-85-0 O=C(Cn1ccnc1[N+]([O-])=O)NCc2ccccc2 -2.602

+271-89-6 c1cccc2occc12 -2.831

#65-85-0 O=C(O)c1ccccc1 -3.531

+104-31-4 O=C(OCCOCCOCCOCCOCCOCCOCCOCCOCCOC)c1ccc(NCCCC)cc1 -0.090

+100-47-0 N#Cc1ccccc1 -3.301

#119-61-9 O=C(c1ccccc1)c2ccccc2 -2.137

+95-16-9 c1cccc2scnc12 -3.633

\*98-88-4 ClC(=O)c1ccccc1 -3.694

+100-51-6 OCc1ccccc1 -4.632

+103-41-3 O=C(OCc1ccccc1)/C=C/c2ccccc2 -0.967

+103-50-4 C(OCc1ccccc1)c2ccccc2 -1.602

+100-46-9 NCc1ccccc1 -6.000

#5638-76-6 CNCCc1ccccn1 -6.000

+378-44-9 OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@@H]3C -1.823

+59170-23-9 COc1cc(ccc1OC)CCNC[C@H](O)COc2cc(C)ccc2 -2.265

+15301-48-1 CCC(=O)N5c1ccccc1N(C4CCN(CCC(C#N)(c2ccccc2)c3ccccc3)CC4)C5=O 1.036

\*103-29-7 C(Cc1ccccc1)c2ccccc2 -0.633

+42576-02-3 Clc2cc(Cl)ccc2Oc1cc(C(=O)OC)c(cc1)[N+]([O-])=O 0.400

+60628-96-8 c1cc(ccc1c2ccccc2)[C@H](c3ccccc3)n4ccnc4 0.959

+28434-01-7 C/C(C)=C/[C@@H]3C(C(=C)CCC=2C=C(Cc1ccccc1)CC=2)C3(C)C 0.523

+58-85-5 O=C1N[C@H]2[C@@H](CCCCC(=O)O)SC[C@@H]2N1 -2.342

+514-65-8 OC(CCN1CCCCC1)(c2ccccc2)C4CC3C=CC4C3 -1.400

+66722-44-9 CC(C)NC[C@H](O)COc1ccc(cc1)COCCOC(C)C -3.350

+56518-41-3 Nc2nc(N)ncc2Cc1cc(OC)c(Br)c(OC)c1 -2.140

\*314-40-9 CC[C@@H](C)N1C(=O)C(Br)=C(C)NC1=O -2.911

#1812-30-2 Brc1ccc2NC(=O)CN=C(c2c1)c3ccccn3 -2.243

+1146-98-1 Brc1ccc(cc1)C3C(=O)c2ccccc2C3=O -0.872

+496-67-3 CC(C)[C@@H](Br)C(=O)NC(N)=O -3.547

\*108-86-1 Brc1ccccc1 -2.649

+75-25-2 BrC(Br)Br -3.491

\*2104-96-3 Clc1cc(OP(=S)(OC)OC)c(Cl)cc1Br 0.523

#4093-35-0 Nc1cc(OC)c(cc1Br)C(=O)NCCN(CC)CC -1.410

+10457-90-6 Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Br)cc3 -1.954

#521-74-4 Oc1c(Br)cc(Br)c2cccnc12 -1.288

+357-57-3 COc1cc2c(cc1OC)N3C(=O)C[C@@H]7OCC=C6CN4CC[C@@]25C3[C@H]7[C@H]6C[C@H]45 -3.505

+54340-62-4 CC(C)(C)NC[C@@H](O)c1cc2cccc(CC)c2o1 -2.330

+41483-43-6 CCNc1nc(C)c(CCCC)c(OS(=O)(=O)N(C)C)n1 -1.342

+14556-46-8 Clc1ccc(C)cc1OC[C@H](O)CNC(C)(C)C -2.869

+52485-79-7 CC(C)(C)[C@@](C)(O)[C@H]1C[C@]74CC[C@]1(OC)[C@@H]5Oc3c(O)ccc2C[C@H]7N(CC[C@@]45c23)CC6CC6 0.197

+36505-84-7 O=C4CC1(CCCC1)CC(=O)N4CCCCN2CCN(CC2)c3ncccn3 -1.330

#23184-66-9 ClCC(=O)N(COCCCC)c1c(cccc1CC)CC -1.362

+653-03-2 CCCC(=O)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 0.783

\*33629-47-9 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N[C@H](C)CC)C(C)(C)C -0.000

+123-72-8 CCCC=O -4.851

+109-74-0 CCCC#N -4.519

+58-08-2 O=C2c1n(C)cnc1N(C)C(=O)N2C -4.334

\*76-22-2 CC2(C)[C@@H]1CC(=O)[C@]2(C)CC1 -3.204

+7689-03-4 CC[C@]1(O)C=2C=C3c4nc5ccccc5cc4CN3C(=O)C=2COC1=O -2.316

+298-46-4 NC(=O)N2c3ccccc3C=Cc1ccccc12 -1.248

#86-74-8 c1cccc2nc3ccccc3c12 -0.255

+10605-21-7 O=C(OC)Nc1nc2ccccc2n1 -1.462

+541-79-7 O[C@@H](NC(=O)OCC)C(Cl)(Cl)Cl -2.877

\*1563-66-2 CNC(=O)Oc1cccc2CC(C)(C)Oc12 -2.505

-24279-91-2 NC(=O)OC[C@@H](OC)C=1C(=O)C(=C(C)C(=O)C=1N2CC2)N3CC3 -3.790

+339-43-5 Nc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC -2.728

+1260-17-9 O[C@H]1[C@H](O)[C@@H](O)[C@H](O[C@@H]1CO)c4c(O)c3C(=O)c2c(C)c(C(=O)O)c(O)cc2C(=O)c3c(O)c4O -3.114

+61422-45-5 O=C1NC(=O)C(F)=CN1C(=O)NCCCCCC -2.086

+72956-09-3 COc4ccccc4OCCNC[C@@H](O)COc2cccc3nc1ccccc1c23 0.234

+138-41-0 O=S(N)(=O)c1ccc(cc1)C(=O)O -4.207

+53994-73-3 ClC=3CS[C@H]2N(C(=O)[C@@H]2NC(=O)[C@H](N)c1ccccc1)C=3C(=O)O -4.000

+34444-01-4 O[C@H](c1ccccc1)C(=O)N[C@H]4C(=O)N3C(=C(CSc2nnnn2C)CS[C@@H]34)C(=O)O -2.667

+25953-19-9 O=C(O)C=3N4C(=O)[C@@H](NC(=O)Cn1cnnn1)[C@H]4SCC=3CSc2nnc(C)s2 -2.330

+35607-66-0 O=C(O)C=2N3C(=O)[C@](NC(=O)Cc1cccs1)(OC)[C@H]3SCC=2COC(N)=O -2.021

+55268-75-2 CO\N=C(\c1ccco1)C(=O)N[C@H]3C(=O)N2C(=C(COC(N)=O)CS[C@@H]23)C(=O)O -2.161

+153-61-7 O=C(O)C=2N3C(=O)[C@@H](NC(=O)Cc1cccs1)[C@H]3SCC=2COC(C)=O -2.199

+38821-53-3 CC=3CS[C@H]2N(C(=O)[C@@H]2NC(=O)[C@H](N)C1=CCC=CC1)C=3C(=O)O -4.328

+133-90-4 Clc1cc(C(=O)O)c(Cl)c(N)c1 -2.845

+305-03-3 O=C(O)CCCc1ccc(cc1)N(CCCl)CCCl -4.093

#56-75-7 O=[N+]([O-])c1ccc(cc1)[C@@H](O)[C@@H](CO)NC(=O)C(Cl)Cl -3.398

+58-25-3 Clc1ccc2N=C(C[N+]([O-])=C(c2c1)c3ccccc3)NC -3.301

\*6164-98-3 Clc1cc(C)c(/N=C/N(C)C)cc1 -2.431

+85-34-7 Clc1c(CC(=O)O)c(Cl)ccc1Cl -2.301

+80-77-3 O=C1CCS(=O)(=O)C(N1C)c2ccc(Cl)cc2 -3.398

+78-95-5 CC(=O)CCl -4.954

#108-90-7 Clc1ccccc1 -2.697

+510-15-6 OC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)C(=O)OCC -1.114

+57-15-8 ClC(Cl)(Cl)C(C)(C)O -3.903

+67-66-3 ClC(Cl)Cl -3.900

#76-06-2 ClC(Cl)(Cl)[N+]([O-])=O -3.210

+148-65-2 Clc2ccc(CN(CCN(C)C)c1ccccn1)s2 -3.303

#58-94-6 NS(=O)(=O)c2cc1c(N=CNS1(=O)=O)cc2Cl -2.425

+54749-90-5 O[C@H]1O[C@H](CO)[C@@H](O)[C@@H](O)[C@H]1NC(=O)N(CCCl)N=O -3.262

\*104-29-0 Clc1ccc(OCC(O)CO)cc1 -4.000

\*461-78-9 Clc1ccc(CC(C)(C)N)cc1 -3.511

+50-53-3 CN(C)CCCN1c3ccccc3Sc2ccc(Cl)cc12 -0.407

\*113-59-7 CN(C)CC\C=C1\c3ccccc3Sc2ccc(Cl)cc12 0.530

+57-62-5 NC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@@]2(O)C1=O)C(=O)c3c(O)ccc(Cl)c3[C@@]4(C)O -2.799

#57-88-5 CC(C)CCC[C@@H](C)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C 1.022

+218-01-9 c1cc4ccccc4c2ccc3ccccc3c12 2.699

+51481-61-9 N#C\N=C(/NC)NCCSCc1ncnc1C -3.972

+118-10-5 O[C@H](C2CC1CCN2C[C@@H]1C=C)c4ccnc3ccccc34 -2.380

+132-60-5 O=C(O)c1cc(nc2ccccc12)c3ccccc3 -2.204

+104-54-1 OC\C=C\c1ccccc1 -3.792

+298-57-7 c1ccccc1C(c2ccccc2)N3CCN(CC3)C/C=C/c4ccccc4 -2.875

+253-66-7 c1cnnc2ccccc12 -4.170

+104-28-9 COc1ccc(/C=C/C(=O)OCCOCC)cc1 -2.699

+85721-33-1 O=C(O)C2=CN(c1cc(c(F)cc1C2=O)N3CCNCC3)C4CC4 -4.477

+81098-60-4 Clc1cc(c(OC)cc1N)C(=O)N[C@H]3CCN(CCCOc2ccc(F)cc2)C[C@H]3OC -0.433

+1195-16-0 O=C1SCC[C@H]1NC(=O)C -5.137

+372-75-8 N[C@@H](CCCNC(N)=O)C(=O)O -4.107

+30544-61-7 O=C(c1ccc(Cl)cc1)N(CCCC(=O)O)c2ccc(OC)cc2 -1.500

+55905-53-8 Clc1cc(c(OC)cc1N)C(=O)NC3CCN(Cc2ccccc2)CC3 -0.590

\*18323-44-9 O[C@@H]1[C@@H](O)[C@@H](O)[C@H](O[C@@H]1SC)C(NC(=O)[C@@H]2C[C@@H](CCC)CN2C)[C@H](C)Cl -1.486

+1159-93-9 CN(C)CCN2c3ccc(Cl)cc3Nc1ccccc1C2=O 0.299

\*25122-41-2 ClCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@@H]3C -1.301

+54063-32-0 ClCC(=O)[C@]2(O)[C@@]3(C)CC(=O)[C@]1(F)[C@]4(C)C=CC(=O)C=C4CC[C@H]1[C@@H]3C[C@@H]2C -1.712

+2030-63-9 Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5 0.648

+533-45-9 ClCCc1scnc1C -3.017

+1622-61-3 [O-][N+](=O)c1ccc2NC(=O)CN=C(c2c1)c3ccccc3Cl -2.000

+4205-90-7 Clc2cccc(Cl)c2NC1=NCCN1 -4.134

+2971-90-6 Oc1c(Cl)c(C)nc(C)c1Cl -1.000

+120-32-1 Oc2ccc(Cl)cc2Cc1ccccc1 -2.173

+33671-46-4 Clc3ccccc3C1=NCC(=O)N(C)c2sc(cc12)CC -1.262

+61-72-3 OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1ccccc1Cl)[C@H]4SC3(C)C -1.143

+5786-21-0 CN1CCN(CC1)C2=Nc4cc(Cl)ccc4Nc3ccccc23 -1.072

+76-57-3 COc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 -3.954

+477-27-0 CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(O)C(=O)C=C12 -3.778

-64-86-8 CC(=O)N[C@H]2CCc3cc(OC)c(OC)c(OC)c3C1=CC=C(OC)C(=O)C=C12 -4.653

+458-35-5 Oc1ccc(cc1OC)/C=C\CO -4.217

+50-22-6 OCC(=O)[C@H]4CC[C@@H]2[C@]4(C)C[C@H](O)[C@@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 -2.299

+486-56-6 CN2C(=O)CC[C@H]2c1cnccc1 -6.000

\*56-72-4 CCOP(=S)(OCC)Oc1ccc2c(c1)OC(=O)C(Cl)=C2C -0.176

+91-64-5 O=C1C=Cc2ccccc2O1 -3.279

+4366-18-1 OC=1c4ccccc4OC(=O)C=1C(COC)C2=C(O)c3ccccc3OC2=O -2.428

+60-27-5 N=C1NC(=O)CN1C -4.904

+21725-46-2 Clc1nc(NCC)nc(NC(C)(C)C#N)n1 -2.230

+460-19-5 N#CC#N -5.179

+82-92-8 CN1CCN(CC1)C(c2ccccc2)c3ccccc3 -3.000

#52-31-3 O=C1NC(=O)NC(=O)C1(CC)C2=CCCCC2 -3.204

+108-93-0 OC1CCCCC1 -4.623

+108-94-1 O=C1CCCCC1 -4.398

\*110-83-8 C1C=CCCC1 -2.328

+120-92-3 O=C1CCCC1 -3.963

+75-19-4 C1CC1 -2.581

+2259-96-3 NS(=O)(=O)c4cc1c(N[C@H](NS1(=O)=O)[C@@H]3C[C@H]2C=C[C@H]3C2)cc4Cl -0.400

+52-90-4 O=C(O)[C@@H](N)CS -5.442

+485-35-8 O=C3C=CC=C2N3C[C@H]1C[C@H]2CNC1 -5.642

+71-30-7 NC=1C=CNC(=O)N=1 -3.903

+75-99-0 CC(Cl)(Cl)C(=O)O -5.701

\*50-29-3 Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl 2.260

+1131-64-2 N=C(N)N1Cc2ccccc2CC1 -4.124

+477-30-5 COc2c3C1=CC=C(OC)C(=O)C=C1[C@@H](CCc3cc(OC)c2OC)NC -3.500

#83-44-3 O=C(O)CC[C@@H](C)[C@H]2CC[C@H]1[C@@H]3CC[C@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@@]12C -1.639

\*64-85-7 OCC(=O)[C@H]3CC[C@H]2[C@@H]4CCC1=CC(=O)CC[C@]1(C)[C@H]4CC[C@]23C -1.775

+50-47-5 CNCCCN2c3ccccc3CCc1ccccc12 -1.768

+382-67-2 OCC(=O)[C@@H]3[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C -1.624

+50-02-2 OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C -1.949

+475-26-3 Fc1ccc(cc1)C(c2ccc(F)cc2)C(Cl)(Cl)Cl 1.081

+124-02-7 C=CCNCC=C -4.934

+333-41-5 Cc1cc(OP(=S)(OCC)OCC)nc(n1)C(C)C -1.602

+57998-68-2 O=C(OCC)NC=1C(=O)C(=C(NC(=O)OCC)C(=O)C=1N2CC2)N3CC3 -3.420

+364-98-7 Clc1ccc2N=C(C)NS(=O)(=O)c2c1 -3.455

+103-49-1 C(NCc1ccccc1)c2ccccc2 -2.893

+1918-00-9 COc1c(c(Cl)ccc1Cl)C(=O)O -3.920

\*2463-84-5 Clc1cc(ccc1OP(=S)(OC)OC)[N+]([O-])=O -1.167

+97-17-6 Clc1cc(Cl)ccc1OP(=S)(OCC)OCC 0.611

+75-71-8 ClC(Cl)(F)F -2.447

+133-53-9 Cc1cc(O)c(Cl)c(C)c1Cl -2.301

\*2164-09-2 Clc1ccc(NC(=O)C(=C)C)cc1Cl -0.929

+66-76-2 OC=3c4ccccc4OC(=O)C=3CC1=C(O)c2ccccc2OC1=O -2.107

+84-17-3 Oc1ccc(cc1)C(=C\C)\C(=C\C)c2ccc(O)cc2 -0.477

+111-42-2 OCCNCCO -6.000

+60-91-3 CCN(CC)CCN1c3ccccc3Sc2ccccc12 1.276

\*109-89-7 CCNCC -6.000

+56-53-1 Oc1ccc(cc1)C(\CC)=C(\CC)c2ccc(O)cc2 -1.079

+35367-38-5 Clc2ccc(NC(=O)NC(=O)c1c(F)cccc1F)cc2 1.097

+22494-42-4 OC(=O)c1cc(ccc1O)c2ccc(F)cc2F -1.161

+579-38-4 CN(c1ccc(O)cc1)C(=O)C(Cl)Cl -2.941

+42399-41-7 CN(C)CCN2c3ccccc3S[C@@H](c1ccc(OC)cc1)[C@@H](OC(C)=O)C2=O -2.667

#59-52-9 OC[C@H](S)CS -4.940

+5221-53-4 Cc1nc(nc(O)c1CCCC)N(C)C -3.079

\*60-51-5 COP(=S)(OC)SCC(=O)NC -4.398

+131-11-3 COC(=O)c1ccccc1C(=O)OC -3.602

\*124-40-3 CNC -6.212

+551-92-8 O=[N+]([O-])c1cnc(C)n1C -4.262

#148-01-6 Cc1c(cc(cc1[N+](=O)[O-])[N+]([O-])=O)C(N)=O -3.000

#88-85-7 O=[N+]([O-])c1cc(cc(c1O)[C@H](C)CC)[N+]([O-])=O -1.716

+520-27-4 COc1ccc(cc1O)C2=CC(=O)c3c(O)cc(cc3O2)O[C@@H]5O[C@H](CO[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O)[C@@H](O)[C@H](O)[C@H]5O -2.611

+537-12-2 Cl.O=C(Nc1ccccc1)OC[C@H](OC(=O)Nc2ccccc2)CN3CCCCC3 -4.000

+82-66-6 O=C2c1ccccc1C(=O)C2C(=O)C(c3ccccc3)c4ccccc4 0.523

+58-73-1 CN(C)CCOC(c1ccccc1)c2ccccc2 -3.486

+915-30-0 O=C(OCC)C3(CCN(CCC(C#N)(c1ccccc1)c2ccccc2)CC3)c4ccccc4 -2.903

+117-34-0 OC(=O)C(c1ccccc1)c2ccccc2 -2.104

+122-39-4 c1ccccc1Nc2ccccc2 -1.724

+101-81-5 c1ccccc1Cc2ccccc2 -1.149

+4147-51-7 CCSc1nc(nc(NC(C)C)n1)NC(C)C -1.204

+3737-09-5 CC(C)N(CC[C@](c1ccccn1)(c2ccccc2)C(N)=O)C(C)C -1.652

\*330-54-1 Clc1ccc(NC(=O)N(C)C)cc1Cl -1.623

+502-55-6 CCOC(=S)SSC(=S)OCC -0.441

+57808-66-9 Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4 0.006

+51-61-6 Oc1ccc(CCN)cc1O -6.000

+1668-19-5 CN(C)CC\C=C1/c3ccccc3OCc2ccccc12 -1.500

+564-25-0 NC(=O)C=4C(=O)[C@@]3(O)C(O)=C2C(=O)c1c(O)cccc1[C@H](C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C -2.799

+58-19-5 O=C3C[C@H]4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)C[C@H]3C -1.164

+548-73-2 Fc1ccc(cc1)C(=O)CCCN2CC=C(CC2)N3c4ccccc4NC3=O -0.624

+527-17-3 CC=1C(=O)C(C)=C(C)C(=O)C=1C -2.646

\*479-18-5 OC[C@@H](O)Cn2cnc1c2C(=O)N(C)C(=O)N1C -5.522

+483-18-1 COc4cc5CCN[C@H](C[C@H]1C[C@H]2c3cc(OC)c(OC)cc3CCN2C[C@@H]1CC)c5cc4OC -2.993

+75847-73-3 OC(=O)[C@@H]2CCCN2C(=O)[C@H](C)N[C@H](CCc1ccccc1)C(=O)OCC -4.215

+72-20-8 ClC1=C(Cl)[C@]2(Cl)C(Cl)(Cl)[C@]1(Cl)[C@@H]3[C@@H]2[C@H]4C[C@@H]3[C@H]5O[C@H]45 0.602

+74011-58-8 O=C(O)C2=CN(CC)c1nc(c(F)cc1C2=O)N3CCNCC3 -4.535

+72301-79-2 CC(C)S(=O)(=O)n1c2cc(ccc2nc1N)\C(=N\O)c3ccccc3 -1.093

+86880-51-5 Oc1ccc(cc1)CC(=O)NCCNC[C@H](O)COc2ccccc2C#N -3.204

\*299-42-3 O[C@H](c1ccccc1)[C@H](C)NC -4.803

+481-29-8 O=C4CC[C@@H]3[C@]4(C)CC[C@H]1[C@H]3CC[C@H]2C[C@@H](O)CC[C@]12C -1.305

+2363-58-8 O[C@H]2CC[C@H]1[C@@H]3CC[C@H]4C[C@@H]5S[C@@H]5C[C@]4(C)[C@H]3CC[C@@]12C -0.079

+474-86-2 Oc3cc4CC=C1[C@H](CC[C@@]2(C)C(=O)CC[C@H]12)c4cc3 -0.149

+149-32-6 OC[C@H](O)[C@H](O)CO -5.785

+50-28-2 Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@H]1O)c4cc3 -0.556

+50-27-1 Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2C[C@@H](O)[C@@H]1O)c4cc3 -2.644

+53-16-7 Oc3cc4CC[C@@H]1[C@H](CC[C@]2(C)C(=O)CC[C@@H]12)c4cc3 -1.477

#55283-68-6 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CC(=C)C)CC)C(F)(F)F 0.523

+75-08-1 CCS -4.193

+141-43-5 NCCO -6.000

+563-12-2 S=P(SCSP(=S)(OCC)OCC)(OCC)OCC -0.301

#23947-60-6 CCNC1=NC(=O)C(CCCC)=C(C)N1 -2.176

+434-03-7 O=C4CC[C@@]3(C)C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)=C4 0.163

+26225-79-6 CS(=O)(=O)Oc1cc2c(cc1)O[C@H](OCC)C2(C)C -1.699

+77-67-8 C[C@@]1(CC)CC(=O)NC1=O -4.593

-86-35-1 O=C2N[C@H](c1ccccc1)C(=O)N2CC -3.723

+93-89-0 O=C(OCC)c1ccccc1 -2.857

+101-97-3 O=C(OCC)Cc1ccccc1 -2.869

#118-61-6 Oc1ccccc1C(=O)OCC -2.867

+75-04-7 CCN -6.000

\*100-41-4 CCc1ccccc1 -2.228

+107-15-3 NCCN -6.000

+76-58-4 CCOc5ccc1C[C@H]2N(C)CC[C@]34c1c5O[C@@H]4[C@@H](O)C=C[C@@H]23 -3.417

\*30544-47-9 FC(F)(F)c1cc(ccc1)Nc2ccccc2C(=O)OCCOCCO -0.204

#33125-97-2 CC(c1ccccc1)n2cncc2C(=O)OCC -1.801

+38260-54-7 CCc1nc(OCC)cc(OP(=S)(OC)OC)n1 -1.602

+2235-90-7 CC[C@@H](N)Cc2cnc1ccccc12 -2.708

+470-82-6 CC2(C)OC1(C)CCC2CC1 -3.544

\*97-53-0 Oc1ccc(cc1OC)CC=C -3.391

+76824-35-6 N/C(N)=N/c1nc(CSCCC(\N)=N/S(N)(=O)=O)cs1 -3.000

+52-85-7 O=S(=O)(N(C)C)c1ccc(OP(=S)(OC)OC)cc1 -2.037

+22224-92-6 Cc1cc(ccc1SC)OP(=O)(NC(C)C)OCC -2.517

+61019-78-1 N#C[C@@](CCCC)(Cn1ccnc1)c2ccccc2 -1.580

+60168-88-9 O[C@@](c1ccccc1Cl)(c2cncnc2)c3ccc(Cl)cc3 -1.146

+36330-85-5 O=C(CCC(=O)O)c1ccc(cc1)c2ccccc2 -0.344

\*458-24-2 FC(F)(F)c1cccc(C[C@H](C)NCC)c1 -2.615

+67227-56-9 Oc1ccc(cc1)[C@H]3CNCCc2c3cc(O)c(O)c2Cl -3.602

+437-38-7 CCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3 -2.301

#55-38-9 Cc1cc(ccc1SC)OP(=S)(OC)OC -0.875

+18046-21-4 O=C(O)Cc1sc(nc1c2ccc(Cl)cc2)c3ccccc3 -0.554

+51630-58-1 Clc1ccc(cc1)C(C(C)C)C(=O)OC(C#N)c3cccc(Oc2ccccc2)c3 1.620

+525-82-6 O=C2C=C(Oc1ccccc12)c3ccccc3 -1.484

+15301-69-6 O=C(OCCN1CCCCC1)c4cccc2c4OC(=C(C)C2=O)c3ccccc3 -1.000

+54143-55-4 FC(F)(F)COc2cc(C(=O)NC[C@@H]1CCCCN1)c(OCC(F)(F)F)cc2 -0.170

+79660-72-3 CN1CCN(CC1)c2c(F)c3c(cc2F)C(=O)C(=CN3CCF)C(=O)O -3.865

+5250-39-5 OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1c(F)cccc1Cl)[C@H]4SC3(C)C -0.945

\*33245-39-5 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCCl)CCC)C(F)(F)F 0.046

+21679-14-1 Nc3nc(F)nc1c3ncn1[C@H]2O[C@H](CO)[C@@H](O)[C@@H]2O -3.548

+78755-81-4 O=C(OCC)c3ncn2c3CN(C)C(=O)c1cc(F)ccc12 -2.107

+52468-60-7 Fc1ccc(cc1)C(c2ccc(F)cc2)N3CCN(CC3)C/C=C/c4ccccc4 0.470

+462-06-6 Fc1ccccc1 -3.188

\*426-13-1 CC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3C[C@H](C)C1=CC(=O)C=C[C@@]12C -1.477

+54910-89-3 FC(F)(F)c2ccc(O[C@@H](CCNC)c1ccccc1)cc2 -1.780

+76-43-7 C[C@]4(O)CC[C@@H]2[C@]4(C)C[C@H](O)[C@]1(F)[C@@]3(C)CCC(=O)C=C3CC[C@H]12 -1.829

\*2709-56-0 FC(F)(F)c2cc3C(=C\CCN1CCN(CCO)CC1)/c4ccccc4Sc3cc2 0.461

+69-23-8 FC(F)(F)c2cc3N(CCCN1CCN(CCO)CC1)c4ccccc4Sc3cc2 -1.493

+5104-49-4 Fc2cc(ccc2c1ccccc1)[C@H](C)C(=O)O -0.903

+1841-19-6 Fc1ccc(cc1)C(CCCN2CCC4(CC2)C(=O)NCN4c3ccccc3)c5ccc(F)cc5 -1.000

+69409-94-5 Clc3cc(ccc3NC(C(=O)OC(C#N)c2cccc(Oc1ccccc1)c2)C(C)C)C(F)(F)F 2.301

+21548-32-3 CCOP(=O)(/N=C1\SCS1)OCC -4.699

+110-00-9 c1ccco1 -4.000

+67-45-8 [O-][N+](=O)c2oc(/C=N/N1CCOC1=O)cc2 -1.602

\*98-01-1 O=Cc1ccco1 -4.886

+54-31-9 NS(=O)(=O)c2cc(c(NCc1ccco1)cc2Cl)C(=O)O -1.864

\*60142-96-3 NCC1(CC(=O)O)CCCCC1 -3.652

-106-24-1 C\C(C)=C\CCC(/C)=C\CO -2.000

+545-26-6 O[C@H]5CC[C@@]3(C)[C@H](CC[C@@H]2[C@@]4(O)C[C@H](O)[C@H](C1=CC(=O)OC1)[C@]4(C)CC[C@@H]23)C5 -2.179

+3820-67-5 OC[C@@H](O)COC(=O)c3ccccc3Nc1ccnc2cc(Cl)ccc12 -4.602

+29094-61-9 Cc1cnc(cn1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3 -1.571

+50-99-7 O[C@H]([C@@H](O)C=O)[C@H](O)[C@H](O)CO -6.079

+77-21-4 CC[C@@]1(CCC(=O)NC1=O)c2ccccc2 -3.000

+10238-21-8 O=C(NC1CCCCC1)NS(=O)(=O)c3ccc(CCNC(=O)c2cc(Cl)ccc2OC)cc3 -0.602

+56-81-5 OCC(O)CO -6.000

#56-40-6 NCC(=O)O -5.396

+126-07-8 O=C2c3c(O[C@@]21C(=CC(=O)C[C@H]1C)OC)c(Cl)c(OC)cc3OC -0.937

+90-05-1 Oc1ccccc1OC -4.272

#93-14-1 OCC(O)COc1ccccc1OC -4.699

+113-00-8 N=C(N)N -3.265

+73-40-5 NC2=Nc1ncnc1C(=O)N2 -3.318

+118-00-3 NC3=Nc1c(ncn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N3 -2.845

+23092-17-3 FC(F)(F)CN2c1ccc(Cl)cc1C(=NCC2=O)c3ccccc3 -0.382

+52-86-8 Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3 -1.146

+442-51-3 COc1ccc3c(c1)nc2c3ccnc2C -0.428

#509-86-4 O=C1NC(=O)NC(=O)C1(CC)C2=CCCCCC2 -2.398

\*76-44-8 ClC2=C(Cl)[C@]3(Cl)[C@@H]1C=C[C@H](Cl)[C@@H]1[C@@]2(Cl)C3(Cl)Cl 0.745

+23560-59-0 ClC1=C(OP(=O)(OC)OC)C2CC=CC12 -3.398

\*118-74-1 Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl 2.208

\*67-72-1 ClC(Cl)(Cl)C(Cl)(Cl)Cl -1.699

+70-30-4 Clc2c(Cc1c(O)c(Cl)cc(Cl)c1Cl)c(O)c(Cl)cc2Cl -2.146

+51235-04-2 CN(C)C2=NC(=O)N(C1CCCCC1)C(=O)N2C -4.519

+84-16-2 Oc1ccc(cc1)[C@@H](CC)[C@@H](CC)c2ccc(O)cc2 -1.079

+56-29-1 C[C@@]1(C(=O)N=C(O)N(C)C1=O)C2=CCCCC2 -2.638

#495-69-2 O=C(NCC(=O)O)c1ccccc1 -3.574

+51-45-6 NCCc1cncn1 -6.000

+71-00-1 N[C@@H](Cc1cncn1)C(=O)O -4.659

+87-00-3 CN3[C@@H]1CC[C@@H]3C[C@H](C1)OC(=O)C(O)c2ccccc2 -4.000

\*461-72-3 O=C1NC(=O)CN1 -4.599

+86-54-4 N\N=C1/NN=Cc2ccccc12 -3.980

+118-08-1 CN2CCc1cc5OCOc5cc1[C@@H]2[C@H]4OC(=O)c3c(OC)c(ccc34)OC -1.477

+58-93-5 NS(=O)(=O)c2cc1c(NCNS1(=O)=O)cc2Cl -2.859

+50-23-7 OCC(=O)[C@@]4(O)CC[C@@H]2[C@]4(C)C[C@H](O)[C@@H]1[C@@]3(C)CCC(=O)C=C3CC[C@H]12 -2.505

+123-31-9 Oc1ccc(O)cc1 -4.857

\*50-19-1 O[C@](COC(N)=O)(CC)c1ccccc1 -4.398

#127-07-1 NC(=O)NO -6.000

+68-94-0 O=C2NC=Nc1ncnc12 -2.845

\*53648-05-8 C[C@@H](C(=O)NO)c1ccc(CC(C)C)cc1 -2.301

+288-32-4 c1cncn1 -5.201

\*496-11-7 c1cccc2CCCc12 -2.037

+74517-78-5 NC(=O)C3(CCCNC(C)C)c1ccccc1c2ccccc23 -0.274

+95-13-6 c1cccc2CC=Cc12 -2.521

#482-89-3 O=C3c4ccccc4N\C3=C2/Nc1ccccc1C2=O -1.127

+120-72-9 c1cccc2nccc12 -3.551

+53-86-1 Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC 0.028

+87-89-8 O[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O)[C@H]1O -5.155

+440-58-4 O=C(C)Nc1c(I)c(c(I)c(CNC(C)=O)c1I)C(=O)O -3.477

+606-17-7 O=C(Nc1c(I)c(c(I)cc1I)C(=O)O)CCCCC(=O)Nc2c(I)c(C(=O)O)c(I)cc2I -2.663

+18181-70-9 Clc1cc(I)c(Cl)cc1OP(=S)(OC)OC 1.000

+66108-95-0 OC[C@@H](O)CNC(=O)c1c(I)c(N(C[C@H](O)CO)C(C)=O)c(I)c(c1I)C(=O)NC[C@H](O)CO -2.029

+60166-93-0 O=C(Nc1c(I)c(c(I)c(c1I)C(=O)NC(CO)CO)C(=O)NC(CO)CO)[C@H](C)O -5.146

+73334-07-3 O=C(Nc1c(I)c(c(I)c(c1I)C(=O)N(C)C[C@H](O)CO)C(=O)NC[C@H](O)CO)COC -1.377

+36734-19-7 O=C2CN(C(=O)NC(C)C)C(=O)N2c1cc(Cl)cc(Cl)c1 -1.143

\*54-92-2 O=C(NNC(C)C)c1ccncc1 -4.428

\*91-56-5 O=C1c2ccccc2NC1=O -4.185

+124-76-5 C[C@@]21CC[C@@H](C[C@H]1O)C2(C)C -3.076

+538-93-2 CC(C)Cc1ccccc1 -1.004

+59-63-2 Cc1cc(no1)C(=O)NNCc2ccccc2 -3.204

+97-54-1 Oc1ccc(cc1OC)\C=C\C -2.551

+25311-71-1 S=P(Oc1ccccc1C(=O)OC(C)C)(NC(C)C)OCC -1.344

+338-95-4 OCC(=O)[C@@]4(O)CC[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3CCC1=CC(=O)C=C[C@@]12C -2.330

+26675-46-7 FC(F)(F)[C@H](Cl)OC(F)F -3.650

+54-85-3 O=C(NN)c1ccncc1 -5.146

+55-22-1 O=C(O)c1ccncc1 -3.716

+498-94-2 O=C(O)C1CCNCC1 -5.501

\*78-59-1 O=C1C=C(C)CC(C)(C)C1 -4.079

+121-91-5 OC(=O)c1cccc(c1)C(=O)O -2.114

+33820-53-0 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)C(C)C 0.959

#119-65-3 c1cccc2ccncc12 -3.655

+59-01-8 O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CN)O[C@@H]3O[C@H]2[C@H](O)[C@@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](N)[C@H]1O)[C@H](N)C[C@@H]2N -6.000

\*853-34-9 CC(=O)CCC2C(=O)N(c1ccccc1)N(C2=O)c3ccccc3 -2.241

\*27762-78-3 OC(O)C(=O)[C@H](C)OCC -5.000

+22071-15-4 C[C@H](C(=O)O)c1cccc(c1)C(=O)c2ccccc2 -1.708

+82-02-0 COc3c1c(OC(C)=CC1=O)c(OC)c2occc23 -3.017

+501-30-4 O=C1C=C(CO)OC=C1O -5.971

+36894-69-6 O=C(N)c1cc(ccc1O)[C@@H](O)CN[C@@H](C)CCc2ccccc2 -2.068

+103890-78-4 CC=1NC(C)=C(C(C=1C(=O)OCC)c2ccccc2/C=C/C(=O)OC(C)(C)C)C(=O)OCC 0.295

+4618-18-2 O[C@H]2[C@H](O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O)[C@@H](CO)O[C@]2(O)CO -5.883

+61-90-5 CC(C)C[C@H](N)C(=O)O -4.332

+14769-73-4 N1=C3SCCN3C[C@@H]1c2ccccc2 -3.049

+47141-42-4 CC(C)(C)NC[C@H](O)COc2cccc1c2CCCC1=O -3.097

+137-58-6 O=C(Nc1c(C)cccc1C)CN(CC)CC -3.613

+154-21-2 O[C@@H]1[C@@H](O)[C@@H](O)[C@@H](O[C@@H]1SC)[C@@H](NC(=O)[C@@H]2C[C@@H](CCC)CN2C)[C@@H](C)O -2.967

\*330-55-2 Clc1ccc(NC(=O)N(C)OC)cc1Cl -1.875

+90-69-7 CN2[C@H](CCC[C@H]2C[C@@H](O)c1ccccc1)CC(=O)c3ccccc3 -1.685

#98079-51-7 O=C(O)C2=CN(CC)c1c(F)c(c(F)cc1C2=O)N3C[C@H](C)NCC3 -4.435

+13010-47-4 O=C(NC1CCCCC1)N(CCCl)N=O -2.045

+91431-42-4 CC(=O)Oc2c1cc(Cl)ccc1c(OC(C)=O)c(OC)c2OC -1.076

+846-49-1 Clc3ccccc3C2=NC(O)C(=O)Nc1ccc(Cl)cc12 -1.903

+59729-31-6 CC(C)N1CCC(CC1)N(c2ccc(Cl)cc2)C(=O)Cc3ccccc3 0.476

+75330-75-5 C[C@@H](CC)C(=O)O[C@H]3C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@H]23 -0.330

+1977-10-2 CN1CCN(CC1)C3=Nc4ccccc4Oc2ccc(Cl)cc23 -0.752

+73-22-3 O=C(O)[C@@H](N)Cc2cnc1ccccc12 -4.127

+487-21-8 Oc2nc(O)nc1nccnc12 -3.097

+59937-28-9 CC(C)OC(=O)C(/C(=O)OC(C)C)=C1/SC=CS1 -0.954

+69-79-4 O[C@H]2[C@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)[C@@H](CO)O[C@@H](O)[C@@H]2O -5.892

+591-27-5 Nc1cccc(O)c1 -4.431

+31431-39-7 O=C(OC)Nc1nc2cc(ccc2n1)C(=O)c3ccccc3 -1.853

+78266-06-5 Cc1cc(C)c(Br)c(C)c1NC(=O)CN(CC(=O)O)CC(=O)O -0.090

+137-05-3 N#CC(=C)C(=O)OC -3.977

+2898-12-6 Clc1ccc2c(c1)C(=NCCN2C)c3ccccc3 -0.491

+977-79-7 CC(=O)[C@@]3(C)CC[C@H]2[C@@H]4C=C(C)C1=CC(=O)CC[C@]1(C)[C@H]4CC[C@@]23C -0.260

-7195-27-9 C[C@@]2(CN(C)S(=O)(=O)c1ccc(Cl)c(c1)S(N)(=O)=O)CCCO2 -1.225

+517-60-2 OC(=O)c1c(c(c(c(c1C(=O)O)C(=O)O)C(=O)O)C(=O)O)C(=O)O -2.559

+71125-38-7 Cc3cnc(NC(=O)C2=C(O)c1ccccc1S(=O)(=O)N2C)s3 -0.854

\*58-27-5 O=C2C=C(C)C(=O)c1ccccc12 -2.204

#1490-04-6 CC(C)[C@H]1CC[C@H](C)C[C@H]1O -2.623

+60-89-9 CN1CCCC(C1)CN2c4ccccc4Sc3ccccc23 -0.747

#57-42-1 CN1CCC(CC1)(C(=O)OCC)c2ccccc2 -3.508

\*57-53-4 O=C(N)OCC(C)(COC(=O)N)CCC -3.672

+54-04-6 COc1c(cc(cc1OC)CCN)OC -4.925

\*57837-19-1 C[C@@H](N(C(=O)COC)c1c(C)cccc1C)C(=O)OC -3.924

+5001-33-2 Oc1ccc(cc1OC)[C@H](O)CNC -6.000

+914-00-1 NC(=O)C=4C(=O)[C@@]3(O)C(O)=C2C(=O)c1c(O)cccc1C(=C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C -3.878

#67-56-1 CO -6.000

+91-80-5 CN(C)CCN(Cc1cccs1)c2ccccn2 -2.779

+72-44-6 Cc1ccccc1N3C(C)=Nc2ccccc2C3=O -0.675

+554-57-4 CN1N=C(S/C1=N/C(C)=O)S(=O)(N)=O -3.544

+100-97-0 C1N3CN2CN(CN1C2)C3 -5.652

+950-37-8 O=C1SC(=NN1CSP(=S)(OC)OC)OC -2.272

\*63-68-3 O=C(O)[C@@H](N)CCSC -4.753

#16752-77-5 C\C(=N\OC(=O)NC)SC -4.763

+59-05-2 O=C(O)[C@H](CCC(=O)O)NC(=O)c1ccc(cc1)N(C)Cc2nc3c(nc2)nc(N)nc3N -3.415

-298-81-7 COc1c3occc3cc2C=CC(=O)Oc12 -1.678

+76-38-0 ClC(Cl)C(F)(F)OC -4.452

+77-41-8 C[C@@]1(CC(=O)N(C)C1=O)c2ccccc2 -3.715

\*134-20-3 Nc1ccccc1C(=O)OC -3.455

+93-58-3 COC(=O)c1ccccc1 -3.322

#93-60-7 COC(=O)c1cccnc1 -4.678

+502-02-3 OS(=O)(=O)c2ccc(/N=N/c1ccc(cc1)N(C)C)cc2 -1.624

+493-52-7 CN(C)c2ccc(/N=N/c1ccccc1C(=O)O)cc2 -0.565

+74-89-5 CN -6.033

#60-34-4 CNN -6.000

+113-45-1 O=C(OC)[C@@H](c1ccccc1)[C@@H]2CCCCN2 -5.303

+364-62-5 Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC -2.301

+51218-45-2 ClCC(=O)N(c1c(C)cccc1CC)[C@H](C)COC -2.724

+17560-51-9 NS(=O)(=O)c2cc3C(=O)N(c1ccccc1C)[C@H](C)Nc3cc2Cl -1.780

+21087-64-9 O=C1C(=NN=C(SC)N1N)C(C)(C)C -3.021

+31112-62-6 O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]2NC(=O)c1c(I)c(NC(C)=O)c(I)c(N(C)C(C)=O)c1I -5.699

\*73573-88-3 C[C@@H](CC)C(=O)O[C@H]3CCC=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@@H]23 -0.681

+7786-34-7 O=P(OC)(OC)OC(/C)=C/C(=O)OC -5.778

\*3704-09-4 C[C@@H]4CC1=CC(=O)CC[C@@H]1[C@H]3CC[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@@H]34 -1.860

+25905-77-5 Cc2cc(nnc2NCCN1CCOCC1)c3ccccc3 -3.373

#10118-90-8 CN(C)c2ccc(O)c1C(=O)C3=C(O)[C@]4(O)C(=O)C(=C(O)[C@@H](N(C)C)[C@@H]4C[C@@H]3Cc12)C(N)=O -4.716

+2385-85-5 ClC53C1(Cl)C4(Cl)C2(Cl)C1(Cl)C(Cl)(Cl)C5(Cl)C2(Cl)C3(Cl)C4(Cl)Cl 1.071

+99-09-2 O=[N+]([O-])c1cccc(N)c1 -3.079

+554-84-7 O=[N+]([O-])c1cccc(O)c1 -4.130

#103-16-2 Oc2ccc(OCc1ccccc1)cc2 -2.400

+5741-22-0 CC(C)NC[C@H](O)COc1ccccc1OC -3.997

+480-16-0 Oc3ccc(C=2Oc1cc(O)cc(O)c1C(=O)C=2O)c(O)c3 -2.398

+57-27-2 Oc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 -2.173

+110-91-8 C1CNCCO1 -6.000

+54-32-0 CC(=O)Oc1cc(C(C)C)c(OCCN(C)C)cc1C -2.509

+108-45-2 Nc1cccc(N)c1 -5.377

#127-19-5 CN(C)C(C)=O -6.000

+42924-53-8 CC(=O)CCc1ccc2cc(ccc2c1)OC -1.862

+42200-33-9 CC(C)(C)NC[C@@H](O)COc2cccc1C[C@@H](O)[C@@H](O)Cc12 -3.921

#62-67-9 Oc5ccc1C[C@H]2N(CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23)CC=C -3.442

+465-65-6 O=C1CC[C@@]5(O)[C@H]2Cc4ccc(O)c3O[C@@H]1[C@]5(CCN2CC=C)c34 -3.152

+434-22-0 O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@H]1O)=C4 -2.509

\*835-31-4 c2cc(CC1=NCCN1)c3ccccc3c2 -1.072

+91-20-3 c1cccc2ccccc12 -1.491

\*15299-99-7 CCN(CC)C(=O)C(C)Oc2cccc1ccccc12 -1.863

+132-66-1 O=C(O)c1ccccc1C(=O)Nc3cccc2ccccc23 -2.301

+131-28-2 O=C(O)c1c(OC)c(OC)ccc1C(=O)Cc2c(cc3OCOc3c2OC)CCN(C)C -2.892

+463-82-1 CC(C)(C)C -1.521

+466-07-9 O=C1C=C(CO1)[C@@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CC[C@@H]2C[C@H](CC[C@@]23C)O[C@@H]4O[C@@H](C)[C@@H](O)[C@H](OC)[C@H]4O -0.838

#54-11-5 CN2CCC[C@H]2c1cnccc1 -6.000

#59-67-6 O=C(O)c1cccnc1 -4.255

+405-22-1 O=[N+]([O-])c1ccc(/C=N/N(CCO)C(N)=O)o1 -2.699

+555-84-0 O=[N+]([O-])c2ccc(/C=N/N1CCNC1=O)o2 -1.993

+6236-05-1 O=[N+]([O-])c1ccc(\C=N\O)o1 -3.000

+13411-16-0 O=[N+]([O-])c2ccc(/C=C/c1cccc(CO)n1)o2 -2.835

-2011-67-8 [O-][N+](=O)c1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3 -1.882

+66085-59-4 CC=1NC(C)=C(C(C=1C(=O)OC(C)C)c2cccc(c2)[N+]([O-])=O)C(=O)OCCOC -1.386

+63675-72-9 CC=1NC(C)=C(C(C=1C(=O)OCC(C)C)c2ccccc2[N+]([O-])=O)C(=O)OC -1.391

+98-95-3 [O-][N+](=O)c1ccccc1 -3.320

\*79-24-3 [O-][N+](=O)CC -4.672

+75-52-5 [O-][N+](C)=O -5.045

+579-10-2 CN(C(C)=O)c1ccccc1 -4.223

#62-75-9 CN(C)N=O -6.000

\*59-89-2 O=NN1CCOCC1 -6.000

+1088-11-5 Clc1ccc2NC(=O)CN=C(c2c1)c3ccccc3 -1.756

#68-22-4 O=C4CC[C@H]3C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)=C4 -0.848

+27314-13-2 FC(F)(F)c1cc(ccc1)N2N=CC(NC)=C(Cl)C2=O -1.528

\*6533-00-2 O=C4CC[C@H]3C(CC[C@@H]2[C@H]3CC[C@]1(CC)[C@H]2CC[C@@]1(O)C#C)=C4 -0.238

+466-97-7 Oc5ccc1C[C@H]2NCC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 -5.408

#941-69-5 O=C2C=CC(=O)N2c1ccccc1 -3.843

\*95-50-1 Clc1ccccc1Cl -2.193

#88-74-4 O=[N+]([O-])c1ccccc1N -3.167

+94-70-2 CCOc1ccccc1N -3.528

+90-43-7 Oc2ccccc2c1ccccc1 -2.845

#16773-42-5 Cc1ncc([N+]([O-])=O)n1C[C@H](O)CCl -3.636

+70-26-8 NCCC[C@H](N)C(=O)O -6.000

+119-93-7 Cc1cc(ccc1N)c2ccc(N)c(C)c2 -3.114

+529-20-4 Cc1ccccc1C=O -3.072

+529-19-1 N#Cc1ccccc1C -2.860

+508-52-1 O[C@@H]3C[C@@]4(O)CC[C@@H]2[C@@]5(O)CC[C@H](C1=CC(=O)OC1)[C@@]5(C)C[C@@H](O)[C@@H]2[C@@]4(CO)[C@H](O)C3 -3.262

+66-79-5 OC(=O)[C@@H]3N4C(=O)[C@@H](NC(=O)c2c(C)onc2c1ccccc1)[C@H]4SC3(C)C -1.444

+19666-30-9 O=C2OC(=NN2c1cc(OC(C)C)c(Cl)cc1Cl)C(C)(C)C 0.155

+21738-42-1 [O-][N+](=O)c1cc2N[C@H](CCc2cc1CO)CNC(C)C -2.914

+23135-22-0 O=C(C(=N\OC(=O)NC)\SC)N(C)C -5.447

\*126-93-2 O=C(N)[C@@]1(CC)O[C@H]1CCC -4.021

\*21256-18-8 OC(=O)CCc1nc(c(o1)c2ccccc2)c3ccccc3 -0.944

+604-75-1 Clc1ccc2NC(=O)[C@H](O)N=C(c2c1)c3ccccc3 -2.253

+131-57-7 O=C(c1ccc(cc1O)OC)c2ccccc2 -1.836

+76-41-5 O=C1CC[C@@]5(O)[C@H]2Cc4ccc(O)c3O[C@@H]1[C@]5(CCN2C)c34 -4.380

+129-20-4 Oc1ccc(cc1)N3C(=O)[C@@H](CCCC)C(=O)N3c2ccccc2 -1.778

+2439-01-2 Cc1ccc2nc3SC(=O)Sc3nc2c1 -0.000

+123-30-8 Nc1ccc(O)cc1 -4.204

+130-85-8 O=C(O)c4cc1ccccc1c(Cc2c3ccccc3cc(C(=O)O)c2O)c4O -5.037

+100-09-4 COc1ccc(cc1)C(=O)O -2.724

+123-63-7 CC1OC(C)OC(C)O1 -5.049

+70-70-2 O=C(CC)c1ccc(O)cc1 -2.538

+508-59-8 O=C2C=C[C@@]3(O)[C@@H](C)CC[C@H]1C(=C)C(=O)O[C@H]1[C@@]23C -4.158

+103-88-8 Brc1ccc(NC(C)=O)cc1 -2.613

\*99-91-2 O=C(C)c1ccc(Cl)cc1 -2.045

+106-37-6 Brc1ccc(Br)cc1 -1.301

+540-36-3 Fc1ccc(F)cc1 -3.086

+70458-92-3 CN1CCN(CC1)c2cc3N(CC)C=C(C(=O)O)C(=O)c3cc2F -4.057

+40487-42-1 [O-][N+](=O)c1c(C)c(C)cc([N+]([O-])=O)c1NC(CC)CC 0.523

+135-48-8 c1c3cc4cc5ccccc5cc4cc3cc2ccccc12 2.967

#87-86-5 Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl -1.146

+115-77-5 OCC(CO)(CO)CO -4.859

+109-66-0 CCCCC -1.580

+76-74-4 O=C1NC(=O)NC(=O)C1(CC)C(C)CCC -2.832

+84-97-9 CN1CCN(CC1)CCCN2c4ccccc4Sc3ccccc23 -0.336

+37924-13-3 O=S(=O)(c1ccccc1)c2cc(C)c(NS(=O)(=O)C(F)(F)F)cc2 -1.778

+52645-53-1 Cl/C(Cl)=C/[C@H]3[C@@H](C(=O)OCc2cccc(Oc1ccccc1)c2)C3(C)C 2.222

+58-39-9 OCCN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 -1.452

+1182-87-2 O=C1C=C(CO1)[C@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CC[C@@H]2C[C@@H](CC[C@@]23C=O)O[C@H]4O[C@@H](C)[C@@H](O)[C@H](OC)[C@H]4O -2.602

+371-40-4 Fc1ccc(N)cc1 -4.049

#85-01-8 c2cc3ccc1ccccc1c3cc2 -0.061

+84-11-7 O=C2c3ccccc3c1ccccc1C2=O -0.875

+92-82-0 n1c3ccccc3nc2ccccc12 -1.204

\*60-12-8 OCCc1ccccc1 -4.346

+103-73-1 CCOc1ccccc1 -2.755

#103-03-7 NC(=O)NNc1ccccc1 -3.453

+108-95-2 Oc1ccccc1 -4.918

+77-09-8 Oc1ccc(cc1)C3(OC(=O)c2ccccc23)c4ccc(O)cc4 -2.602

+143-74-8 Oc1ccc(cc1)C3(OS(=O)(=O)c2ccccc23)c4ccc(O)cc4 -2.886

+92-84-2 c1ccc2Sc3ccccc3Nc2c1 -0.201

+26002-80-2 C/C(C)=C/[C@@H]3[C@H](C(=O)OCc2cccc(Oc1ccccc1)c2)C3(C)C 2.013

+135-67-1 c1ccc2Oc3ccccc3Nc2c1 -0.328

#673-31-4 NC(=O)OCCCc1ccccc1 -3.072

#435-97-2 OC=1c3ccccc3OC(=O)C=1[C@H](CC)c2ccccc2 -1.111

\*86-34-0 O=C2N(C)C(=O)C[C@@H]2c1ccccc1 -3.846

#122-09-8 NC(C)(C)Cc1ccccc1 -4.270

#122-79-2 O=C(C)Oc1ccccc1 -3.667

+101-84-8 c1ccccc1Oc2ccccc2 -1.255

#139-66-2 c1ccccc1Sc2ccccc2 -0.910

+122-78-1 O=CCc1ccccc1 -3.481

+103-82-2 OC(=O)Cc1ccccc1 -4.220

\*63-91-2 N[C@@H](Cc1ccccc1)C(=O)O -4.430

#50-33-9 O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2 -1.677

+100-63-0 NNc1ccccc1 -5.104

\*64-10-8 O=C(N)Nc1ccccc1 -4.230

+509-67-1 CN5CC[C@@]32c6c4ccc(OCCN1CCOCC1)c6O[C@H]2[C@@H](O)C=C[C@H]3[C@H]5C4 -4.301

+2310-17-0 CCOP(=S)(OCC)SCN1c2ccc(Cl)cc2OC1=O -0.484

\*732-11-6 COP(=S)(OC)SCN2C(=O)c1ccccc1C2=O -1.387

+13171-21-6 O=P(OC)(OC)OC(\C)=C(/Cl)C(=O)N(CC)CC -6.000

#253-52-1 c1cccc2cnncc12 -4.699

+85-41-6 O=C1NC(=O)c2ccccc12 -2.556

#57-47-6 CNC(=O)Oc1cc2c(cc1)N(C)[C@H]3N(C)CC[C@]23C -3.890

#98-98-6 O=C(O)c1ccccn1 -5.982

+75-97-8 CC(C)(C)C(C)=O -4.279

+13523-86-9 CC(C)NCC(O)COc2cccc1nccc12 -3.897

+540-38-5 Ic1ccc(O)cc1 -2.631

+84-04-8 NC(=O)C1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 1.432

+1893-33-0 Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)(C(N)=O)N3CCCCC3 -1.912

#110-85-0 C1CNCCN1 -6.000

\*110-89-4 C1CCCCN1 -6.000

+94-62-2 O=C(/C=C/C=C/c1ccc2OCOc2c1)N3CCCCC3 -1.602

+120-57-0 O=Cc1ccc2OCOc2c1 -3.544

+2531-04-6 CN1CCC(CC1)N2NC(=C(CC)C2=O)c3ccccc3 -2.707

+54-91-1 O=C(CCBr)N1CCN(CC1)C(=O)CCBr -3.396

#7491-74-9 O=C1CCCN1CC(=O)N -4.919

+55837-27-9 O=C(O)c2cc(c(Oc1ccccc1)c(c2)N3CCCC3)S(N)(=O)=O -0.369

+302-41-0 N#CC(CCN1CCC(CC1)(C(N)=O)N2CCCCC2)(c3ccccc3)c4ccccc4 0.309

+72732-56-0 COc3cc(Cc1cnc2nc(N)nc(N)c2c1C)c(OC)cc3 -2.121

+36322-90-4 OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 -1.362

\*100-01-6 O=[N+]([O-])c1ccc(N)cc1 -2.862

+100-02-7 O=[N+]([O-])c1ccc(O)cc1 -4.064

+156-43-4 CCOc1ccc(N)cc1 -3.876

+106-50-3 Nc1ccc(N)cc1 -4.568

#92-69-3 Oc1ccc(cc1)c2ccccc2 -1.750

+55268-74-1 O=C1CN(C[C@@H]2c3ccccc3CCN12)C(=O)C4CCCCC4 -2.602

+53-03-2 OCC(=O)[C@@]3(O)CC[C@H]2[C@@H]4CCC1=CC(=O)C=C[C@]1(C)[C@H]4C(=O)C[C@@]23C -2.494

+145-13-1 CC(=O)[C@H]4CC[C@@H]3[C@]4(C)CC[C@H]2[C@H]3CC=C1C[C@@H](O)CC[C@@]12C -0.849

+511-45-5 OC(CCN1CCCCC1)(c2ccccc2)c3ccccc3 -1.519

#59-46-1 Nc1ccc(cc1)C(=O)OCCN(CC)CC -3.975

+671-16-9 CC(C)NC(=O)c1ccc(CNNC)cc1 -3.152

+67747-09-5 O=C(N(CCOc1c(Cl)cc(Cl)cc1Cl)CCC)n2ccnc2 -1.531

#58-38-8 CN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 -1.176

#32809-16-8 Clc1cc(cc(Cl)c1)N2C(=O)[C@]3(C)C[C@@]3(C)C2=O -0.653

+26399-36-0 CCCN(CC1CC1)c2c(cc(cc2[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O 1.000

+62666-20-0 Clc1ccc(cc1)/C(=N\CCCC(N)=O)c2cc(F)ccc2O -1.851

+57-83-0 CC(=O)[C@H]3CC[C@H]2[C@@H]4CCC1=CC(=O)CC[C@]1(C)[C@H]4CC[C@]23C -0.945

#147-85-3 O=C(O)[C@@H]1CCCN1 -5.210

+1918-16-7 CC(C)N(C(=O)CCl)c1ccccc1 -2.845

+551-27-9 OC(=O)[C@@H]2N3C(=O)[C@@H](NC(=O)C(CC)Oc1ccccc1)[C@H]3SC2(C)C -1.356

+362-29-8 CCC(=O)c1cc2N(CC(C)N(C)C)c3ccccc3Sc2cc1 0.343

+123-38-6 CCC=O -5.486

+79-05-0 CCC(N)=O -5.691

+107-12-0 CCC#N -5.013

+93-55-0 O=C(CC)c1ccccc1 -3.301

+2078-54-8 CC(C)c1cccc(C(C)C)c1O -2.093

+525-66-6 CC(C)NC[C@@H](O)COc2cccc1ccccc12 -1.790

+121-79-9 Oc1cc(cc(O)c1O)C(=O)OCCC -3.544

+107-10-8 CCCN -6.000

+115-07-1 C=CC -2.301

+466-06-8 O=C1C=CC(=CO1)[C@@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CCC2=C[C@H](CC[C@@]23C)O[C@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O -1.769

#438-60-8 CNCCCC2c3ccccc3C=Cc1ccccc12 -0.017

+2537-29-3 O=C1NC(=O)NC(=O)C1(C[C@@H](C)O)CC=C -4.547

+603-00-9 C[C@@H](O)Cn2cnc1c2C(=O)N(C)C(=O)N1C -6.000

+66-97-7 O=C1C=Cc2cc3ccoc3cc2O1 -3.286

+91-18-9 n1ccnc2ncncc12 -5.155

+53-79-2 COc1ccc(cc1)C[C@@H](N)C(=O)N[C@H]4[C@@H](CO)O[C@@H](n3cnc2c3ncnc2N(C)C)[C@@H]4O -1.702

#81-54-9 O=C2c1ccccc1C(=O)c3c2c(O)cc(O)c3O -0.806

+24691-76-7 CC=2OCCCC=2C(=O)Nc1ccccc1 -2.778

+290-37-9 c1cnccn1 -5.338

+13457-18-6 O=C(OCC)c1cn2nc(cc2nc1C)OP(=S)(OCC)OCC -0.623

+129-00-0 c1ccc2ccc3cccc4ccc1c2c34 0.870

+289-80-5 c1cccnn1 -6.000

+110-86-1 c1ccccn1 -6.000

+58-14-0 CCc1nc(N)nc(N)c1c2ccc(Cl)cc2 -2.083

\*123-75-1 C1CCCN1 -6.000

+36735-22-5 Fc3ccccc3C2=NCC(=S)N(CC(F)(F)F)c1ccc(Cl)cc12 -0.127

+91-63-4 Cc1ccc2ccccc2n1 -2.698

+73-49-4 NS(=O)(=O)c1cc2C(=O)N[C@@H](Nc2cc1Cl)CC -2.176

+130-95-0 COc1cc2c(cc1)nccc2[C@@H](O)[C@@H]4C[C@@H]3CCN4C[C@@H]3C=C -2.699

+81-64-1 O=C2c1ccccc1C(=O)c3c2c(O)ccc3O 1.017

#91-22-5 c1cccc2cccnc12 -3.786

+91-19-0 c1cccc2nccnc12 -5.820

#100-76-5 C1CN2CCC1CC2 -4.862

+58994-96-0 O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CNC(=O)N(CCCl)N=O)O[C@@H]1OC -3.954

+66357-35-5 [O-][N+](=O)\C=C(/NC)NCCSCc1ccc(CN(C)C)o1 -4.393

\*80125-14-0 CCN2CCC[C@H]2CNC(=O)c1c(OC)ccc(Br)c1OC -1.869

+81-88-9 [Cl-].O=C(O)c4ccccc4C=1c3ccc(cc3OC2=CC(\C=CC=12)=[N+](/CC)CC)N(CC)CC -4.079

+36791-04-5 NC(=O)c1ncn(n1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -4.676

\*84057-95-4 CCCN2CCCC[C@@H]2C(=O)Nc1c(C)cccc1C -1.760

+35834-26-5 CN(C)[C@H]3C[C@@H](C)O[C@@H](O[C@@H]1[C@@H](C)[C@H](O)CC(=O)O[C@H](CC)[C@@H](C)[C@@H]2O[C@@]2(C)C=CC(=O)[C@H](C)C[C@@H]1CC=O)[C@H]3O -1.464

+83-79-4 C=C(C)[C@@H]2Oc3ccc1C(=O)[C@H]4c5cc(OC)c(OC)cc5OC[C@H]4Oc1c3C2 0.699

\*81-07-2 O=C2NS(=O)(=O)c1ccccc12 -3.602

+94-59-7 C=CCc1ccc2OCOc2c1 -2.083

-138-52-3 OCc2ccccc2O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O -4.602

\*90-02-8 O=Cc1ccccc1O -4.230

+87-17-2 O=C(Nc1ccccc1)c2ccccc2O -1.740

+69-72-7 OC(=O)c1ccccc1O -3.350

+552-94-3 O=C(Oc1ccccc1C(=O)O)c2ccccc2O -2.041

\*107-97-1 CNCC(=O)O -5.477

#3366-95-8 Cc1ncc([N+]([O-])=O)n1CC(O)C -4.137

+50-67-9 Oc1cc2c(cc1)ncc2CCN -4.301

+138-59-0 O[C@@H]1CC(=C[C@@H](O)[C@H]1O)C(=O)O -5.176

\*93-72-1 Clc1cc(OC(C)C(=O)O)c(Cl)cc1Cl -1.851

\*79902-63-9 CC(C)(CC)C(=O)O[C@H]3C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@H]23 0.116

+532-32-1 [Na+].[O-]C(=O)c1ccccc1 -5.745

+3930-20-9 O=S(C)(=O)Nc1ccc(cc1)[C@H](O)CNC(C)C -3.741

+1404-64-4 CC=1NC(=O)NC(=O)C=1/C=C/C(=O)N[C@H](CO)CS(=O)CSC -3.873

\*90-39-1 C3CCCN4C[C@H]2C[C@H](CN1CCCC[C@@H]12)[C@H]34 -3.483

+52-01-7 CC(=O)S[C@@H]4CC1=CC(=O)CC[C@]1(C)[C@H]5CC[C@@]3(C)[C@@H](CC[C@]23CCC(=O)O2)[C@H]45 -1.342

+521-18-6 O=C3C[C@H]4CC[C@@H]2[C@H](CC[C@]1(C)[C@H]2CC[C@@H]1O)[C@@]4(C)CC3 -5.720

+18883-66-4 O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1NC(=O)N(C)N=O -3.705

+57-24-9 O=C2C[C@H]7OCC=C6CN4CC[C@@]53c1ccccc1N2[C@@H]3[C@H]7[C@H]6C[C@@H]45 -2.204

\*100-42-5 C=Cc1ccccc1 -2.491

+56030-54-7 CCC(=O)N(c1ccccc1)C2(COC)CCN(CC2)CCc3cccs3 -1.881

+41744-40-5 OC(=O)[C@@H]2N3C(=O)[C@H](NC(=O)[C@@H](c1ccccc1)S(=O)(=O)O)[C@H]3SC2(C)C -1.841

+17784-12-2 O=C1N=C(C=CN1CC)NS(=O)(=O)c2ccc(N)cc2 -3.243

+2447-57-6 O=S(=O)(Nc1ncnc(OC)c1OC)c2ccc(N)cc2 -3.431

+94-19-9 O=S(=O)(Nc1nnc(CC)s1)c2ccc(N)cc2 -3.512

+57-67-0 Nc1ccc(cc1)S(=O)(=O)/N=C(\N)N -3.342

+95-06-7 C=C(Cl)CSC(=S)N(CC)CC -2.000

#57-68-1 O=S(=O)(Nc1nc(C)cc(C)n1)c2ccc(N)cc2 -3.176

+723-46-6 Cc2cc(NS(=O)(=O)c1ccc(N)cc1)no2 -2.785

+80-35-3 O=S(=O)(Nc1ccc(OC)nn1)c2ccc(N)cc2 -2.167

#63-74-1 Nc1ccc(cc1)S(=O)(N)=O -3.875

+121-57-3 Nc1ccc(cc1)S(O)(=O)=O -4.033

+144-83-2 O=S(=O)(Nc1ccccn1)c2ccc(N)cc2 -2.428

+59-40-5 Nc1ccc(cc1)S(=O)(=O)Nc2cnc3ccccc3n2 -0.875

+72-14-0 O=S(=O)(Nc1nccs1)c2ccc(N)cc2 -2.572

+515-49-1 Nc1ccc(cc1)S(=O)(=O)NC(N)=S -4.041

+57-96-5 O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3 -1.494

+515-64-0 Cc2cc(NS(=O)(=O)c1ccc(N)cc1)nc(C)n2 -3.210

\*38194-50-2 CS(=O)c1ccc(cc1)/C=C3/c2ccc(F)cc2C(CC(=O)O)=C3C -3.477

+73384-60-8 CS(=O)c3ccc(c1nc2cccnc2n1)c(OC)c3 -3.155

+53583-79-2 CCN2CCC[C@@H]2CNC(=O)c1cc(ccc1OC)S(=O)(=O)CC -2.860

\*103628-46-2 CNS(=O)(=O)Cc1cc2c(cc1)ncc2CCN(C)C -4.330

+87-90-1 ClN1C(=O)N(Cl)C(=O)N(Cl)C1=O -4.079

+321-64-2 Nc1c3ccccc3nc2CCCCc12 -2.336

+4267-05-4 NS(=O)(=O)c2cc1c(N[C@@H](NS1(=O)=O)C(Cl)(Cl)Cl)cc2Cl -1.641

+124-72-1 FC(F)(F)[C@H](Br)F -3.356

#5902-51-2 O=C1NC(C)=C(Cl)C(=O)N1C(C)(C)C -2.851

+23031-25-6 Oc1cc(cc(O)c1)[C@@H](O)CNC(C)(C)C -5.328

+58-22-0 O=C4CC[C@@]3(C)C(CC[C@@H]2[C@@H]3CC[C@@]1(C)[C@H]2CC[C@@H]1O)=C4 -1.369

+60-54-8 NC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@]2(O)C1=O)C(=O)c3c(O)cccc3[C@@]4(C)O -2.364

+116-29-0 Clc1cc(c(Cl)cc1Cl)S(=O)(=O)c2ccc(Cl)cc2 1.108

+109-99-9 C1CCCO1 -6.000

\*142-68-7 C1CCCCO1 -4.904

\*632-22-4 CN(C)C(=O)N(C)C -6.000

+10379-14-3 Clc1ccc2c(c1)C(=NCC(=O)N2C)C3=CCCCC3 -1.422

#50-35-1 O=C1NC(=O)CCC1N3C(=O)c2ccccc2C3=O -2.736

+115-37-7 COC1=CC=C3[C@H]2Cc4ccc(OC)c5O[C@@H]1[C@]3(CCN2C)c45 -2.833

+467-98-1 O=C3C=CC4[C@H]2Cc1ccc(OC)c(O)c1[C@@]4(CCN2C)C3 -3.602

+91-79-2 CN(C)CCN(Cc1ccsc1)c2ccccn2 -3.647

#83-67-0 Cn1cnc2c1C(=O)NC(=O)N2C -2.519

+58-55-9 O=C2c1ncnc1N(C)C(=O)N2C -3.867

+148-79-8 n1c3ccccc3nc1c2cscn2 -1.699

+77-27-0 O=C1NC(=S)NC(=O)C1(CC=C)[C@H](C)CCC -1.694

+288-47-1 c1cncs1 -4.731

\*473-30-3 O=S(=O)(c1cnc(N)s1)c2ccc(N)cc2 -2.602

+59669-26-0 CN(SN(C)C(=O)O\N=C(\C)SC)C(=O)O\N=C(\C)SC -1.544

+154-42-7 NC2=Nc1ncnc1C(=S)N2 -4.560

+110-02-1 c1cccs1 -3.479

+108-98-5 Sc1ccccc1 -2.922

+84-06-0 CC(=O)OCCN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 -0.950

+50-52-2 CN4CCCCC4CCN1c3ccccc3Sc2ccc(SC)cc12 1.469

+5591-45-7 CN(C)S(=O)(=O)c2cc3C(=C\CCN1CCN(C)CC1)\c4ccccc4Sc3cc2 0.119

+62-56-6 NC(N)=S -5.152

+492-22-8 O=C1c3ccccc3Sc2ccccc12 -0.061

+137-26-8 CN(C)C(=S)SSC(=S)N(C)C -1.477

+72-19-5 O=C(O)[C@@H](N)[C@@H](C)O -4.987

+50-89-5 CC1=CN(C(=O)NC1=O)[C@H]2C[C@H](O)[C@@H](CO)O2 -3.901

\*65-71-4 CC1=CNC(=O)NC1=O -3.582

+89-83-8 CC(C)c1ccc(C)cc1O -2.954

+76-61-9 CC(C)c1cc(c(C)cc1O)C3(OS(=O)(=O)c2ccccc23)c4cc(C(C)C)c(O)cc4C -2.041

+32527-55-2 OCCN1CCN(CC1)C(=O)CN2c3cc(Cl)ccc3SC2=O -2.869

+26839-75-8 O[C@H](COc1nsnc1N2CCOCC2)CNC(C)(C)C -3.438

+1156-19-0 Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2CCCCCC2 -1.816

+59-98-3 c2cc(CC1=NCCN1)ccc2 -2.572

#64-77-7 Cc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC -2.037

-4201-22-3 Cc2cc(Cl)c(NC1=NCCN1)cc2 -4.061

+728-88-1 C[C@H](CN1CCCCC1)C(=O)c2ccc(C)cc2 -2.290

+108-88-3 Cc1ccccc1 -2.721

+68-76-8 O=C1C=C(C(=O)C(=C1N2CC2)N3CC3)N4CC4 -5.595

+24017-47-8 CCOP(=S)(OCC)Oc1ncn(n1)c2ccccc2 -1.591

\*133-67-5 NS(=O)(=O)c2cc1c(N[C@H](NS1(=O)=O)C(Cl)Cl)cc2Cl -2.903

+112-24-3 NCCNCCNCCN -6.679

+121-44-8 CCN(CC)CC -4.867

+280-57-9 C1CN2CCN1CC2 -5.653

\*51-18-3 n1c(nc(nc1N2CC2)N3CC3)N4CC4 -5.602

+1420-06-0 c1ccccc1C(N2CCOCC2)(c3ccccc3)c4ccccc4 1.699

+117-89-5 FC(F)(F)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 -1.086

+146-54-3 FC(F)(F)c1cc2N(CCCN(C)C)c3ccccc3Sc2cc1 0.757

\*1582-09-8 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)C(F)(F)F 0.735

+70-00-8 FC(F)(F)C1=CN(C(=O)NC1=O)[C@H]2C[C@H](O)[C@@H](CO)O2 -3.193

#616-68-2 O=C(Nc1c(C)cc(C)cc1C)CN(CC)CC -2.324

+552-30-7 O=C(O)c1ccc2C(=O)OC(=O)c2c1 -3.017

#84-96-8 CN(C)CC(C)CN1c3ccccc3Sc2ccccc12 0.026

+738-70-5 Nc2nc(N)ncc2Cc1cc(OC)c(OC)c(OC)c1 -2.602

+52128-35-5 COc1cc(cc(OC)c1OC)NCc2ccc3nc(N)nc(N)c3c2C -1.497

\*91-81-6 CN(C)CCN(Cc1ccccc1)c2ccccn2 -2.769

+217-59-4 c3cccc4c1ccccc1c2ccccc2c34 1.386

+519-73-3 c1ccccc1C(c2ccccc2)c3ccccc3 0.178

+486-12-4 Cc1ccc(cc1)C(=C\CN2CCCC2)\c3ccccn3 -1.874

+552-63-6 OC[C@@H](C(=O)O)c1ccccc1 -4.301

+61-54-1 NCCc2cnc1ccccc12 -4.519

+69-33-0 Nc3ncnc1c3ccn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -3.477

+51-67-2 Oc1ccc(CCN)cc1 -4.017

+60-18-4 Oc1ccc(C[C@H](N)C(=O)O)cc1 -2.680

+58-96-8 O=C1NC(=O)N(C=C1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -4.787

\*66644-81-3 C=CCN2CCC[C@@H]2CNC(=O)c1cc(cc(OC)c1OC)S(N)(=O)=O -2.332

+52-53-9 COc1cc(ccc1OC)[C@@](C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C -0.650

+1929-77-7 O=C(SCCC)N(CCC)CCC -1.954

+18542-37-5 O[C@H]3C[C@@]1(COC(=O)C(=C)[C@@H]1[C@H]2OC(=O)C(=C)[C@@H]23)C=C -4.471

+50471-44-8 O=C1N(C(=O)O[C@@]1(C)C=C)c2cc(Cl)cc(Cl)c2 -0.415

\*81-81-2 CC(=O)CC(C1=C(O)c2ccccc2OC1=O)c3ccccc3 -1.230

+69-89-6 O=C1NC(=O)Nc2ncnc12 -1.839

+90-47-1 O=C1c3ccccc3Oc2ccccc12 -0.655

+14293-44-8 O=S(N)(=O)c1cc(c(O)cc1Cl)C(=O)Nc2c(C)cccc2C -1.763

+146-48-5 O=C(OC)[C@H]2[C@@H](O)CC[C@H]3CN4CCc1c5ccccc5nc1[C@@H]4C[C@@H]23 -2.442

**Table S4**

**The numerical data on toxicity towards rats (mg/kg, pLD50) for drug-like substances. Split 1**

+79-00-5 ClCC(Cl)Cl -2.922

+87-61-6 Clc1cccc(Cl)c1Cl -3.262

-524-42-5 O=C1c2ccccc2C=CC1=O -2.398

\*108-70-3 Clc1cc(Cl)cc(Cl)c1 -2.903

+106-99-0 C=CC=C -3.739

-534-07-6 ClCC(=O)CCl -1.301

+102-06-7 N=C(Nc1ccccc1)Nc2ccccc2 -2.509

#130-15-4 O=C2C=CC(=O)c1ccccc12 -2.279

-112-53-8 CCCCCCCCCCCCO -4.107

-288-88-0 c1nncn1 -3.243

#90-15-3 Oc2cccc1ccccc12 -3.272

#108-03-2 [O-][N+](=O)CCC -2.658

+92-43-3 O=C1CCN(N1)c2ccccc2 -2.301

-118-79-6 Brc1cc(Br)cc(Br)c1O -3.301

+88-06-2 Clc1cc(Cl)cc(Cl)c1O -2.914

#118-96-7 Cc1c(cc(cc1[N+](=O)[O-])[N+]([O-])=O)[N+]([O-])=O -2.783

+120-83-2 Clc1cc(Cl)c(O)cc1 -1.672

#367-25-9 Fc1ccc(N)c(F)c1 -2.914

-97-02-9 O=[N+]([O-])c1cc(ccc1N)[N+]([O-])=O -2.455

-51-28-5 O=[N+]([O-])c1cc(ccc1O)[N+]([O-])=O -1.477

-108-48-5 Cc1cccc(C)n1 -2.602

-695-34-1 Cc1ccnc(N)c1 -2.301

-96-50-4 Nc1nccs1 -2.681

\*110-43-0 CC(=O)CCCCC -3.223

+149-30-4 Sc1nc2ccccc2s1 -2.000

+115-19-5 C#CC(C)(C)O -3.290

+135-19-3 Oc1ccc2ccccc2c1 -3.292

+79-46-9 CC(C)[N+]([O-])=O -2.857

\*122-99-6 OCCOc1ccccc1 -3.100

+95-76-1 Nc1cc(Cl)c(Cl)cc1 -2.736

#13466-78-9 CC2(C)[C@H]1CC=C(C)C[C@@H]12 -3.681

+584-02-1 CCC(O)CC -3.272

+89796-99-6 Clc2cccc(Cl)c2Nc1ccccc1CC(=O)OCC(=O)O -2.114

-642-83-1 O=C1O[C@@H]2[C@H](OC(C)=O)C(=O)O[C@@H]2[C@H]1OC(C)=O -4.000

-152-72-7 [O-][N+](=O)c1ccc(cc1)[C@@H](CC(C)=O)C2=C(O)c3ccccc3OC2=O -2.710

-75-07-0 CC=O -2.820

-60-35-5 CC(N)=O -3.845

#103-84-4 O=C(C)Nc1ccccc1 -2.903

+968-81-0 O=C(NC1CCCCC1)NS(=O)(=O)c2ccc(cc2)C(C)=O -3.301

-75-05-8 CC#N -3.391

+98-86-2 CC(=O)c1ccccc1 -2.911

+616-91-1 CC(=O)N[C@@H](CS)C(O)=O -3.703

+72420-38-3 C[C@]1(OC(=CC1=O)C(=O)O)c2ccccc2 -3.477

+55079-83-9 Cc1c(C)c(/C=CC(\C)=C\C=C\C(\C)=C\C(=O)O)c(C)cc1OC -3.602

+79-06-1 C=CC(N)=O -2.093

+59277-89-3 NC2=Nc1c(ncn1COCCO)C(=O)N2 -4.301

-281-23-2 C1C3CC2CC1CC(C2)C3 -4.000

-73-24-5 NC=1NC=NC2=NC=NC=12 -2.356

-56287-74-2 Cc1ccccc1N3C(=Nc2ccc(N)cc2C3=O)CF -2.396

\*74258-86-9 O=C(N[C@@H](Cc1ccccc1)C(=O)O)[C@@H]2CCCN2C(=O)[C@H](C)CSC(C)=O -3.699

+54965-21-8 O=C(OC)Nc1nc2ccc(cc2n1)SCCC -3.380

-18559-94-9 OCc1cc(ccc1O)[C@@H](O)CNC(C)(C)C -2.820

+22131-79-9 Clc1cc(ccc1OCC=C)CC(=O)O -3.021

-116-06-3 CC(C)(\C=N\OC(=O)NC)SC -0.699

-309-00-2 ClC3=C(Cl)[C@@]4(Cl)[C@@H]2[C@@H]([C@@H]1C[C@H]2C=C1)[C@]3(Cl)C4(Cl)Cl -1.591

+33178-86-8 C=CCN(C1=NCCN1)c2c(Cl)cccc2Cl -2.699

+5486-77-1 O=C(NCCN(CC)CC)c1ccc(Cl)cc1OCC=C -3.477

+107-11-9 C=CCN -2.009

+39718-89-3 O=C(O)[C@H](C)c1ccc(NCC(=C)C)cc1 -2.740

-768-94-5 NC12CC3CC(C1)CC(C2)C3 -2.954

+539-21-9 N=C(N)N\N=C1\C=C/C(=N\NC(N)=S)C=C1 -2.875

+51022-69-6 CC(=O)OCC(=O)[C@]56OC1(CCCC1)O[C@@H]6C[C@H]4C3CCC2=CC(=O)C=C[C@]2(C)[C@@]3(F)[C@@H](O)C[C@@]45C -3.301

+32887-01-7 OC(=O)[C@@H]2N3C(=O)[C@@H](/N=C/N1CCCCCC1)[C@H]3SC2(C)C -4.000

#834-12-8 CSc1nc(NCC)nc(NC(C)C)n1 -2.706

+642-44-4 O=C1N(CC=C)C(N)=CC(=O)N1CC -3.362

-58-15-1 CN(C)C=2C(=O)N(c1ccccc1)N(C)C=2C -2.455

#50-48-6 CN(C)CC\C=C1\c3ccccc3CCc2ccccc12 -2.505

+68302-57-8 CC(C)c1cc2C(=O)c3cc(c(N)nc3Oc2cc1)C(=O)O -4.000

+14028-44-5 Clc1ccc2Oc4ccccc4N=C(c2c1)N3CCNCC3 -2.496

\*134-37-2 Nc1cc(ccc1)N2C=CC=CC2=O -3.362

-300-62-9 NC(C)Cc1ccccc1 -1.477

-99464-64-9 O=C(OCC)O[C@@H](C)OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 -2.873

+29883-15-6 O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]3OC[C@H]2O[C@@H](O[C@H](C#N)c1ccccc1)[C@H](O)[C@@H](O)[C@@H]2O -2.607

+31698-14-3 N=C1N=C2O[C@H]3[C@H](O)[C@@H](CO)O[C@H]3N2C=C1 -3.845

+62-53-3 Nc1ccccc1 -2.398

-72432-10-1 O=C2CCCN2C(=O)c1ccc(OC)cc1 -3.653

-100-66-3 COc1ccccc1 -3.568

+60-80-0 O=C2C=C(C)N(C)N2c1ccccc1 -3.232

+52-46-0 C1CN1p2(np(np(n2)(N3CC3)N4CC4)(N5CC5)N6CC6)N7CC7 -1.991

-63968-64-9 O=C4O[C@H]2O[C@@]1(C)CC[C@@H]3[C@]2(OO1)[C@@H](CC[C@H]3C)[C@H]4C -3.746

+22839-47-0 O=C(O)C[C@@H](N)C(=O)N[C@H](Cc1ccccc1)C(=O)OC -4.000

-68844-77-9 Fc1ccc(cc1)Cn4c5ccccc5nc4NC3CCN(CCc2ccc(OC)cc2)CC3 -3.408

+29122-68-7 CC(C)NCC(O)COc1ccc(cc1)CC(N)=O -3.301

-51-55-8 CN3C1CCC3CC(C1)OC(=O)C(CO)c2ccccc2 -2.699

-62973-76-6 Cn2c(cnc2/C=C/c1ccnc(N)n1)[N+]([O-])=O -3.881

+1649-18-9 Fc1ccc(cc1)C(=O)CCCN2CCN(CC2)c3ccccn3 -2.389

-58581-89-8 Clc1ccc(cc1)CC3=NN(C(=O)c2ccccc23)[C@@H]4CCCN(C)CC4 -2.491

\*1830-32-6 CCN(CC)C(=O)CSc1ccc(Cl)nn1 -3.190

-103-33-3 N(=N/c1ccccc1)\c2ccccc2 -3.000

+27589-33-9 NS(=O)(=O)c2cc(c(NCc1cccs1)cc2Cl)c3nnnn3 -3.406

-78110-38-0 [NH3+]c1nc(cs1)\C(=N\OC(C)(C)C(=O)O)C(=O)N[C@@H]2C(=O)N(S([O-])(=O)=O)[C@H]2C -4.000

-275-51-4 c1cccc2cccc2c1 -3.602

-1134-47-0 Clc1ccc(cc1)C(CN)CC(=O)O -2.161

+101-27-9 Clc1cc(NC(=O)OCC#CCCl)ccc1 -2.722

+20187-55-7 O=C(O)COc3nn(Cc1ccccc1)c2ccccc23 -3.079

+22781-23-3 CNC(=O)Oc1cccc2OC(C)(C)Oc12 -1.602

+17804-35-2 O=C(OC)Nc2nc1ccccc1n2C(=O)NCCCC -4.000

+51234-28-7 O=C(O)[C@@H](C)c1cc2nc(oc2cc1)c3ccc(Cl)cc3 -2.072

+100-52-7 O=Cc1ccccc1 -3.114

-3562-84-3 Brc1cc(cc(Br)c1O)C(=O)c2c3ccccc3oc2CC -2.394

+71-43-2 c1ccccc1 -2.968

+17243-39-9 CNCC24CCC(c1ccccc12)c3ccccc34 -2.778

\*65-85-0 O=C(O)c1ccccc1 -3.230

+119-61-9 O=C(c1ccccc1)c2ccccc2 -4.000

+95-16-9 c1cccc2scnc12 -2.580

+98-88-4 ClC(=O)c1ccccc1 -3.279

-156-08-1 CN(Cc1ccccc1)[C@@H](C)Cc2ccccc2 -2.204

-53-89-4 CN1CCC(CC1)N3NC(=C(Cc2ccccc2)C3=O)c4ccccc4 -3.431

-100-51-6 OCc1ccccc1 -3.090

+103-41-3 O=C(OCc1ccccc1)/C=C/c2ccccc2 -3.743

+103-50-4 C(OCc1ccccc1)c2ccccc2 -3.398

-5638-76-6 CNCCc1ccccn1 -3.786

+41859-67-0 O=C(NCCc1ccc(OC(C)(C)C(=O)O)cc1)c2ccc(Cl)cc2 -3.034

+15301-48-1 CCC(=O)N5c1ccccc1N(C4CCN(CCC(C#N)(c2ccccc2)c3ccccc3)CC4)C5=O -2.149

-103-29-7 C(Cc1ccccc1)c2ccccc2 -3.655

+42576-02-3 Clc2cc(Cl)ccc2Oc1cc(C(=O)OC)c(cc1)[N+]([O-])=O -3.806

+60628-96-8 c1cc(ccc1c2ccccc2)[C@H](c3ccccc3)n4ccnc4 -3.165

-60662-16-0 CN(C)CCN(C)n2cc(c1ccccc12)c3ccccc3 -3.064

-69047-39-8 Clc1ccc(cc1)OC(C)(C)C(=O)OC(COC(=O)c2cccnc2)COC(=O)c3cccnc3 -3.602

+28434-01-7 C/C(C)=C/[C@@H]3C(C(=C)CCC=2C=C(Cc1ccccc1)CC=2)C3(C)C -3.095

#514-65-8 OC(CCN1CCCCC1)(c2ccccc2)C4CC3C=CC4C3 -2.875

#56518-41-3 Nc2nc(N)ncc2Cc1cc(OC)c(Br)c(OC)c1 -3.400

-314-40-9 CC[C@@H](C)N1C(=O)C(Br)=C(C)NC1=O -2.807

-1812-30-2 Brc1ccc2NC(=O)CN=C(c2c1)c3ccccn3 -3.290

+496-67-3 CC(C)[C@@H](Br)C(=O)NC(N)=O -3.000

+108-86-1 Brc1ccccc1 -3.377

-75-25-2 BrC(Br)Br -2.970

+2104-96-3 Clc1cc(OP(=S)(OC)OC)c(Cl)cc1Br -3.204

\*4093-35-0 Nc1cc(OC)c(cc1Br)C(=O)NCCN(CC)CC -2.736

\*10457-90-6 Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Br)cc3 -2.555

+65002-17-7 O=C(N[C@H](CS)C(=O)O)C(C)(C)S -3.591

#841-73-6 O=C2N(C1CCCCC1)C(=O)NC(=O)[C@H]2CCCC -3.047

-51333-22-3 OCC(=O)[C@@]45O[C@@H](O[C@H]5C[C@@H]3[C@@H]2CCC1=CC(=O)C=C[C@]1(C)[C@H]2[C@@H](O)C[C@@]34C)CCC -3.505

-57982-78-2 CC(C)(C)N1CCC(CC1)(c2ccccc2)c3ccccc3 -2.217

+36798-79-5 C\C(C)=CC(\C)=N\N=C1/NN=Cc2ccccc12 -2.792

-41483-43-6 CCNc1nc(C)c(CCCC)c(OS(=O)(=O)N(C)C)n1 -3.602

-23184-66-9 ClCC(=O)N(COCCCC)c1c(cccc1CC)CC -3.241

-653-03-2 CCCC(=O)c2cc3N(CCCN1CCN(C)CC1)c4ccccc4Sc3cc2 -2.616

-55837-18-8 CC[C@H](C(=O)O)c1ccc(cc1)CC(C)C -3.204

\*33629-47-9 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N[C@H](C)CC)C(C)(C)C -3.398

#123-72-8 CCCC=O -3.396

+109-74-0 CCCC#N -1.699

-64241-34-5 O=C(OCC)NNc1ccc(nn1)N(C[C@@H](C)O)CC -3.314

+58-08-2 O=C2c1n(C)cnc1N(C)C(=O)N2C -2.283

+32222-06-3 C=C1C(\C[C@@H](O)CC1O)=C\C=C3\CCC[C@@]2(C)C3CC[C@@H]2C(C)CCCC(C)(C)O 0.208

+36104-80-0 CN(C)C(=O)OC2N=C(c1cc(Cl)ccc1N(C)C2=O)c3ccccc3 -3.602

+7689-03-4 CC[C@]1(O)C=2C=C3c4nc5ccccc5cc4CN3C(=O)C=2COC1=O -2.185

\*298-46-4 NC(=O)N2c3ccccc3C=Cc1ccccc12 -3.292

+10605-21-7 O=C(OC)Nc1nc2ccccc2n1 -3.806

+77-23-6 CCN(CC)CCOCCOC(=O)C1(CCCC1)c2ccccc2 -2.176

-638-23-3 OC(=O)[C@@H](N)CSCC(O)=O -4.176

-1563-66-2 CNC(=O)Oc1cccc2CC(C)(C)Oc12 -0.699

+24279-91-2 NC(=O)OC[C@@H](OC)C=1C(=O)C(=C(C)C(=O)C=1N2CC2)N3CC3 -1.436

-339-43-5 Nc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC -3.643

-61422-45-5 O=C1NC(=O)C(F)=CN1C(=O)NCCCCCC -2.428

-5942-95-0 NC(=O)C4(CCN(CCCN2c3ccccc3CCc1ccccc12)CC4)N5CCCCC5 -3.011

-53716-49-7 O=C(O)C(C)c1ccc2c3cc(Cl)ccc3nc2c1 -1.869

-2037-95-8 O=C2NC(=O)Oc1ccccc12 -2.875

\*53994-73-3 ClC=3CS[C@H]2N(C(=O)[C@@H]2NC(=O)[C@H](N)c1ccccc1)C=3C(=O)O -4.301

+79350-37-1 Nc1scc(n1)/C(=N\OCC(=O)O)C(=O)N[C@@H]3C(=O)N2C(=C(C=C)CS[C@@H]23)C(=O)O -4.000

+35607-66-0 O=C(O)C=2N3C(=O)[C@](NC(=O)Cc1cccs1)(OC)[C@H]3SCC=2COC(N)=O -4.000

-51762-05-1 N[C@H](C1C=CCC=C1)C(=O)N[C@@H]3C(=O)N2C(=C(OC)CS[C@@H]23)C(=O)O -4.352

-55268-75-2 CO\N=C(\c1ccco1)C(=O)N[C@H]3C(=O)N2C(=C(COC(N)=O)CS[C@@H]23)C(=O)O -4.000

+38821-53-3 CC=3CS[C@H]2N(C(=O)[C@@H]2NC(=O)[C@H](N)C1=CCC=CC1)C=3C(=O)O -4.079

-133-90-4 Clc1cc(C(=O)O)c(Cl)c(N)c1 -3.544

#305-03-3 O=C(O)CCCc1ccc(cc1)N(CCCl)CCCl -1.881

-56-75-7 O=[N+]([O-])c1ccc(cc1)[C@@H](O)[C@@H](CO)NC(=O)C(Cl)Cl -3.398

-5588-20-5 O=C1N[C@@H](C(=O)N1SC(Cl)(Cl)Cl)[C@H](CC)CCCC -3.066

\*58-25-3 Clc1ccc2N=C(C[N+]([O-])=C(c2c1)c3ccccc3)NC -2.593

-6164-98-3 Clc1cc(C)c(/N=C/N(C)C)cc1 -2.204

+85-34-7 Clc1c(CC(=O)O)c(Cl)ccc1Cl -3.250

+80-77-3 O=C1CCS(=O)(=O)C(N1C)c2ccc(Cl)cc2 -2.782

+78-95-5 CC(=O)CCl -2.000

\*108-90-7 Clc1ccccc1 -3.045

#510-15-6 OC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)C(=O)OCC -2.845

+67-66-3 ClC(Cl)Cl -2.842

+76-06-2 ClC(Cl)(Cl)[N+]([O-])=O -2.398

+59-32-5 Clc1ccc(cc1)CN(CCN(C)C)c2ccccn2 -2.964

+58-94-6 NS(=O)(=O)c2cc1c(N=CNS1(=O)=O)cc2Cl -4.000

\*461-78-9 Clc1ccc(CC(C)(C)N)cc1 -2.398

+50-53-3 CN(C)CCCN1c3ccccc3Sc2ccc(Cl)cc12 -2.152

+113-59-7 CN(C)CC\C=C1\c3ccccc3Sc2ccc(Cl)cc12 -2.301

-72-80-0 Oc1c(Cl)cc(Cl)c2ccc(C)nc12 -2.820

+73963-72-1 O=C1CCc2cc(ccc2N1)OCCCCc4nnnn4C3CCCCC3 -3.699

-51481-61-9 N#C\N=C(/NC)NCCSCc1ncnc1C -3.699

-104-54-1 OC\C=C\c1ccccc1 -3.301

+298-57-7 c1ccccc1C(c2ccccc2)N3CCN(CC3)C/C=C/c4ccccc4 -3.813

#28657-80-9 O=C(O)C2=NN(CC)c1cc3OCOc3cc1C2=O -3.558

\*58473-74-8 Brc1cc(/C=C/C(=O)NCC)ccc1 -3.647

-85721-33-1 O=C(O)C2=CN(c1cc(c(F)cc1C2=O)N3CCNCC3)C4CC4 -3.301

+81098-60-4 Clc1cc(c(OC)cc1N)C(=O)N[C@H]3CCN(CCCOc2ccc(F)cc2)C[C@H]3OC -3.620

-30544-61-7 O=C(c1ccc(Cl)cc1)N(CCCC(=O)O)c2ccc(OC)cc2 -3.301

-30299-08-2 O=C(O)[C@@](C)(CC)Oc1ccc(cc1)C2(CCCCC2)c3ccc(O[C@@](C)(CC)C(=O)O)cc3 -3.602

\*14437-41-3 Clc2ccc(NC(=O)c1cc(I)cc(I)c1OC(C)=O)cc2 -3.699

-2030-63-9 Clc1ccc(cc1)NC3=CC4=Nc2ccccc2N(C4=C\C3=N\C(C)C)c5ccc(Cl)cc5 -3.924

-671-95-4 O=S(N)(=O)c1cc(ccc1Cl)S(N)(=O)=O -2.531

-37693-01-9 Clc2cc(Cl)ccc2Cc1cc(ccc1O)C(C)(C)CC(C)(C)C -3.602

\*5310-55-4 CN(C)CCC[C@@H]2c3ccccc3Nc1ccc(Cl)cc12 -2.579

-911-45-5 CCN(CCOc1ccc(cc1)/C(c2ccccc2)=C(/Cl)c3ccccc3)CC -3.760

+1622-61-3 [O-][N+](=O)c1ccc2NC(=O)CN=C(c2c1)c3ccccc3Cl -4.176

-4205-90-7 Clc2cccc(Cl)c2NC1=NCCN1 -1.828

+2971-90-6 Oc1c(Cl)c(C)nc(C)c1Cl -4.255

-68206-94-0 O=C(OCC)COc2ccc1c(OC(=O)C(CCN(CC)CC)=C1C)c2Cl -3.097

\*120-32-1 Oc2ccc(Cl)cc2Cc1ccccc1 -3.230

+57808-65-8 Clc2cc(NC(=O)c1cc(I)cc(I)c1O)c(C)cc2[C@H](C#N)c3ccc(Cl)cc3 -2.418

-2058-52-8 CN1CCN(CC1)C3=Nc4ccccc4Sc2ccc(Cl)cc23 -2.447

+33671-46-4 Clc3ccccc3C1=NCC(=O)N(C)c2sc(cc12)CC -3.165

+23593-75-1 Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4 -2.850

+24166-13-0 Clc1ccccc1C34OCCN4CC(=O)Nc2ccc(Cl)cc23 -3.250

+5786-21-0 CN1CCN(CC1)C2=Nc4cc(Cl)ccc4Nc3ccccc23 -2.400

#76-57-3 COc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 -2.630

-66575-29-9 CC(=O)O[C@H]2[C@@H](O)[C@@H]1[C@](C)([C@@H](O)CCC1(C)C)[C@@]3(O)C(=O)C[C@](C)(C=C)O[C@]23C -3.407

-56-72-4 CCOP(=S)(OCC)Oc1ccc2c(c1)OC(=O)C(Cl)=C2C -1.114

-91-64-5 O=C1C=Cc2ccccc2O1 -2.467

\*483-63-6 CCN(C(=O)\C=C\C)c1ccccc1C -3.176

+21725-46-2 Clc1nc(NCC)nc(NC(C)(C)C#N)n1 -2.173

+456-59-7 O=C(O[C@H]1C[C@@H](C)CC(C)(C)C1)[C@H](O)c2ccccc2 -3.699

\*512-16-3 OC1(CCCCC1)[C@H](CC)C(=O)O -3.683

\*108-93-0 OC1CCCCC1 -3.146

+68-41-7 N[C@@H]1CONC1=O -3.699

-2259-96-3 NS(=O)(=O)c4cc1c(N[C@H](NS1(=O)=O)[C@@H]3C[C@H]2C=C[C@H]3C2)cc4Cl -3.699

+7199-29-3 NC(=O)C2c3ccccc3CCc1ccccc12 -3.380

\*52-90-4 O=C(O)[C@@H](N)CS -3.276

+17230-88-5 C#C[C@]3(O)CC[C@H]2[C@@H]4CCC1=Cc5oncc5C[C@]1(C)[C@H]4CC[C@]23C -4.230

-50-29-3 Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl -1.940

#14817-09-5 NC(=O)c1cc(OC)c(OCCCCCCCCCC)c(c1)OC -3.217

+83-44-3 O=C(O)CC[C@@H](C)[C@H]2CC[C@H]1[C@@H]3CC[C@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@@]12C -3.000

+50-47-5 CNCCCN2c3ccccc3CCc1ccccc12 -2.574

-50-02-2 OCC(=O)[C@]3(O)[C@@]4(C)C[C@H](O)[C@@]2(F)[C@@H](CCC1=CC(=O)C=C[C@@]12C)[C@@H]4C[C@H]3C -3.477

+124-02-7 C=CCNCC=C -2.762

-333-41-5 Cc1cc(OP(=S)(OCC)OCC)nc(n1)C(C)C -1.820

-364-98-7 Clc1ccc2N=C(C)NS(=O)(=O)c2c1 -2.991

#1918-00-9 COc1c(c(Cl)ccc1Cl)C(=O)O -3.017

+2463-84-5 Clc1cc(ccc1OP(=S)(OC)OC)[N+]([O-])=O -2.453

+97-17-6 Clc1cc(Cl)ccc1OP(=S)(OCC)OCC -2.236

+120-97-8 Clc1c(cc(cc1Cl)S(N)(=O)=O)S(N)(=O)=O -4.003

\*2164-09-2 Clc1ccc(NC(=O)C(=C)C)cc1Cl -3.255

-66-76-2 OC=3c4ccccc4OC(=O)C=3CC1=C(O)c2ccccc2OC1=O -2.398

+702-54-5 CCC1(CC)COC(=O)NC1=O -1.851

\*109-89-7 CCNCC -2.732

+56-53-1 Oc1ccc(cc1)C(\CC)=C(\CC)c2ccc(O)cc2 -3.477

-20170-20-1 CN(C)[C@H](C)C(=O)Nc2cc(nn2c1ccccc1)c3ccccc3 -2.911

#28782-42-5 O=C(O)C3(CCN(CCC(C#N)(c1ccccc1)c2ccccc2)CC3)c4ccccc4 -2.173

#35367-38-5 Clc2ccc(NC(=O)NC(=O)c1c(F)cccc1F)cc2 -3.667

+22494-42-4 OC(=O)c1cc(ccc1O)c2ccc(F)cc2F -2.593

#5221-53-4 Cc1nc(nc(O)c1CCCC)N(C)C -3.371

-60-51-5 COP(=S)(OC)SCC(=O)NC -1.778

-131-11-3 COC(=O)c1ccccc1C(=O)OC -3.833

+124-40-3 CNC -2.844

-148-01-6 Cc1c(cc(cc1[N+](=O)[O-])[N+]([O-])=O)C(N)=O -2.778

-88-85-7 O=[N+]([O-])c1cc(cc(c1O)[C@H](C)CC)[N+]([O-])=O -1.398

+82-66-6 O=C2c1ccccc1C(=O)C2C(=O)C(c3ccccc3)c4ccccc4 -0.176

+58-73-1 CN(C)CCOC(c1ccccc1)c2ccccc2 -2.591

-972-02-1 OC(CCCN1CCCCC1)(c2ccccc2)c3ccccc3 -2.911

#915-30-0 O=C(OCC)C3(CCN(CCC(C#N)(c1ccccc1)c2ccccc2)CC3)c4ccccc4 -2.344

\*117-34-0 OC(=O)C(c1ccccc1)c2ccccc2 -3.744

+122-39-4 c1ccccc1Nc2ccccc2 -3.049

+101-81-5 c1ccccc1Cc2ccccc2 -3.352

+4147-51-7 CCSc1nc(nc(NC(C)C)n1)NC(C)C -3.591

-58-32-2 OCCN(CCO)c2nc1c(nc(nc1c(n2)N3CCCCC3)N(CCO)CCO)N4CCCCC4 -3.924

-3737-09-5 CC(C)N(CC[C@](c1ccccn1)(c2ccccc2)C(N)=O)C(C)C -2.522

-330-54-1 Clc1ccc(NC(=O)N(C)C)cc1Cl -3.007

-502-55-6 CCOC(=S)SSC(=S)OCC -2.681

+74639-40-0 CC(=O)N[C@@H](CCSC)C(=O)NCCc1cc(OC(=O)OCC)c(cc1)OC(=O)OCC -3.301

-1593-77-7 C[C@H]1CN(C[C@@H](C)O1)C2CCCCCCCCCCC2 -3.422

+57808-66-9 Clc4cc5NC(=O)N(C3CCN(CCCN1c2ccccc2NC1=O)CC3)c5cc4 -3.720

+1668-19-5 CN(C)CC\C=C1/c3ccccc3OCc2ccccc12 -2.167

+3094-09-5 FC1=CN(C(=O)NC1=O)[C@@H]2O[C@H](C)[C@@H](O)[C@H]2O -3.530

-69975-86-6 O=C2c1n(cnc1N(C)C(=O)N2C)CC3OCCO3 -2.985

+564-25-0 NC(=O)C=4C(=O)[C@@]3(O)C(O)=C2C(=O)c1c(O)cccc1[C@H](C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C -3.301

+82413-20-5 Oc1cccc(c1)C(/c2ccc(OCCN(C)C)cc2)=C(/CC)c3ccccc3 -3.653

-548-73-2 Fc1ccc(cc1)C(=O)CCCN2CC=C(CC2)N3c4ccccc4NC3=O -2.875

#17692-31-8 O[C@@H](CN1CCN(CC1)c2ccccc2)CO -2.875

+3176-03-2 O[C@@H]3CC[C@]4(O)[C@H]2Cc1ccc(OC)c(OC)c1[C@@]4(CCN2C)C3 -2.530

-90101-16-9 O=C3OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)N3c4ccccn4 -3.157

+23651-95-8 Oc1ccc(cc1O)[C@@H](O)[C@H](N)C(=O)O -4.000

+90729-43-4 CC(C)(C)c1ccc(cc1)C(=O)CCCN2CCC(CC2)OC(c3ccccc3)c4ccccc4 -3.602

+95-04-5 CC\C(=C\C)C(=O)NC(N)=O -3.398

-72-20-8 ClC1=C(Cl)[C@]2(Cl)C(Cl)(Cl)[C@]1(Cl)[C@@H]3[C@@H]2[C@H]4C[C@@H]3[C@H]5O[C@H]45 -0.477

-55726-47-1 CCCCCCCCCCCCCCCCCCCCCC(=O)NC1=NC(=O)N(C=C1)[C@@H]2O[C@H](CO)[C@@H](O)[C@@H]2O -3.000

+74011-58-8 O=C(O)C2=CN(CC)c1nc(c(F)cc1C2=O)N3CCNCC3 -3.699

-73121-56-9 O[C@H]2CC(=O)[C@@H](C/C=C=C\CCC(=O)OC)[C@@H]2\C=C/[C@@H](O)COc1ccccc1 -0.204

-82159-09-9 OC(=O)CN2C(=O)C(=CC(\C)=C\c1ccccc1)\SC2=S -0.724

\*299-42-3 O[C@H](c1ccccc1)[C@H](C)NC -2.778

+32665-36-4 O[C@@H](CCN2CCN(C[C@H](OC)c1ccccc1)CC2)c3ccccc3 -2.806

+84611-23-4 O=C1SCC[C@H]1NC(=O)CSCC(=O)O -4.000

+64204-55-3 O=C(CN1CCNCC1)NC2CCCCC2 -3.591

+50-27-1 Oc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2C[C@@H](O)[C@@H]1O)c4cc3 -3.301

+55283-68-6 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CC(=C)C)CC)C(F)(F)F -4.000

#304-84-7 Oc1ccc(cc1OC)C(=O)N(CC)CC -2.188

-75-08-1 CCS -2.834

\*141-43-5 NCCO -3.236

#563-12-2 S=P(SCSP(=S)(OCC)OCC)(OCC)OCC -1.114

+23947-60-6 CCNC1=NC(=O)C(CCCC)=C(C)N1 -3.602

-26225-79-6 CS(=O)(=O)Oc1cc2c(cc1)O[C@H](OCC)C2(C)C -3.053

+77-15-6 CN1CCC[C@@](CC1)(C(=O)OCC)c2ccccc2 -2.550

-77-67-8 C[C@@]1(CC)CC(=O)NC1=O -3.260

-86-35-1 O=C2N[C@H](c1ccccc1)C(=O)N2CC -3.176

+93-89-0 O=C(OCC)c1ccccc1 -3.322

\*101-97-3 O=C(OCC)Cc1ccccc1 -3.519

-118-61-6 Oc1ccccc1C(=O)OCC -3.121

+75-04-7 CCN -2.602

-100-41-4 CCc1ccccc1 -3.544

#107-15-3 NCCN -3.079

\*76-58-4 CCOc5ccc1C[C@H]2N(C)CC[C@]34c1c5O[C@@H]4[C@@H](O)C=C[C@@H]23 -2.908

#21715-46-8 Clc1ccc2N=C(NCC)O[C@@](C)(c2c1)c3ccccc3 -3.176

+40054-69-1 Clc1ccccc1C4=NCc2nnc(C)n2c3sc(cc34)CC -3.545

+41340-25-4 O=C(O)C[C@]3(CC)OCCc2c3nc1c(cccc12)CC -1.973

-30544-47-9 FC(F)(F)c1cc(ccc1)Nc2ccccc2C(=O)OCCOCCO -2.465

-38260-54-7 CCc1nc(OCC)cc(OP(=S)(OC)OC)n1 -3.255

-470-82-6 CC2(C)OC1(C)CCC2CC1 -3.394

\*97-53-0 Oc1ccc(cc1OC)CC=C -3.286

-53370-90-4 NC(=O)c1ccccc1OCCCCCC -3.699

+52479-85-3 Oc2ccc(C(=O)c1cc(O)c(O)c(O)c1)c(O)c2O -3.154

-76824-35-6 N/C(N)=N/c1nc(CSCCC(\N)=N/S(N)(=O)=O)cs1 -3.607

+52-85-7 O=S(=O)(N(C)C)c1ccc(OP(=S)(OC)OC)cc1 -1.447

+3102-00-9 CCCCOC[C@@H](O)COc1ccccc1 -3.375

+25451-15-4 NC(=O)OCC(COC(N)=O)c1ccccc1 -3.699

-5728-52-9 OC(=O)Cc1ccc(cc1)c2ccccc2 -2.215

+22224-92-6 Cc1cc(ccc1SC)OP(=O)(NC(C)C)OCC -0.903

+61019-78-1 N#C[C@@](CCCC)(Cn1ccnc1)c2ccccc2 -3.201

+60168-88-9 O[C@@](c1ccccc1Cl)(c2cncnc2)c3ccc(Cl)cc3 -3.398

+36330-85-5 O=C(CCC(=O)O)c1ccc(cc1)c2ccccc2 -2.301

-458-24-2 FC(F)(F)c1cccc(C[C@H](C)NCC)c1 -2.114

+49562-28-9 O=C(c1ccc(Cl)cc1)c2ccc(OC(C)(C)C(=O)OC(C)C)cc2 -3.301

-437-38-7 CCC(=O)N(C2CCN(CCc1ccccc1)CC2)c3ccccc3 -1.255

+55-38-9 Cc1cc(ccc1SC)OP(=S)(OC)OC -2.255

-18046-21-4 O=C(O)Cc1sc(nc1c2ccc(Cl)cc2)c3ccccc3 -2.612

-51630-58-1 Clc1ccc(cc1)C(C(C)C)C(=O)OC(C#N)c3cccc(Oc2ccccc2)c3 -1.846

+79660-72-3 CN1CCN(CC1)c2c(F)c3c(cc2F)C(=O)C(=CN3CCF)C(=O)O -3.602

+31430-15-6 Fc1ccc(cc1)C(=O)c2cc3nc(NC(=O)OC)nc3cc2 -3.408

+33245-39-5 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCCl)CCC)C(F)(F)F -3.468

+86386-73-4 OC(Cn1cncn1)(Cn2cncn2)c3ccc(F)cc3F -3.104

+78755-81-4 O=C(OCC)c3ncn2c3CN(C)C(=O)c1cc(F)ccc12 -3.623

#56430-99-0 FC(F)(F)c1cccc(c1)[C@](O)(CC)c2ccccc2 -3.349

-462-06-6 Fc1ccccc1 -3.643

+54910-89-3 FC(F)(F)c2ccc(O[C@@H](CCNC)c1ccccc1)cc2 -2.916

+40507-23-1 Fc1ccc(cc1)C3=NC(=O)N(c2cc(C)ccc23)C(C)C -3.477

\*17617-23-1 Fc3ccccc3C2=NCC(=O)N(CCN(CC)CC)c1ccc(Cl)cc12 -2.991

+5104-49-4 Fc2cc(ccc2c1ccccc1)[C@H](C)C(=O)O -2.068

-27060-91-9 Fc1ccccc1[C@@]34OCCN4CC(=O)N(CCO)c2ccc(Cl)cc23 -3.778

+69409-94-5 Clc3cc(ccc3NC(C(=O)OC(C#N)c2cccc(Oc1ccccc1)c2)C(C)C)C(F)(F)F -2.417

+6064-83-1 OP(=O)(O)Oc1ccccc1C(=O)O -3.043

+5598-52-7 Clc1cc(Cl)c(Cl)nc1OP(=O)(OC)OC -2.939

+21548-32-3 CCOP(=O)(/N=C1\SCS1)OCC -0.672

+67-45-8 [O-][N+](=O)c2oc(/C=N/N1CCOC1=O)cc2 -3.368

+98-01-1 O=Cc1ccco1 -1.813

-54-31-9 NS(=O)(=O)c2cc(c(NCc1ccco1)cc2Cl)C(=O)O -3.415

-64318-79-2 O[C@H]1CC(=O)[C@@H](CCCC/C=C/C(=O)OC)[C@@H]1/C=C/[C@@H](O)C(C)(C)CCCC -1.752

-106-24-1 C\C(C)=C\CCC(/C)=C\CO -3.556

-3820-67-5 OC[C@@H](O)COC(=O)c3ccccc3Nc1ccnc2cc(Cl)ccc12 -3.362

+26944-48-9 O[C@H]3[C@]1(C)CC[C@H](C1(C)C)[C@@H]3NC(=O)NS(=O)(=O)c2ccc(C)cc2 -4.255

\*21187-98-4 Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2C[C@H]3CCC[C@@H]3C2 -3.477

+50-99-7 O[C@H]([C@@H](O)C=O)[C@H](O)[C@H](O)CO -4.412

\*77-21-4 CC[C@@]1(CCC(=O)NC1=O)c2ccccc2 -2.778

+10238-21-8 O=C(NC1CCCCC1)NS(=O)(=O)c3ccc(CCNC(=O)c2cc(Cl)ccc2OC)cc3 -4.301

+56-81-5 OCC(O)CO -4.100

+56-40-6 NCC(=O)O -3.899

-339-44-6 O=S(=O)(Nc1ncc(cn1)OCCOC)c2ccccc2 -3.491

-126-07-8 O=C2c3c(O[C@@]21C(=CC(=O)C[C@H]1C)OC)c(Cl)c(OC)cc3OC -4.000

-90-05-1 Oc1ccccc1OC -2.716

-93-14-1 OCC(O)COc1ccccc1OC -3.179

-55-65-2 N=C(N)NCCN1CCCCCCC1 -3.021

+3093-35-4 ClCC(=O)[C@]45OC(C)(C)O[C@@H]5C[C@@H]3[C@]4(C)C[C@H](O)[C@@]2(F)[C@H]3CCC1=CC(=O)CC[C@@]12C -3.699

-52-86-8 Fc1ccc(cc1)C(=O)CCCN2CCC(O)(CC2)c3ccc(Cl)cc3 -2.107

+777-11-7 Clc1cc(OCC#CI)c(Cl)cc1Cl -3.748

-59128-97-1 Fc1ccccc1[C@@]34OCCN4CC(=O)Nc2ccc(Br)cc23 -3.456

+7237-81-2 CCCCCCC(COC(=O)c1cccnc1)(COC(=O)c2cccnc2)COC(=O)c3cccnc3 -3.699

-509-86-4 O=C1NC(=O)NC(=O)C1(CC)C2=CCCCCC2 -3.699

-76-44-8 ClC2=C(Cl)[C@]3(Cl)[C@@H]1C=C[C@H](Cl)[C@@H]1[C@@]2(Cl)C3(Cl)Cl -1.602

-23560-59-0 ClC1=C(OP(=O)(OC)OC)C2CC=CC12 -1.982

-118-74-1 Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl -4.000

+67-72-1 ClC(Cl)(Cl)C(Cl)(Cl)Cl -3.649

-70-30-4 Clc2c(Cc1c(O)c(Cl)cc(Cl)c1Cl)c(O)c(Cl)cc2Cl -1.748

+51235-04-2 CN(C)C2=NC(=O)N(C1CCCCC1)C(=O)N2C -3.228

+84-16-2 Oc1ccc(cc1)[C@@H](CC)[C@@H](CC)c2ccc(O)cc2 -3.301

-71-00-1 N[C@@H](Cc1cncn1)C(=O)O -4.176

-848-53-3 Clc1ccc(cc1)[C@H](c2ccccc2)N3CCCN(C)CC3 -2.690

+3105-97-3 CCN(CC)CCNc1ccc(CO)c2Sc3ccccc3C(=O)c12 -2.991

+86-54-4 N\N=C1/NN=Cc2ccccc12 -1.954

+58-93-5 NS(=O)(=O)c2cc1c(NCNS1(=O)=O)cc2Cl -3.439

-123-31-9 Oc1ccc(O)cc1 -2.480

\*50-19-1 O[C@](COC(N)=O)(CC)c1ccccc1 -2.783

-127-07-1 NC(=O)NO -3.760

+68-88-2 Clc1ccc(cc1)[C@@H](c2ccccc2)N3CCN(CC3)CCOCCO -2.924

-50847-11-5 CC(C)C(=O)c1c2ccccn2nc1C(C)C -3.127

#78919-13-8 O[C@@H]2C[C@@H]1C\C(C[C@@H]1[C@H]2/C=C/[C@@H](O)[C@H](C)CC#CC)=C\CCCC(=O)O -2.000

-288-32-4 c1cncn1 -2.342

#26807-65-8 NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN2c3ccccc3CC2C -3.477

-120-72-9 c1cccc2nccc12 -3.000

-53-86-1 Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC -0.384

+26844-12-2 O=C(NC3CCN(CCc1cnc2ccccc12)CC3)c4ccccc4 -3.255

+440-58-4 O=C(C)Nc1c(I)c(c(I)c(CNC(C)=O)c1I)C(=O)O -3.845

+18181-70-9 Clc1cc(I)c(Cl)cc1OP(=S)(OC)OC -3.367

+66108-95-0 OC[C@@H](O)CNC(=O)c1c(I)c(N(C[C@H](O)CO)C(C)=O)c(I)c(c1I)C(=O)NC[C@H](O)CO -4.301

#5560-72-5 CN(C)CCCn3c1CCCCCCc1c2ccccc23 -2.889

-36734-19-7 O=C2CN(C(=O)NC(C)C)C(=O)N2c1cc(Cl)cc(Cl)c1 -3.544

#54-92-2 O=C(NNC(C)C)c1ccncc1 -2.562

-89667-40-3 O=C(O)CCCC\C=C(\c1cccnc1)c2ccccc2 -3.301

\*124-76-5 C[C@@]21CC[C@@H](C[C@H]1O)C2(C)C -3.716

#59-63-2 Cc1cc(no1)C(=O)NNCc2ccccc2 -2.447

+97-54-1 Oc1ccc(cc1OC)\C=C\C -3.193

-25311-71-1 S=P(Oc1ccccc1C(=O)OC(C)C)(NC(C)C)OCC -1.324

-54-85-3 O=C(NN)c1ccncc1 -3.097

-55-22-1 O=C(O)c1ccncc1 -3.699

\*57021-61-1 O=C(Nc1c(C)cccc1C)C2=CC=CNC2=O -3.778

+78-59-1 O=C1C=C(C)CC(C)(C)C1 -3.272

-121-91-5 OC(=O)c1cccc(c1)C(=O)O -4.017

+33820-53-0 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)C(C)C -3.699

-119-65-3 c1cccc2ccncc12 -2.556

#55453-87-7 O=C(O)Cc1ccc2OCc3ccccc3C(=O)c2c1 -2.155

\*59-01-8 O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CN)O[C@@H]3O[C@H]2[C@H](O)[C@@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](N)[C@H]1O)[C@H](N)C[C@@H]2N -4.000

-853-34-9 CC(=O)CCC2C(=O)N(c1ccccc1)N(C2=O)c3ccccc3 -2.857

-22071-15-4 C[C@H](C(=O)O)c1cccc(c1)C(=O)c2ccccc2 -1.795

+82-02-0 COc3c1c(OC(C)=CC1=O)c(OC)c2occc23 -1.838

-36894-69-6 O=C(N)c1cc(ccc1O)[C@@H](O)CN[C@@H](C)CCc2ccccc2 -3.301

#103890-78-4 CC=1NC(C)=C(C(C=1C(=O)OCC)c2ccccc2/C=C/C(=O)OC(C)(C)C)C(=O)OCC -2.944

-4618-18-2 O[C@H]2[C@H](O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O)[C@@H](CO)O[C@]2(O)CO -4.259

+84057-84-1 Clc1cccc(c1Cl)c2nnc(N)nc2N -2.312

-14769-73-4 N1=C3SCCN3C[C@@H]1c2ccccc2 -2.681

-137-58-6 O=C(Nc1c(C)cccc1C)CN(CC)CC -2.501

\*154-21-2 O[C@@H]1[C@@H](O)[C@@H](O)[C@@H](O[C@@H]1SC)[C@@H](NC(=O)[C@@H]2C[C@@H](CCC)CN2C)[C@@H](C)O -3.000

\*330-55-2 Clc1ccc(NC(=O)N(C)OC)cc1Cl -3.059

+98079-51-7 O=C(O)C2=CN(CC)c1c(F)c(c(F)cc1C2=O)N3C[C@H](C)NCC3 -3.580

-13010-47-4 O=C(NC1CCCCC1)N(CCCl)N=O -1.845

+50264-69-2 O=C(O)c3nn(Cc1ccc(Cl)cc1Cl)c2ccccc23 -3.230

-53179-11-6 CN(C)C(=O)C(CCN1CCC(O)(CC1)c2ccc(Cl)cc2)(c3ccccc3)c4ccccc4 -1.991

#846-49-1 Clc3ccccc3C2=NC(O)C(=O)Nc1ccc(Cl)cc12 -3.653

\*59729-31-6 CC(C)N1CCC(CC1)N(c2ccc(Cl)cc2)C(=O)Cc3ccccc3 -2.597

-848-75-9 Clc3ccccc3C2=N[C@@H](O)C(=O)N(C)c1ccc(Cl)cc12 -4.000

#1977-10-2 CN1CCN(CC1)C3=Nc4ccccc4Oc2ccc(Cl)cc23 -2.179

+73-22-3 O=C(O)[C@@H](N)Cc2cnc1ccccc12 -4.204

-59937-28-9 CC(C)OC(=O)C(/C(=O)OC(C)C)=C1/SC=CS1 -3.315

+69-79-4 O[C@H]2[C@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)[C@@H](CO)O[C@@H](O)[C@@H]2O -4.542

\*591-27-5 Nc1cccc(O)c1 -2.966

+10262-69-8 CNCCCC24CCC(c1ccccc12)c3ccccc34 -2.881

+22232-71-9 Clc1ccc(cc1)[C@]4(O)c2ccccc2C3=NCCN34 -1.560

-31431-39-7 O=C(OC)Nc1nc2cc(ccc2n1)C(=O)c3ccccc3 -2.854

-569-65-3 Cc1cccc(c1)CN2CCN(CC2)[C@@H](c3ccc(Cl)cc3)c4ccccc4 -3.243

#2013-58-3 NC(=O)C=4C(=O)[C@]3(O)C(O)=C2C(=O)c1c(O)ccc(Cl)c1C(=C)[C@H]2[C@H](O)[C@H]3[C@@H](C=4O)N(C)C -3.301

#51-68-3 Clc1ccc(OCC(=O)OCCN(C)C)cc1 -3.415

-137-05-3 N#CC(=C)C(=O)OC -3.204

\*2898-12-6 Clc1ccc2c(c1)C(=NCCN2C)c3ccccc3 -2.954

+7195-27-9 C[C@@]2(CN(C)S(=O)(=O)c1ccc(Cl)c(c1)S(N)(=O)=O)CCCO2 -4.000

+5118-29-6 CN(C)CC\C=C2/c1ccccc1C(C)(C)c3ccccc23 -2.230

-71628-96-1 CN(C)[C@H]6[C@H](O)[C@@H]5Oc3c(cc(O)c4C(=O)c2c(O)c1c(C[C@](C)(O)C[C@H]1OC)cc2C(=O)c34)[C@](C)(O5)[C@H]6O -3.252

#57-42-1 CN1CCC(CC1)(C(=O)OCC)c2ccccc2 -2.210

+70-07-5 COc2ccccc2OC[C@@H]1CNC(=O)O1 -3.582

+17854-59-0 O=C3c4ccccc4Oc2c3ccc(OC)c2CN1CCCCC1 -2.262

+57-53-4 O=C(N)OCC(C)(COC(=O)N)CCC -2.900

\*89-57-6 OC(=O)c1cc(N)ccc1O -3.447

+72-33-3 COc3cc4CC[C@@H]2[C@H](CC[C@@]1(C)[C@H]2CC[C@@]1(O)C#C)c4cc3 -4.000

+57837-19-1 C[C@@H](N(C(=O)COC)c1c(C)cccc1C)C(=O)OC -2.753

+586-06-1 Oc1cc(cc(O)c1)[C@H](O)CNC(C)C -3.528

+926-93-2 C[C@@H](NC(=S)NNC(=S)NC)C=C -3.000

-67-56-1 CO -3.750

-72-44-6 Cc1ccccc1N3C(C)=Nc2ccccc2C3=O -2.267

+950-37-8 O=C1SC(=NN1CSP(=S)(OC)OC)OC -1.301

-63-68-3 O=C(O)[C@@H](N)CCSC -4.556

+16752-77-5 C\C(=N\OC(=O)NC)SC -1.167

-59-05-2 O=C(O)[C@H](CCC(=O)O)NC(=O)c1ccc(cc1)N(C)Cc2nc3c(nc2)nc(N)nc3N -2.130

-298-81-7 COc1c3occc3cc2C=CC(=O)Oc12 -2.898

-76-38-0 ClC(Cl)C(F)(F)OC -3.556

#134-20-3 Nc1ccccc1C(=O)OC -3.464

#93-58-3 COC(=O)c1ccccc1 -3.071

+74-89-5 CN -2.000

+60-34-4 CNN -1.505

-113-45-1 O=C(OC)[C@@H](c1ccccc1)[C@@H]2CCCCN2 -2.565

+1084-65-7 NS(=O)(=O)c2cc1c(CCCS1(=O)=O)cc2C -4.204

\*364-62-5 Nc1cc(OC)c(cc1Cl)C(=O)NCCN(CC)CC -2.875

-51218-45-2 ClCC(=O)N(c1c(C)cccc1CC)[C@H](C)COC -3.342

-17560-51-9 NS(=O)(=O)c2cc3C(=O)N(c1ccccc1C)[C@H](C)Nc3cc2Cl -3.699

\*21087-64-9 O=C1C(=NN=C(SC)N1N)C(C)(C)C -3.041

-31112-62-6 O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]2NC(=O)c1c(I)c(NC(C)=O)c(I)c(N(C)C(C)=O)c1I -4.301

-7786-34-7 O=P(OC)(OC)OC(/C)=C/C(=O)OC -0.477

+31868-18-5 Clc1ccccc1[C@@]34OC[C@@H](C)N4CC(=O)Nc2ccc(Cl)cc23 -3.653

+24219-97-4 CN1C[C@H]3N(CC1)c4ccccc4Cc2ccccc23 -2.966

\*22916-47-8 Clc1ccc(c(Cl)c1)[C@H](OCc2ccc(Cl)cc2Cl)Cn3ccnc3 -2.740

-59467-70-8 Fc4ccccc4C2=NCc1cnc(C)n1c3ccc(Cl)cc23 -2.332

-78415-72-2 N#CC1=CC(=C(C)NC1=O)c2ccncc2 -1.959

-2385-85-5 ClC53C1(Cl)C4(Cl)C2(Cl)C1(Cl)C(Cl)(Cl)C5(Cl)C2(Cl)C3(Cl)C4(Cl)Cl -2.371

+50924-49-7 NC(=O)c1ncn(c1O)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -3.454

-99-09-2 O=[N+]([O-])c1cccc(N)c1 -2.728

+554-84-7 O=[N+]([O-])c1cccc(O)c1 -2.516

\*2210-63-1 O=C2NN(c1ccccc1)C(=O)[C@H]2CCCC -3.243

-6536-18-1 CC4=C(CN2CCO[C@H](c1ccccc1)[C@@H]2C)C(=O)N(c3ccccc3)N4C -2.398

-57-27-2 Oc5ccc1C[C@H]2N(C)CC[C@@]34c1c5O[C@H]4[C@@H](O)C=C[C@@H]23 -2.525

\*110-91-8 C1CNCCO1 -3.161

#108-45-2 Nc1cccc(N)c1 -2.447

+55294-15-0 O=C1CC(N)=NN1[C@H](C)c2ccc(Cl)c(Cl)c2 -3.193

+127-19-5 CN(C)C(C)=O -3.633

-42924-53-8 CC(=O)CCc1ccc2cc(ccc2c1)OC -3.589

+42200-33-9 CC(C)(C)NC[C@@H](O)COc2cccc1C[C@@H](O)[C@@H](O)Cc12 -3.724

+91-20-3 c1cccc2ccccc12 -2.690

+15299-99-7 CCN(CC)C(=O)C(C)Oc2cccc1ccccc12 -3.699

-132-66-1 O=C(O)c1ccccc1C(=O)Nc3cccc2ccccc23 -3.914

+128-53-0 O=C1C=CC(=O)N1CC -1.398

+27848-84-6 Brc1cc(cnc1)C(=O)OC[C@@H]3C[C@]4(OC)c5cccc2c5c(cn2C)C[C@H]4N(C)C3 -3.077

-54-11-5 CN2CCC[C@H]2c1cnccc1 -1.699

+59-67-6 O=C(O)c1cccnc1 -3.845

+555-84-0 O=[N+]([O-])c2ccc(/C=N/N1CCNC1=O)o2 -3.226

-23256-30-6 O=S2(=O)C[C@H](C)N(/N=C/c1ccc(o1)[N+]([O-])=O)CC2 -3.607

-75530-68-6 CC=1NC(C#N)=C(C(C=1C(=O)OC(C)C)c2cccc(c2)[N+]([O-])=O)C(=O)OC -3.193

\*2011-67-8 [O-][N+](=O)c1ccc2c(c1)C(=NCC(=O)N2C)c3ccccc3 -2.987

#66085-59-4 CC=1NC(C)=C(C(C=1C(=O)OC(C)C)c2cccc(c2)[N+]([O-])=O)C(=O)OCCOC -3.437

-63675-72-9 CC=1NC(C)=C(C(C=1C(=O)OCC(C)C)c2ccccc2[N+]([O-])=O)C(=O)OC -3.099

+98-95-3 [O-][N+](=O)c1ccccc1 -2.543

-79-24-3 [O-][N+](=O)CC -3.041

-75-52-5 [O-][N+](C)=O -2.973

-76963-41-2 CN(C)Cc1nc(CSCCNC(=C\[N+]([O-])=O)\NC)cs1 -3.218

-62-75-9 CN(C)N=O -1.568

+59-89-2 O=NN1CCOCC1 -2.450

-24526-64-5 Nc3cccc1c3CN(C)C[C@@H]1c2ccccc2 -2.427

+27314-13-2 FC(F)(F)c1cc(ccc1)N2N=CC(NC)=C(Cl)C2=O -3.903

\*6533-00-2 O=C4CC[C@H]3C(CC[C@@H]2[C@H]3CC[C@]1(CC)[C@H]2CC[C@@]1(O)C#C)=C4 -3.700

+941-69-5 O=C2C=CC(=O)N2c1ccccc1 -1.763

-120-34-3 Nc1ccc(cc1)S(=O)(=O)NC(=O)c2ccc(C)c(C)c2 -3.447

+1843-05-6 O=C(c1ccc(cc1O)OCCCCCCCC)c2ccccc2 -4.000

#95-50-1 Clc1ccccc1Cl -2.699

+88-74-4 O=[N+]([O-])c1ccccc1N -3.204

#90-43-7 Oc2ccccc2c1ccccc1 -3.301

\*16773-42-5 Cc1ncc([N+]([O-])=O)n1C[C@H](O)CCl -3.250

+70667-26-4 O[C@@H]1CC(=O)[C@H](CC(=O)CCCCC(=O)OC)[C@H]1/C=C/[C@@H](O)C[C@@H](C)CCCC -1.643

-529-19-1 N#Cc1ccccc1C -3.505

#19666-30-9 O=C2OC(=NN2c1cc(OC(C)C)c(Cl)cc1Cl)C(C)(C)C -3.544

-21738-42-1 [O-][N+](=O)c1cc2N[C@H](CCc2cc1CO)CNC(C)C -1.477

\*23135-22-0 O=C(C(=N\OC(=O)NC)\SC)N(C)C -0.398

-126-93-2 O=C(N)[C@@]1(CC)O[C@H]1CCC -3.097

+53-39-4 O=C2C[C@H]3CC[C@H]1[C@@H]4CC[C@](C)(O)[C@]4(C)CC[C@@H]1[C@@]3(C)CO2 -4.000

+21256-18-8 OC(=O)CCc1nc(c(o1)c2ccccc2)c3ccccc3 -3.650

-60607-34-3 O=C5Nc1ccccc1N5CCCN2CCN(CC2)C(c3ccccc3)c4ccccc4 -3.149

+604-75-1 Clc1ccc2NC(=O)[C@H](O)N=C(c2c1)c3ccccc3 -3.903

+24143-17-7 Clc1ccc2NC(=O)CN3C[C@@H](C)O[C@]3(c2c1)c4ccccc4 -3.602

\*468-61-1 CCC(CC)(C(=O)OCCOCCN(CC)CC)c1ccccc1 -2.262

-33765-68-3 CC[C@H]3C[C@H]2[C@@H]4CCC1=CC(=O)CC[C@@H]1[C@H]4CC[C@]2(C)[C@H]3O -4.083

\*959-14-8 CCN(CC)CCc1nc(no1)c2ccccc2 -3.301

+131-57-7 O=C(c1ccc(cc1O)OC)c2ccccc2 -3.869

-2277-92-1 Clc2c(C(=O)Nc1cc(Cl)cc(Cl)c1O)c(O)c(Cl)cc2Cl -3.000

-153-87-7 COc3cc4nc(C)c(CCN1CCN(CC1)c2ccccc2)c4cc3OC -3.000

#129-20-4 Oc1ccc(cc1)N3C(=O)[C@@H](CCCC)C(=O)N3c2ccccc2 -2.517

+2439-01-2 Cc1ccc2nc3SC(=O)Sc3nc2c1 -3.041

-123-30-8 Nc1ccc(O)cc1 -2.574

-123-63-7 CC1OC(C)OC(C)O1 -3.185

-14255-87-9 O=C(OC)Nc1nc2ccc(cc2n1)CCCC -1.602

-7542-37-2 N[C@@H]4[C@@H](O)[C@H](O)[C@@H](CO)O[C@@H]4O[C@@H]3[C@@H](N)C[C@H](N)[C@H](O)[C@H]3O[C@H]2O[C@H](CO)[C@@H](O[C@H]1O[C@@H](CN)[C@@H](O)[C@H](O)[C@H]1N)[C@H]2O -4.335

+2152-34-3 NC1=NC(=O)[C@@H](O1)c2ccccc2 -2.639

+40487-42-1 [O-][N+](=O)c1c(C)c(C)cc([N+]([O-])=O)c1NC(CC)CC -3.021

+87-86-5 Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl -1.431

-115-77-5 OCC(CO)(CO)CO -4.290

+109-66-0 CCCCC -2.602

\*96513-83-6 CC(C)N(CC[C@@](CC(C)C)(c1ccccn1)C(N)=O)C(C)C -3.041

-76-74-4 O=C1NC(=O)NC(=O)C1(CC)C(C)CCC -2.097

+84-97-9 CN1CCN(CC1)CCCN2c4ccccc4Sc3ccccc23 -2.699

+37924-13-3 O=S(=O)(c1ccccc1)c2cc(C)c(NS(=O)(=O)C(F)(F)F)cc2 -2.801

+52645-53-1 Cl/C(Cl)=C/[C@H]3[C@@H](C(=O)OCc2cccc(Oc1ccccc1)c2)C3(C)C -2.583

+58-39-9 OCCN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 -2.502

-371-40-4 Fc1ccc(N)cc1 -2.620

-3735-90-8 CCN(CC)CCSC(=O)N(c1ccccc1)c2ccccc2 -2.568

-60-12-8 OCCc1ccccc1 -3.253

+108-95-2 Oc1ccccc1 -2.501

+26002-80-2 C/C(C)=C/[C@@H]3[C@H](C(=O)OCc2cccc(Oc1ccccc1)c2)C3(C)C -4.000

-59-96-1 C[C@H](COc1ccccc1)N(Cc2ccccc2)CCCl -3.398

#673-31-4 NC(=O)OCCCc1ccccc1 -3.045

+435-97-2 OC=1c3ccccc3OC(=O)C=1[C@H](CC)c2ccccc2 -2.301

\*101-84-8 c1ccccc1Oc2ccccc2 -3.389

\*122-78-1 O=CCc1ccccc1 -3.190

+103-82-2 OC(=O)Cc1ccccc1 -3.352

+50-33-9 O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2 -2.389

-100-63-0 NNc1ccccc1 -2.274

#92-12-6 CN(C)CCOc2ccccc2Cc1ccccc1 -3.146

+64-10-8 O=C(N)Nc1ccccc1 -3.301

#553-69-5 O[C@H](CNc1ccccn1)c2ccccc2 -2.879

+2310-17-0 CCOP(=S)(OCC)SCN1c2ccc(Cl)cc2OC1=O -1.929

-732-11-6 COP(=S)(OC)SCN2C(=O)c1ccccc1C2=O -1.966

-13171-21-6 O=P(OC)(OC)OC(\C)=C(/Cl)C(=O)N(CC)CC -0.903

+57-47-6 CNC(=O)Oc1cc2c(cc1)N(C)[C@H]3N(C)CC[C@]23C -0.653

-21755-66-8 C(CN1CCCCC1)N(Cc2ccccn2)c3ccccc3 -2.906

+32828-81-2 O=C(NCc1cccnc1)c3cc(C(=O)NCc2cccnc2)c(OC)cc3 -3.477

-75-97-8 CC(C)(C)C(C)=O -2.785

-52463-83-9 Clc1ccc2c(c1)C(=NCC(=O)N2CC#C)c3ccccc3 -3.765

-13523-86-9 CC(C)NCC(O)COc2cccc1nccc12 -2.420

-84-04-8 NC(=O)C1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 -2.792

+1893-33-0 Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)(C(N)=O)N3CCCCC3 -2.204

+3819-00-9 CC(=O)c2cc3N(CCCN1CCC(CCO)CC1)c4ccccc4Sc3cc2 -2.591

#110-85-0 C1CNCCN1 -3.279

#110-89-4 C1CCCCN1 -2.602

#94-62-2 O=C(/C=C/C=C/c1ccc2OCOc2c1)N3CCCCC3 -2.711

\*120-57-0 O=Cc1ccc2OCOc2c1 -3.431

-54-91-1 O=C(CCBr)N1CCN(CC1)C(=O)CCBr -2.342

+467-60-7 OC(c1ccccc1)(c2ccccc2)[C@@H]3CCCCN3 -2.255

#17243-64-0 O=C(OCC)/C=C2/S[C@H](N1CCCCC1)C(=O)N2CC -3.513

+55837-27-9 O=C(O)c2cc(c(Oc1ccccc1)c(c2)N3CCCC3)S(N)(=O)=O -3.748

+302-41-0 N#CC(CCN1CCC(CC1)(C(N)=O)N2CCCCC2)(c3ccccc3)c4ccccc4 -2.505

\*72732-56-0 COc3cc(Cc1cnc2nc(N)nc(N)c2c1C)c(OC)cc3 -3.067

#36322-90-4 OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 -2.334

-31793-07-4 O=C(O)[C@@H](C)c1cc(Cl)c(cc1)N2CC=CC2 -2.545

-33817-20-8 CC(C)(C)C(=O)OCOC(=O)[C@@H]2N3C(=O)[C@H](NC(=O)[C@H](N)c1ccccc1)[C@H]3SC2(C)C -3.778

+63394-05-8 Clc1ccc(cc1)OC(C)(C)C(=O)NC(=O)NCN2CCOCC2 -3.602

+64218-02-6 OC\C=C(/C)CC\C=C(/CC\C=C(/C)CC\C=C(/C)C)CO -4.037

#100-01-6 O=[N+]([O-])c1ccc(N)cc1 -2.875

+100-02-7 O=[N+]([O-])c1ccc(O)cc1 -2.305

-801-52-5 NC(=O)OC[C@@H]3C=1C(=O)C(N)=C(C)C(=O)C=1N2C[C@@H]4N(C)[C@@H]4[C@]23OC -1.833

+156-43-4 CCOc1ccc(N)cc1 -2.732

-106-50-3 Nc1ccc(N)cc1 -1.903

+52549-17-4 O=C(O)[C@@H](C)c1cc2Cc3cccnc3Oc2cc1 -1.775

-55268-74-1 O=C1CN(C[C@@H]2c3ccccc3CCN12)C(=O)C4CCCCC4 -3.453

+23288-49-5 CC(C)(C)c2cc(SC(C)(C)Sc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C)cc(c2O)C(C)(C)C -3.699

+67747-09-5 O=C(N(CCOc1c(Cl)cc(Cl)cc1Cl)CCC)n2ccnc2 -3.204

-58-38-8 CN1CCN(CC1)CCCN2c4ccccc4Sc3ccc(Cl)cc23 -3.255

+23249-97-0 O=C(O)CCc1nc2ccccc2n1 -3.230

+32809-16-8 Clc1cc(cc(Cl)c1)N2C(=O)[C@]3(C)C[C@@]3(C)C2=O -3.845

+26399-36-0 CCCN(CC1CC1)c2c(cc(cc2[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O -3.257

-62666-20-0 Clc1ccc(cc1)/C(=N\CCCC(N)=O)c2cc(F)ccc2O -3.130

+1918-16-7 CC(C)N(C(=O)CCl)c1ccccc1 -2.851

\*123-38-6 CCC=O -3.149

+107-12-0 CCC#N -1.591

#2078-54-8 CC(C)c1cccc(C(C)C)c1O -2.699

-525-66-6 CC(C)NC[C@@H](O)COc2cccc1ccccc12 -2.820

\*121-79-9 Oc1cc(cc(O)c1O)C(=O)OCCC -3.322

\*107-10-8 CCCN -2.568

+101-40-6 C[C@H](NC)CC1CCCCC1 -1.919

\*22760-18-5 CC(C)N2c1cc(C)ccc1C(=NC2=O)c3ccccc3 -2.880

+466-06-8 O=C1C=CC(=CO1)[C@@H]6CC[C@@]5(O)[C@]6(C)CC[C@H]3[C@@H]5CCC2=C[C@H](CC[C@@]23C)O[C@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O -1.748

\*438-60-8 CNCCCC2c3ccccc3C=Cc1ccccc12 -2.380

+603-00-9 C[C@@H](O)Cn2cnc1c2C(=O)N(C)C(=O)N1C -2.663

+24691-76-7 CC=2OCCCC=2C(=O)Nc1ccccc1 -4.176

+15686-83-6 CN2CCCN=C2/C=C/c1cccs1 -2.230

-13457-18-6 O=C(OCC)c1cn2nc(cc2nc1C)OP(=S)(OCC)OCC -2.338

-129-00-0 c1ccc2ccc3cccc4ccc1c2c34 -3.431

+110-86-1 c1ccccn1 -2.950

-58-14-0 CCc1nc(N)nc(N)c1c2ccc(Cl)cc2 -2.643

-77-04-3 CCC1(CC)C(=O)C=CNC1=O -2.892

\*123-75-1 C1CCCN1 -2.477

+1018-71-9 Clc2cncc2c1cccc(Cl)c1[N+]([O-])=O -3.301

-36735-22-5 Fc3ccccc3C2=NCC(=S)N(CC(F)(F)F)c1ccc(Cl)cc12 -3.699

+91-63-4 Cc1ccc2ccccc2n1 -3.090

-81-64-1 O=C2c1ccccc1C(=O)c3c2c(O)ccc3O -3.699

\*91-22-5 c1cccc2cccnc12 -2.520

+100-76-5 C1CN2CCC1CC2 -1.910

-58994-96-0 O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CNC(=O)N(CCCl)N=O)O[C@@H]1OC -1.667

#66357-35-5 [O-][N+](=O)\C=C(/NC)NCCSCc1ccc(CN(C)C)o1 -3.699

-73573-42-9 Oc1ccc(cc1OC)/C=C/C(=O)O[C@@H]3C[C@@H]4CN5CCc2c6ccc(OC)cc6nc2[C@H]5C[C@H]4[C@H](C(=O)OC)[C@H]3OC -4.176

-36791-04-5 NC(=O)c1ncn(n1)[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -3.431

+25546-65-0 N[C@@H]3[C@@H](O)[C@H](O)[C@@H](CN)O[C@@H]3O[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O)[C@H]2O[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O -4.000

+106266-06-2 CC=5N=C1CCCCN1C(=O)C=5CCN2CCC(CC2)c4noc3cc(F)ccc34 -1.753

\*83-79-4 C=C(C)[C@@H]2Oc3ccc1C(=O)[C@H]4c5cc(OC)c(OC)cc5OC[C@H]4Oc1c3C2 -1.778

-94-59-7 C=CCc1ccc2OCOc2c1 -3.290

\*90-02-8 O=Cc1ccccc1O -2.716

\*89-73-6 O=C(NO)c1ccccc1O -3.699

+69-72-7 OC(=O)c1ccccc1O -2.950

+92-61-5 COc1cc2C=CC(=O)Oc2cc1O -3.580

-28523-86-6 FC(F)(F)C(OCF)C(F)(F)F -4.033

-69353-22-6 Cc1cc2O[C@@]4(C)CC[C@@]5(C)[C@@H](C)CCC[C@@]53CO[C@@H](c2c(O)c1)[C@@H]34 -3.000

#93-72-1 Clc1cc(OC(C)C(=O)O)c(Cl)cc1Cl -2.813

+154-82-5 O=C(COc1ccc(CCC)cc1OC)N2CCN(CC2)C(=O)COc3ccc(CCC)cc3OC -3.011

#79902-63-9 CC(C)(CC)C(=O)O[C@H]3C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@H]23 -3.647

+90-39-1 C3CCCN4C[C@H]2C[C@H](CN1CCCC[C@@H]12)[C@H]34 -2.982

-52-01-7 CC(=O)S[C@@H]4CC1=CC(=O)CC[C@]1(C)[C@H]5CC[C@@]3(C)[C@@H](CC[C@]23CCC(=O)O2)[C@H]45 -3.000

+57-24-9 O=C2C[C@H]7OCC=C6CN4CC[C@@]53c1ccccc1N2[C@@H]3[C@H]7[C@H]6C[C@@H]45 -0.371

-100-42-5 C=Cc1ccccc1 -3.423

+58095-31-1 NC(=O)N[C@@H]2CCC(=O)c1sccc12 -3.699

+95-06-7 C=C(Cl)CSC(=S)N(CC)CC -2.929

+723-46-6 Cc2cc(NS(=O)(=O)c1ccc(N)cc1)no2 -3.792

+80-35-3 O=S(=O)(Nc1ccc(OC)nn1)c2ccc(N)cc2 -3.438

+63-74-1 Nc1ccc(cc1)S(=O)(N)=O -3.591

-121-57-3 Nc1ccc(cc1)S(O)(=O)=O -4.090

+144-83-2 O=S(=O)(Nc1ccccn1)c2ccc(N)cc2 -4.199

-59-40-5 Nc1ccc(cc1)S(=O)(=O)Nc2cnc3ccccc3n2 -3.137

-599-79-1 O=S(=O)(Nc1ccccn1)c3ccc(/N=N/c2cc(C(=O)O)c(O)cc2)cc3 -4.193

-515-49-1 Nc1ccc(cc1)S(=O)(=O)NC(N)=S -3.477

+57-96-5 O=C4C(CCS(=O)c1ccccc1)C(=O)N(c2ccccc2)N4c3ccccc3 -2.554

+38194-50-2 CS(=O)c1ccc(cc1)/C=C3/c2ccc(F)cc2C(CC(=O)O)=C3C -2.422

+73384-60-8 CS(=O)c3ccc(c1nc2cccnc2n1)c(OC)c3 -2.498

+54767-75-8 CC(C)Sc1ccc(cc1)[C@H](O)[C@H](C)NCCCCCCCC -3.241

+40828-46-4 O=C(c1ccc(cc1)[C@H](C)C(=O)O)c2cccs2 -1.849

+27470-51-5 O=C(O)CCC(=O)OCC2(CCCC)C(=O)N(c1ccccc1)N(C2=O)c3ccccc3 -3.230

\*87-90-1 ClN1C(=O)N(Cl)C(=O)N(Cl)C1=O -2.609

#321-64-2 Nc1c3ccccc3nc2CCCCc12 -1.845

\*82989-25-1 O=C(OCCCC)C(=O)Nc1cccc(c1)c2nnnn2 -3.602

-59804-37-4 OC=2c1sccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3 -1.898

+5902-51-2 O=C1NC(C)=C(Cl)C(=O)N1C(C)(C)C -3.230

-37686-84-3 CCN(CC)C(=O)N[C@H]1C[C@@H]2c3cccc4ncc(C[C@@H]2N(C)C1)c34 -2.000

+60-54-8 NC(=O)C1=C(O)[C@@H](N(C)C)[C@@H]2C[C@H]4C(=C(O)[C@]2(O)C1=O)C(=O)c3c(O)cccc3[C@@]4(C)O -2.907

#116-29-0 Clc1cc(c(Cl)cc1Cl)S(=O)(=O)c2ccc(Cl)cc2 -2.753

#109-99-9 C1CCCO1 -3.217

+632-22-4 CN(C)C(=O)N(C)C -2.900

\*50-35-1 O=C1NC(=O)CCC1N3C(=O)c2ccccc2C3=O -2.053

-115-37-7 COC1=CC=C3[C@H]2Cc4ccc(OC)c5O[C@@H]1[C@]3(CCN2C)c45 -2.057

#83-67-0 Cn1cnc2c1C(=O)NC(=O)N2C -3.102

-54504-70-0 Clc1ccc(cc1)OC(C)(C)C(=O)OCCn3cnc2c3C(=O)N(C)C(=O)N2C -4.230

+58-55-9 O=C2c1ncnc1N(C)C(=O)N2C -2.352

+148-79-8 n1c3ccccc3nc1c2cscn2 -3.318

-59669-26-0 CN(SN(C)C(=O)O\N=C(\C)SC)C(=O)O\N=C(\C)SC -1.820

-110-02-1 c1cccs1 -3.146

+108-98-5 Sc1ccccc1 -1.665

-50-52-2 CN4CCCCC4CCN1c3ccccc3Sc2ccc(SC)cc12 -2.998

-5591-45-7 CN(C)S(=O)(=O)c2cc3C(=C\CCN1CCN(C)CC1)\c4ccccc4Sc3cc2 -2.857

-62-56-6 NC(N)=S -2.097

+137-26-8 CN(C)C(=S)SSC(=S)N(C)C -2.748

\*655-05-0 CN(C)C1=NC(=O)[C@@H](O1)c2ccccc2 -3.477

+89-83-8 CC(C)c1ccc(C)cc1O -2.991

-32527-55-2 OCCN1CCN(CC1)C(=O)CN2c3cc(Cl)ccc3SC2=O -3.556

\*57648-21-2 Fc1ccc(cc1)C(=O)CCCN2CCC(CC2)N3c4ccccc4NC3=S -2.365

#444-27-9 O=C(O)C1CSCN1 -2.942

-65899-73-2 Clc3sccc3CO[C@H](Cn1ccnc1)c2ccc(Cl)cc2Cl -2.886

+2205-73-4 CC(=O)S[C@@H]3CC1=CC(=O)C[C@H](SC(C)=O)[C@]1(C)[C@H]4CC[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@H]34 -4.000

+4991-65-5 Oc1cc2OC(=O)Sc2cc1 -2.801

+55837-29-1 CCCN(CCC)C(=O)[C@@H](NC(=O)c1ccccc1)Cc2ccc(OCCN(CC)CC)cc2 -2.903

+14679-73-3 O=C(OCC)NNc2nncc1ccccc12 -2.502

+22345-47-7 COc1ccc(cc1OC)C3=NN=C(C)[C@@H](CC)c2cc(OC)c(cc23)OC -2.916

+1156-19-0 Cc1ccc(cc1)S(=O)(=O)NC(=O)NN2CCCCCC2 -3.699

-64-77-7 Cc1ccc(cc1)S(=O)(=O)NC(=O)NCCCC -3.396

-50838-36-3 Cc1cc(ccc1)N(C)C(=S)Oc2ccc4c(c2)[C@@H]3CC[C@@H]4C3 -3.255

#29218-27-7 OC[C@@H]2CN(c1cccc(C)c1)C(=O)O2 -3.088

#728-88-1 C[C@H](CN1CCCCC1)C(=O)c2ccc(C)cc2 -3.161

+108-88-3 Cc1ccccc1 -2.803

+89778-26-7 CN(C)CCOc1ccc(cc1)\C(c2ccccc2)=C(/CCCl)c3ccccc3 -3.230

+27203-92-5 O[C@@]1(CCCC[C@@H]1CN(C)C)c2cc(OC)ccc2 -2.358

+53902-12-8 COc1cc(ccc1OC)/C=C/C(=O)Nc2ccccc2C(=O)O -3.041

-15421-84-8 CCN(CC)c1cc(C)nc2ncnn12 -2.371

-19794-93-5 Clc1cccc(c1)N2CCN(CC2)CCCN3N=C4C=CC=CN4C3=O -2.839

#24017-47-8 CCOP(=S)(OCC)Oc1ncn(n1)c2ccccc2 -1.756

+10310-32-4 O[C@H]2[C@@H](OCc1ccccc1)[C@H](O[C@H]2OCC)[C@H](COCc3ccccc3)OCc4ccccc4 -4.301

-87-10-5 Oc1c(cc(Br)cc1Br)C(=O)Nc2ccc(Br)cc2 -2.613

#133-67-5 NS(=O)(=O)c2cc1c(N[C@H](NS1(=O)=O)C(Cl)Cl)cc2Cl -3.748

-101-20-2 Clc2ccc(NC(=O)Nc1ccc(Cl)cc1)cc2Cl -4.539

-112-24-3 NCCNCCNCCN -3.398

#121-44-8 CCN(CC)CC -2.663

+280-57-9 C1CN2CCN1CC2 -3.230

+51-18-3 n1c(nc(nc1N2CC2)N3CC3)N4CC4 -1.114

+1420-06-0 c1ccccc1C(N2CCOCC2)(c3ccccc3)c4ccccc4 -1.919

-749-13-3 FC(F)(F)c1cccc(c1)C3(O)CCN(CCCC(=O)c2ccc(F)cc2)CC3 -2.146

+146-54-3 FC(F)(F)c1cc2N(CCCN(C)C)c3ccccc3Sc2cc1 -2.267

#1582-09-8 [O-][N+](=O)c1cc(cc([N+]([O-])=O)c1N(CCC)CCC)C(F)(F)F -3.286

+322-79-2 O=C(C)Oc1cc(ccc1C(=O)O)C(F)(F)F -2.604

-13647-35-3 N#C[C@@H]2C[C@]4(C)C5CC[C@@]1(C)C(CC[C@@H]1O)C5CC[C@]43O[C@@H]3C2=O -4.176

+84-96-8 CN(C)CC(C)CN1c3ccccc3Sc2ccccc12 -2.322

+738-70-5 Nc2nc(N)ncc2Cc1cc(OC)c(OC)c(OC)c1 -3.724

+635-41-6 O=C(c1cc(OC)c(OC)c(OC)c1)N2CCOCC2 -3.255

+69900-72-7 O[C@H](/C=C\[C@@H]1[C@H](C\C=C\CCCC(=O)O)C(=O)C[C@@H]1C)C(C)(C)CCCC -1.342

#73803-48-2 NS(=O)(=O)c1cc(ccc1Cl)C(=O)NN3C[C@@H]4[C@@H]2CC[C@H](C2)[C@@H]4C3 -3.903

-14504-73-5 COc1c5OCOc5cc2CCN(C)[C@@H](c12)[C@H]4OC(=O)c3c(N)c(OCC)c(OCC)c(OCC)c34 -4.176

-22089-22-1 O=P1(OCCCN1CCCl)N(CCCl)CCCl -2.305

+69-33-0 Nc3ncnc1c3ccn1[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O -1.204

-4171-13-5 CC[C@@H](C(N)=O)[C@H](C)CC -2.881

+52-53-9 COc1cc(ccc1OC)[C@@](C#N)(CCCN(C)CCc2ccc(OC)c(OC)c2)C(C)C -2.212

\*1929-77-7 O=C(SCCC)N(CCC)CCC -3.079

+81840-15-5 O=C(c1ccc(OC)c(OC)c1)N2CCN(CC2)c3cc4CCC(=O)Nc4cc3 -3.880

#46817-91-8 CCOc2ccccc2OC[C@@H]1CNCCO1 -3.301

\*50471-44-8 O=C1N(C(=O)O[C@@]1(C)C=C)c2cc(Cl)cc(Cl)c2 -4.000

-81-81-2 CC(=O)CC(C1=C(O)c2ccccc2OC1=O)c3ccccc3 -0.204

#14293-44-8 O=S(N)(=O)c1cc(c(O)cc1Cl)C(=O)Nc2c(C)cccc2C -3.215

+7361-61-7 Cc2cccc(C)c2NC1=NCCCS1 -2.114

-56775-88-3 Brc1ccc(cc1)C(=C\CN(C)C)/c2cccnc2 -2.954

-1222-57-7 CS(=O)(=O)c1ccc(cc1)c2cn3ccccc3n2 -3.569

-43200-80-2 CN1CCN(CC1)C(=O)O[C@H]4c2nccnc2C(=O)N4c3ccc(Cl)cn3 -2.918

+26615-21-4 CN(C)CCOC1=Cc3ccccc3Sc2ccc(Cl)cc12 -2.486

**Table S5**

**The numerical data on ACE-inhibitory potency of peptides (pIC50). Split 1**

+1. AAP 4.520

+2. AFL 4.190

+3. AGS 3.280

+4. AIP 3.460

+5. AKK 5.500

+6. AVF 2.670

#7. AVP 3.470

+8. DFG 4.350

+9. DLP 5.320

+10. FAP 5.420

+11. FGK 3.800

+12. FNQ 3.470

+13. FQP 4.920

+14. FWN 4.740

+15. GHG 3.910

+16. GKP 3.450

+17. GPA 3.390

\*18. GPM 4.770

+19. GRP 4.700

+20. GVW 3.620

#21. IEY 3.740

+22. IFL 4.350

+23. ILP 3.570

#24. IPA 3.850

+25. IQP 5.420

\*26. IRA 5.190

+27. IRP 5.740

+28. IYP 4.210

\*29. KLP 3.300

+30. LAY 5.410

#31. LKY 5.000

+32. LKY 6.110

+33. LLP 4.240

+34. LNP 4.370

+35. LQP 5.980

+36. LQQ 4.000

+37. LRP 6.680

+38. LSP 5.770

+39. LVY 5.740

+40. MAW 4.790

+41. MYY 5.020

+42. PAP 4.060

+43. PYP 3.660

+44. RFH 3.480

+45. RIY 4.550

+46. RVY 3.690

+47. SHP 3.550

+48. TAP 5.460

+49. TVY 4.820

+50. VAP 5.700

+51. VAV 3.590

+52. VIY 5.350

+53. VKK 2.980

#54. VLP 3.490

+55. VMP 4.540

\*56. VRK 3.150

+57. VRP 5.660

+58. VSP 5.000

+59. VWY 5.030

\*60. VYP 4.360

+61. YVP 3.700

+62. AGP 3.250

+63. ASP 3.620

#64. AVV 4.180

+65. FGG 4.080

+66. GHF 2.960

+67. GPL 5.580

#68. GTW 3.330

+69. IKP 5.600

+70. IPP 5.300

+71. IVY 4.830

+72. LAA 4.890

+73. LLF 4.100

+74. LPP 5.020

+75. LSA 5.110

+76. MRW 6.220

+77. PLP 3.370

+78. RPR 3.420

\*79. VAA 4.890

\*80. VAY 4.800

+81. VKP 5.430

+82. VPP 5.050

#83. VVY 4.660

+84. ALPH 2.740

\*85. ACHP 3.440

+86. AGSS 3.170

+87. AHHP 3.070

#88. AIPP 3.050

#89. AIYK 3.670

#90. ALPM 3.030

\*91. ALPP 3.550

+92. FVAP 5.000

+93. FYQQ 4.600

#94. GLYP 3.720

+95. GRPR 3.330

+96. GVYP 3.850

+97. HHTF 4.080

#98. IAIP 3.330

#99. IRPV 4.510

+100. KFYG 4.040

#101. KTAP 4.430

+102. LIYP 5.000

+103. LNPA 3.510

#104. LPHF 3.170

+105. LPLP 3.140

+106. LQKW 4.460

+107. LVRT 2.610

+108. LVYP 3.770

+109. PAQK 4.000

#110. QPIP 3.070

+111. RHQG 3.480

+112. RPVQ 3.520

+113. SPYP 3.070

+114. SQPK 3.450

+115. SVAK 3.000

\*116. VLRP 6.050

+117. VPAF 3.240

#118. VVRP 4.090

+119. VYAP 5.210

+120. WHHT 3.960

+121. YGGY 5.470

+122. YLLF 3.760

\*123. YPHK 3.000

+124. YPRY 4.760

+125. YNKL 4.680

#126. YRPY 3.490

+127. AGSP 4.430

+128. AHSY 4.940

+129. FCVL 4.700

+130. GDAP 4.650

+131. GWAP 5.410

+132. IYPR 5.000

+133. LHLP 3.680

+134. LPHA 3.250

+135. LSPA 3.500

\*136. NILP 3.250

+137. SLPQ 3.480

+138. VIIF 5.060

+139. VWIS 4.520

+140. YKYY 4.190

+141. ALPHA 4.100

\*142. AVPYP 4.100

#143. AVVRP 4.130

+144. GRVMP 3.600

+145. GVHHA 4.140

#146. HLPLP 4.390

+147. HPIKH 2.900

\*148. IAIPP 3.220

+149. IRAQQ 3.800

+150. IRPVQ 5.850

\*151. IWHHT 5.290

+152. KAPVA 4.330

+153. KDYRL 4.580

+154. LALPP 3.100

+155. LKPNM 4.770

+156. MLPAY 5.800

+157. MRWRD 5.680

+158. NLHLP 3.380

\*159. PQPIP 3.470

+160. PSFQP 4.140

#161. PTPAP 4.480

+162. PTPVP 3.590

#163. QKTAP 4.520

+164. SKVPP 4.130

#165. VAWKL 4.500

+166. VHIPP 5.000

#167. VHLPP 4.740

+168. VLPIP 4.510

+169. VLPYP 4.440

+170. FFVAP 5.220

+171. HPFAQ 3.330

+172. IPAIN 3.360

\*173. IYPRY 5.070

+174. LVQGS 4.360

+175. PLIYP 5.360

#176. PVPQP 3.960

+177. SLVYP 4.400

+178. VLIVP 5.770

\*179. CWLPVY 4.650

+180. DYGLYP 4.210

+181. ENLLRF 4.080

+182. FCVLRP 4.910

+183. GLDIQK 3.240

+184. GVYPHK 5.800

+185. IFVPAF 5.470

+186. IKPLNY 4.370

+187. KPPETV 4.620

+188. LAHKAL 3.210

+189. LAYFYP 4.190

+190. LHLPGP 5.720

+191. LHLPLL 5.460

+192. LHLPLP 5.260

+193. LHLWLP 5.050

#194. LHLYLP 4.720

+195. LRIPVA 6.420

+196. PAVVLP 4.350

#197. PAVVRP 4.740

#198. PPPVHL 3.960

\*199. PQEVLP 3.040

+200. PQNILP 3.360

\*201. PTHIDW 4.890

+202. PTHIKW 5.740

+203. PVRAVP 3.770

+204. PYVRYL 5.620

+205. QLLKLK 3.470

+206. QPLIYP 5.440

+207. RPKHPI 4.390

\*208. TTMPLW 4.920

+209. TTMPLW 4.290

+210. VAGTWY 2.770

+211. VHLPPP 3.700

+212. VLPIPQ 2.280

+213. VLPYPV 3.380

+214. VPQPIP 3.540

+215. VRGPFP 3.230

+216. VTPALR 4.080

+217. VYPFPG 3.660

+218. YALPHA 5.010

+219. YQQPVL 3.550

+220. YSQQQQ 3.070

+221. FALPQY 5.370

+222. HIKWGD 4.300

+223. KFAWPQ 3.750

\*224. LHLPAP 5.220

+225. LHLPYP 5.640

+226. MYPGIA 3.190

+227. PHQIYP 4.520

#228. PTHIAW 6.410

+229. PTHVAW 5.820

+230. QSLVYP 4.390

+231. TGPIPN 3.500

+232. TVDQHQ 3.740

+233. VPFGVG 3.470

+234. WSKVVL 3.810