|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sno | Structure | smiles | BE |  |
| 1 |  | [H]C1=CC=C(NC(C2=CC=CS2)=N3)C3=C1 | -6.0 | Benzimidazoles from Aryl Alkyl Ketones and 2‑Amino Anilines by an  Iodine Catalysed Oxidative C(CO)−C(alkyl) Bond Cleavage  Surendar Reddy Bathula  J. Org. Chem. 2017, 82, 4422−4428 |
| 2 |  | [H]C1=CC=C(NC(C2=CC(OC)=C(OC)C(OC)=C2)=N3)C3=C1 | -7.5 |  |
| 3 |  | CC1=CC=C2C(NC(C3=CC(OC)=C(OC)C=C3)=N2)=C1 | -6.8 |  |
| 4 |  | [H]C(C=C1)=CC=C1C2=NC3=C(N2)C=C([H])C=C3 | -7.4 |  |
| 5 |  | [H]C(C=C1)=CC=C1C2=NC3=C(N2)C=C(C)C=C3 | -7.5 |  |
| 6 |  | [H]C(C=C1)=CC=C1C2=NC3=C(N2)C=C(C(C4=CC=CC=C4)=O)C=C3 | -8.6 |  |
| 7 |  | C/C([H])=C\C1=CN=C(C2=CC=C(C)C=C2)N1 | -6.8 |  |
| 8 |  | CC(C=C1)=CC=C1C2=NC3=C(N2)C=C(Cl)C=C3 | -7.5 |  |
| 9 |  | CC(C=C1)=CC=C1C2=NC3=C(N2)C=C(F)C=C3 | -7.8 |  |
| 10 |  | CC(C=C1)=CC=C1C2=NC3=C(N2)C=C(C(C4=CC=CC=C4)=O)C=C3 | -9.5 |  |
| 11 |  | [H]C1=CC(NC(C2=CC=C(C(C)(C)C)C=C2)=N3)=C3C=C1 | -7.3 |  |
| 12 |  | [H]C1=CC(NC(C2=CC=C(OC)C=C2)=N3)=C3C=C1 | -6.7 |  |
| 13 |  | COC(C=C1)=CC=C1C2=NC3=C(N2)C=C(C(C4=CC=CC=C4)=O)C=C3 | -8.4 |  |
| 14 |  | FC(C=C1)=CC=C1C2=NC3=C(N2)C=C([H])C=C3 | -7.6 |  |
| 15 |  | FC(C=C1)=CC=C1C2=NC3=C(N2)C=C(C)C=C3 | -7.7 |  |
| 16 |  | FC(C=C1)=CC=C1C2=NC3=C(N2)C=C(C(C4=CC=CC=C4)=O)C=C3 | -9.0 |  |
| 17 |  | ClC(C=C1)=CC=C1C2=NC3=C(N2)C=C([H])C=C3 | -7.6 |  |
| 18 |  | ClC(C=C1)=CC=C1C2=NC3=C(N2)C=C([H])C=C3 | -7.6 |  |
| 19 |  | BrC(C=C1)=CC=C1C2=NC3=C(N2)C=C([H])C=C3 | -7.5 |  |
| 20 |  | [H]C1=CC(NC(C2=CC=C([N+]([O-])=O)C=C2)=N3)=C3C=C1 | -8.4 |  |
| 21 |  | ClC1=C(C2=NC(C=CC([H])=C3)=C3N2)C=CC=C1 | -7.4 |  |
| 22 |  | [H]C1=CC2=C(C=C1)N=C(N2)C3=C(OC)C=C(OC)C=C3 | -7.1 |  |
| 23 |  | CC1=CC2=C(C=C1)N=C(N2)C3=C(OC)C=C(OC)C=C3 | -7.3 |  |
| 24 |  | ClC1=C(C2=NC(C=CC([H])=C3)=C3N2)C=CC(Cl)=C1 | -7.1 |  |
| 25 |  | [H]C1=CC2=C(C=C1)N=C(N2)C3=C(OC)C=CC=C3 | -7.5 |  |
| 26 |  | [R]C1=C(C2=NC(C=CC(C(C3=CC=CC=C3)=O)=C4)=C4N2)C=CC=C1 | -8.9 |  |
| 27 |  | [H]C1=CC2=C(C=C1)N=C(N2)C3=CC(C(F)(F)F)=CC=C3 | -8.0 |  |
| 28 |  | [H]C1=CC2=C(C=C1)N=C(N2)C3=CC(Br)=CC=C3 | -7.4 |  |
| 29 |  | CC1=CC2=C(C=C1)N=C(N2)C3=CC([N+]([O-])=O)=CC=C3.[R] | -8.1 |  |
| 30 |  | CC1=CC2=C(C=C1)N=C(N2)C3=CC(OC)=C(OC)C=C3 | -7.3 |  |
| 31 |  | COC1=C(OC)C(OC)=CC(C2=NC(C=CC=C3)=C3N2)=C1 | -7.2 |  |
| 32 |  | O=[S@](CC1=C(C)C(OC)=C(C)C=N1)C2=NC3=CC=C(OC)C=C3N2 | -7.6 | Oxidative Cyclization Approach to Benzimidazole Libraries  Daniel C. Schmitt  ACS Comb. Sci. 2020, 22, 1−5 |
| 33 |  | O=C1CC(C)C(C2=CC=C3C(NC(C4=CC=C(OC)C=C4)=N3)=C2)=NN1 | -8.5 |  |
| 34 |  | COC1=C2C(NC(C3=CC=CC=C3)=N2)=CC=C1 | -7.0 |  |
| 35 |  | FC1=C2C(NC(C3=CC=CC=C3)=N2)=CC=C1 | -7.0 |  |
| 36 |  | C=C(NC(OC(C)C)=O)/C=C(NCCN=C)\C | -5.3 |  |
| 37 |  | [C-]#[N+]C1=CC2=C(NC(C3=CC=CC=C3)=N2)C=C1 | -7.1 |  |
| 38 |  | FC1=C(NC2=CC=C(Br)C=C2F)C(C(NOCCO)=O)=CC3=C1N=CN3 | -7.8 |  |
| 39 |  | FC1=C2C(NC(C3=CC=CC=C3)=N2)=CC(F)=C1F | -7.9 |  |
| 40 |  | O=S(C1=C2C(NC(C3=CC=CC=C3)=N2)=CC=C1)(C)=O | -7.8 |  |
| 41 |  | O=S(C1=CC=C(NC(C2=CC=CC=C2)=N3)C3=C1)(C)=O | -7.8 |  |
| 42 |  | FC1=C(NC(C2=CC=CC=C2)=N3)C3=CC=C1 | -6.9 |  |
| 43 |  | CC1=C(NC(C2=CC=CC=C2)=N3)C3=CC(C)=C1 | -7.6 |  |
| 44 |  | CC1=CC=C2C(NC(C3=CC=CC=C3)=N2)=C1 | -7.0 |  |
| 45 |  | O=C1C=CC=CN1C2=C(NC(C3=CC=CC=C3)=N4)C4=CC=C2 | -8.5 |  |
| 46 |  | COC1=CC(NC(C2=CC=CC=C2)=N3)=C3C=C1 | -7.1 |  |
| 47 |  | CC(OC(N(C)C1=CC(NC(C2=CC=CC=C2)=N3)=C3C=C1)=O)(C)C | -7.4 |  |
| 48 |  | C1(C2=NC=CC=C2)=CC(NC(C3=CC=CC=C3)=N4)=C4C=C1 | -8.4 |  |
| 49 |  | C1(C=N2)=CC3=C(NC(C4=CC=CC=C4)=N3)C=C1N2CC5=CC=CC=C5 | -9.4 |  |
| 50 |  | C12=CC3=C(NC(C4=CC=CC=C4)=N3)C=C1SN=C2 | -7.7 |  |
| 51 |  | CC(N1CCC2=CC3=C(NC(C4=CC=CC=C4)=N3)C=C21)=O | -7.7 |  |
| 52 |  | C12=CN=CC=C1N=C(C3=CC=CC=C3)N2 | -7.3 |  |
| 53 |  | C12=NC=CC=C1N=C(C3=CC=CC=C3)N2 | -7.2 |  |
| 54 |  | C12=CC=CN=C1N=C(C3=CC=CC=C3)N2 | -7.3 |  |
| 55 |  | FC1=C2C(NC(C3=CC=CC=C3)=N2)=CN=C1 | -7.7 |  |
| 56 |  | CC1=CC2=C(NC(C3=CC=CC=C3)=N2)C=N1 | -6.9 |  |
| 57 |  | CC1=NC(NC(C2=CC=CC=C2)=N3)=C3C=C1 | -7.1 |  |
| 58 |  | C12=NC=NC=C1N=C(C3=CC=CC=C3)N2 | -7.1 |  |
| 59 |  | C1(COC2CC2)=NC=C(NC(C3=CC=CC=C3)=N4)C4=C1 | -7.4 |  |
| 60 |  | BrC1=CC=C2N=C3CCC=CC3N2C1 | -6.2 |  |
| 61 |  | C12=CC=CC=C1N=C(C3=CC=CC=C3)N2 | -7.4 | Diversity Oriented Synthesis of  Benzimidazole and Benzoxa/(thia)zole  Libraries through Polymer-Supported  Hypervalent Iodine Reagent  Atul Kumar  *Journal of Combinatorial Chemistry*, *2009 Vol. 11, No. 2* |
| 62 |  | CC1=CC=C(NC(C2=CC=CC=C2)=N3)C3=C1 | -7.0 |  |
| 63 |  | C12=CC=CC=C1NC(C3=CNC4=C3C=CC=C4)=N2 | -8.3 |  |
| 64 |  | FC1=CC=C(NC(C2=CC=CC=C2)=N3)C3=C1 | -6.9 |  |
| 65 |  | FC1=CC=C(NC(C2=CC=CN=C2)=N3)C3=C1 | -6.9 |  |
| 66 |  | CC1=CC=C(NC(C2=CC=CN=C2)=N3)C3=C1 | -7.2 |  |
| 67 |  | C12=CC=CC=C1N=C(C3=CC=CN=C3)N2 | -7.1 |  |
| 68 |  | C12=CC=CC=C1N=C(C3CCCCC3)N2 | -7.5 |  |
| 69 |  | CC1=CC=C(NC(CCCCC)=N2)C2=C1 | -6.2 |  |
| 70 |  | CCCCCC1=NC2=CC=CC=C2N1 | -6.2 |  |
| 71 |  | C12=CC=CC=C1N=C(C3=CC=CC=C3)O2 | -7.4 |  |
| 72 |  | CC1=CC=C(OC(C2=CC=CC=C2)=N3)C3=C1 | -7.4 |  |
| 73 |  | ClC1=CC=C2C(N=C(C3=CC=CC=C3)O2)=C1 | -7.0 |  |
| 74 |  | C12=CC=CC=C1N=C(C3=CC=CN=C3)N2 | -7.1 |  |
| 75 |  | ClC1=CC=CC=C1C2=NC3=CC=CC=C3O2 | -7.1 |  |
| 76 |  | COC1=CC=C(OC(C2=CC=CC=C2)=N3)C3=C1 | -7.0 |  |
| 77 |  | COC1=C(OC)C=C(OC(C2=CC=CC=C2)=N3)C3=C1 | -7.2 |  |
| 78 |  | ClC1=CC=C2C(N=C(C3=CC=CC(N(O)O)=C3)O2)=C1 | -8.1 |  |
| 79 |  | CC1=CC=C2C(N=C(C3=CC=CC=C3Cl)O2)=C1 | -7.0 |  |
| 80 |  | CC1=CC=C(OC(C2=CC=C(N(O)O)C=C2)=N3)C3=C1 | -8.1 |  |
| 81 |  | FC1=CC=C(N=C(C2=CC=CC=C2)O3)C3=C1 | -6.7 |  |
| 82 |  | CCCCCC1=NC2=CC=CC=C2O1 | -6.1 |  |
| 83 |  | C12CCCCC1OC(C3=CC=CC=C3)=N2 | -7.2 |  |
| 84 |  | C12=CC=CC=C1SC(C3=CC=CC=C3)=N2 | -7.1 |  |
| 85 |  | ClC1=CC=C2C(N=C(C3=CC=CC=C3)S2)=C1 | -6.6 |  |
| 86 |  | ClC1=CC=CC=C1C2=NC3=CC=CC=C3S2 | -7.0 |  |
| 87 |  | COC1=CC=C2C(N=C(C3=CC=CC=C3)S2)=C1 | -6.8 |  |
| 88 |  | COC1=C(OC)C=C2C(N=C(C3=CC=CC=C3)S2)=C1 | -7.5 |  |
| 89 |  | PC1=C(C#N)C2=NC3=C(C=CC=C3)N2C(N4CCN([H])CC4)=C1 | -7.3 | Antimalarial Pyrido[1,2-a]benzimidazoles  Kelly Chibale  J. Med. Chem. 2011, 54, 4581–4589 |
| 90 |  | N#CC1=C(C)C=C(N2CCN(CC3=CC=CC=C3)CC2)N4C1=NC5=C4C=CC=C5 | -8.7 |  |
| 91 |  | NCCN(CC)C1=CC(C(F)(F)F)=C(C#N)C2=NC3=C(C=CC=C3)N21 | -6.9 |  |
| 92 |  | CCN(CCN(C)C)C1=CC(C(F)(F)F)=C(C#N)C2=NC3=C(C=CC=C3)N21 | -7.5 |  |
| 93 |  | CCN(CCN(CC)CC)C1=CC(C(F)(F)F)=C(C#N)C2=NC3=C(C=CC=C3)N21 | -8.0 |  |
| 94 |  | CC1=CC=CC=C1C2=NC3=CC=CC=C3N2CC4=C(C)C=CC=C4 | -8.0 | 1,2-Disubstituted Benzimidazoles by the Iron Catalyzed Cross-  Dehydrogenative Coupling of Isomeric o‑Phenylenediamine  Substrates  Frank W. Foss  J. Org. Chem. 2020, 85, 1991−2009 |
| 95 |  | CC1=CC(CN2C(C3=CC(C)=CC=C3)=NC4=CC=CC=C42)=CC=C1 | -9.6 |  |
| 96 |  | CC(C=C1)=CC=C1C2=NC3=CC=CC=C3[N]2.C | -6.0 |  |
| 97 |  | OC(C=CC=C1)=C1CN2C(C3=CC=CC=C3O)=NC4=CC=CC=C42 | -8.2 |  |
| 98 |  | FC(C=C1)=CC=C1CN2C(C3=CC=C(F)C=C3)=NC4=CC=CC=C42 | -8.4 |  |
| 99 |  | CC1=C(C)C=C(N=C(C2=CC=CC=C2)N3CC4=CC=CC=C4)C3=C1 | -7.7 |  |
| 100 |  | FC1=C(F)C=C(N=C(C2=CC=CC=C2)N3CC4=CC=CC=C4)C3=C1 | -8.3 |  |
| 101 |  | C=CC1=CC=C(N=C(C2=CC=CC=C2)N3CC4=CC=CC=C4)C3=C1 | -8.4 |  |
| 102 |  | C12=NC=CC=C1N(CC3=CC=CC=C3)C(C4=CC=CC=C4)=N2 | -7.9 |  |
| 103 |  | C=CCN1C(C=C)=NC2=CC=CC=C21 | -6.8 |  |
| 104 |  | CC1=NC2=CC=CC=C2N1CC | -5.5 |  |
| 105 |  | CCCCN1C(CCC)=NC2=CC=CC=C21 | -5.8 |  |
| 106 |  | C12=CC=CC=C1N(CC3CC3)C(C4CC4)=N2 | -6.3 |  |
| 107 |  | C12=CC=CC=C1N(CC3CCCCC3)C(C4CCCCC4)=N2 | -8.1 |  |
| 108 |  | CN1C(C2=CC=CC=C2)=NC3=CC=CC=C31 | -7.0 |  |
| 109 |  | CCCCN1C(C2=CC=CC=C2)=NC3=CC=CC=C31 | -6.8 |  |
| 110 |  | C/C=C1CN=C(C2=CC=C(C(OC)=O)C=C2)N\1CC3=CC=CC=C3 | -7.3 |  |
| 111 |  | O=C(C(C=C1)=CC=C1CN2C(C3=CC=CC=C3)=NC4=CC=CC=C42)OC | -8.8 |  |
| 112 |  | C=CCCN1C2=CC(C3=NC(C=CC=C4)=C4N3C)=CC(C)=C2N=C1CCC.O=C(C5=CC=CC=C5)O | -5.9 |  |
| 113 |  | FC(C=C1)=CC=C1CN2C3=CC=CC=C3N=C2[N]4=CC=C(NC5=NCC(C=N5)=O)C=C4 | -9.0 |  |
| 114 |  | O=C(N(C)C)CN1C2=CC(C)=CC=C2N=C1C3=CC=C(C)C=C3 | -7.7 |  |
| 115 |  | C12=CC=CC=C1N3C(CCC3)=N2 | -6.3 | Synthesis of N-Heterocyclic Ring Systems Containing  1,2-Fused Benzimidazole Moieties |
| 116 |  | C12=CC=CC=C1N3C(CCCC3)=N2 | -6.6 |  |
| 117 |  | C12=CC=CC=C1N3C(CCCCC3)=N2 | -6.9 |  |
| 118 |  | CN1C(C)=NC2=CC=CC=C21 | -6.5 |  |
| 119 |  |  |  | Synthesis of Bis-benzimidazoles  LILLIANL I-YENW ANGA ND NADELETMN |
| 120 |  | [H]C1=CC([No][No])=CC2=C1NC(CCC3=NC4=CC([N+]([O-])=O)=CC=C4N3)=N2 | -6.0 |  |
| 121 |  | [H]C1=C2C(N=C(C)N2)=CC(Cl)=C1.C=CCl.[H] | -6.6 |  |
| 122 |  | [H]C1=C2C(N=C(CCC3=NC(C=C(OCC)C=C4[H])=C4N3)N2)=CC(OCC)=C1 | -8.7 |  |
| 123 |  | NC1=C2C(N=C(CCC3=NC(C=C(Cl)C=C4N)=C4N3)N2)=CC(Cl)=C1 | -9.3 |  |
| 124 |  | [H]C1=C2C(N=C(CCCCC3=NC=C(C[H])N3)N2)=CC(C)=C1.[CH3] | -6.0 |  |
| 125 |  | [H]C1=C2C(N=C(CCCCC3=NC(C=C([N+]([O-])=O)C=C4[H])=C4N3)N2)=CC([N+]([O-])=O)=C1 | -7.9 |  |
| 126 |  | [H]C1=C2C(N=C(CCCCC3=NC(C=C(Cl)C=C4[H])=C4N3)N2)=CC(Cl)=C1 | -8.9 |  |
| 127 |  | [H]C1=C2C(N=C(CCCCC3=NC(C=C(N)C=C4[H])=C4N3)N2)=CC(N)=C1 | -8.2 |  |
| 128 |  | [H]C1=C2C(N=C(CCCCC3=NC(C=C([NH2 .2HCl])C=C4[H])=C4N3)N2)=CC([NH2][ClH2])=C1 |  |  |
| 129 |  | ClC1=CC([N+]([O-])=O)=C2C(N=C(CCCCC3=NC(C=C(Cl)C=C4[N+]([O-])=O)=C4N3)N2)=C1 | -7.9 |  |
| 130 |  | NC1=C2C(N=C(CCCCC3=NC(C=C(Cl)C=C4N)=C4N3)N2)=CC(Cl)=C1 | -9.0 |  |
| 131 |  | [H]C1=C2C(N=C(CCCCCCC3=NC(C=C(C)C=C4[H])=C4N3)N2)=CC(C)=C1 | -8.8 |  |
| 132 |  | [H]C1=C2C(N=C(CCCCCCC3=NC(C=C([N+]([O-])=O)C=C4[H])=C4N3)N2)=CC([N+]([O-])=O)=C1 | -7.7 |  |
| 133 |  | [H]C1=C2C(N=C(CCCCCCC3=NC(C=C(Cl)C=C4[H])=C4N3)N2)=CC(Cl)=C1 | -8.2 |  |
| 134 |  | ClC1=CC([N+]([O-])=O)=C2C(N=C(CCCCCCC3=NC(C=C(Cl)C=C4[N+]([O-])=O)=C4N3)N2)=C1 | -9.4 |  |
| 135 |  | [H]C1=C2C(N=C(CCCCCCCCC3=NC(C=C(C)C=C4[H])=C4N3)N2)=CC(C)=C1 | -8.0 |  |
| 136 |  | [H]C1=C2C(N=C(CCCCCCCCC3=NC(C=C(Cl)C=C4[H])=C4N3)N2)=CC(Cl)=C1 | -8.5 |  |
| 137 |  | [H]C1=C2C(N=C(C(O)C(C3=NC(C=C([H])C=C4[H])=C4N3)O)N2)=CC([H])=C1 | -8.7 |  |
| 138 |  | [H]C1=C2C(N=C(C(O)C(C3=NC(C=C(C)C=C4[H])=C4N3)O)N2)=CC(C)=C1 | -9.4 |  |
| 139 |  | [H]C1=C2C(N=C(C(O)C(C3=NC(C=C(OCC)C=C4[H])=C4N3)O)N2)=CC(OCC)=C1 | -9.1 |  |
| 140 |  | [H]C1=C2C(N=C(C(O)C(C3=NC(C=C(Cl)C=C4[H])=C4N3)O)N2)=CC(Cl)=C1 | -9.2 |  |
| 141 |  | [H]C1=CC2=C(NC(CCSCCC3=NC4=CC([H])=CC([H])=C4N3)=N2)C=C1 | -6.3 |  |
| 142 |  | [H]C1=C2C(N=C(C3=C(C4=NC(C=C(Cl)C=C5[H])=C5N4)C=CC=C3)N2)=CC(Cl)=C1 | -8.7 |  |
| 143 |  | CC1=CC(NC(CCC2=CC=CC=C2)=N3)=C3C=C1C | -8.4 | 11 |
| 144 |  | CC1=CC(NC(CCC2=CC(Cl)=CC(Cl)=C2)=N3)=C3C=C1C | -8.9 |  |
| 145 |  | FC1=CC(NC(CCC2=CC=CC=C2)=N3)=C3C=C1 | -7.7 |  |
| 146 |  | FC1=CC(NC(CCC2=CC(Cl)=CC(Cl)=C2)=N3)=C3C=C1 | -6.9 |  |
| 147 |  | ClC1=CC(NC(CCC2=CC=CC=C2)=N3)=C3C([N+]([O-])=O)=C1 | -8.0 |  |
| 148 |  | ClC1=CC(NC(CCC2=CC(Cl)=CC(Cl)=C2)=N3)=C3C([N+]([O-])=O)=C1 | -7.8 |  |
| 149 |  | CC1=CC(NC(C=CC2=CC=CC=C2)=N3)=C3C=C1C | -7.1 |  |
| 150 |  | ClC1=CC(NC(C=CC2=CC=CC=C2)=N3)=C3C([N+]([O-])=O)=C1 | -7.4 |  |
| 151 |  | FC1=CC(NC(C=CC2=CC=CC=C2)=N3)=C3C([N+]([O-])=O)=C1 | -7.3 |  |
| 152 |  | CC1=CC(N(S(=O)(C)=O)C(CCC2=CC=CC=C2)=N3)=C3C=C1C | -8.5 |  |
| 153 |  | CC1=CC(N(S(=O)(C)=O)C(CCC2=CC(Cl)=CC(Cl)=C2)=N3)=C3C=C1C | -8.0 |  |
| 154 |  | FC1=CC(N(S(=O)(C)=O)C(CCC2=CC=CC=C2)=N3)=C3C=C1 | -7.8 |  |
| 155 |  | FC1=CC(N(S(=O)(C)=O)C(CCC2=CC(Cl)=CC(Cl)=C2)=N3)=C3C=C1 | -6.9 |  |
| 156 |  | CC1=CC(N(S(=O)(C2=CC=CC=C2)=O)C(CCC3=CC=CC=C3)=N4)=C4C=C1C | -9.4 |  |
| 157 |  | CC1=CC(N(S(=O)(C2=CC=CC=C2)=O)C(CCC3=CC(Cl)=CC(Cl)=C3)=N4)=C4C=C1C | -9.0 |  |
| 158 |  | FC1=CC(N(S(=O)(C2=CC=CC=C2)=O)C(CCC3=CC(Cl)=CC(Cl)=C3)=N4)=C4C=C1 | -8.2 |  |
| 159 |  | FC1=CC(N(S(=O)(C2=CC=CC=C2)=O)C(CCC3=CC=CC=C3)=N4)=C4C=C1 | -8.1 |  |
| 160 |  | CC1=CC(N(S(=O)(C)=O)C(C=CC2=CC=CC=C2)=N3)=C3C=C1 | -7.2 |  |
| 161 |  | FC1=CC(N(S(=O)(C)=O)C(C=CC2=CC=CC=C2)=N3)=C3C=C1 | -7.4 |  |
| 162 |  | CC1=CC(N(S(=O)(C2=CC=CC=C2)=O)C(C=CC3=CC=CC=C3)=N4)=C4C=C1C | -8.6 |  |
| 163 |  | FC1=CC(N(S(=O)(C2=CC=CC=C2)=O)C(C=CC3=CC=CC=C3)=N4)=C4C=C1 | -8.2 |  |
| 164 |  | C12=CC3=C(NC(C=CC4=CC=CC=C4)=N3)C=C1C=CC=C2 | -8.1 |  |
| 165 |  | C12=CC3=C(NC(CCC4=CC=CC=C4)=N3)C=C1C=CC=C2 | -9.0 |  |
| 166 |  | ClC1=CC(Cl)=CC(CCC2=NC3=C(N2)C=C4C(C=CC=C4)=C3)=C1 | -9.7 |  |
| 167 |  | CC1=CC2=CC3=C(NC(CCCC4=CC=CC=C4)=N3)C=C2C=C1C | -10.3 |  |
| 168 |  | ClC1=CC2=CC3=C(NC(CCCC4=CC=CC=C4)=N3)C=C2C=C1Cl | -8.4 |  |
| 169 |  | CC1=CC2=C(NC(CCCC3=CC=CC=C3)=N2)C=C1C | -8.4 |  |
| 170 |  | CC1=CC2=C(NC(CCCC3=CC=CC=C3)=N2)C=C1 | -7.1 |  |
| 171 |  | FC1=CC(NC(CCCC2=CC=CC=C2)=N3)=C3C=C1 | -7.2 |  |
| 172 |  | ClC1=CC(NC(CCCC2CCCCC2)=N3)=C3C=C1Cl | -7.9 |  |
| 173 |  | FC1=CC(NC(CCCC2CCCCC2)=N3)=C3C=C1 | -7.3 |  |
| 174 |  | FC1=CC(N(S(=O)(C)=O)C(CCCC2=CC=CC=C2)=N3)=C3C=C1 | -8.0 |  |
| 175 |  | FC1=CC(N(S(=O)(C2=CC=CC=C2)=O)C(CCCC3=CC=CC=C3)=N4)=C4C=C1 | -8.6 |  |
| 176 |  | ClC1=CC2=C(N(S(=O)(C3=CC=CC=C3)=O)C(CCC4CCCCC4)=N2)C=C1 | -7.9 |  |
| 177 |  | BrC1=CC2=C(N(S(=O)(C3=CC=CC=C3)=O)C(CCC4CCCCC4)=N2)C=C1 | -8.1 |  |
| 178 |  | CC1=C(C)C=C(N(S(=O)(C2=CC=CC=C2)=O)C(CCC3CCCCC3)=N4)C4=C1 | -8.1 |  |
| 179 |  | O=C(CC1=CC(Br)=CN1)NCC2=CC=CC(CN(C=N3)C4=C3C=CC([H])=C4)=C2 | -8.3 |  |
| 180 |  | O=C(CC1=CC(Br)=CN1)OCC2=CC=CC(CN(C=N3)C4=C3C=CC([H])=C4)=C2 | -7.9 |  |
| 181 |  | O=C(CC1=CC=CN1)NCC2=CC=CC(CN(C=N3)C4=C3C=CC([H])=C4)=C2 | -8.6 |  |
| 182 |  | O=C(CC1=CC=CO1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -8.0 |  |
| 183 |  | O=C(CC1=CC=CS1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -8.1 |  |
| 184 |  | O=C(CC1=CC2=C(C=CC=C2)O1)NCC3=CC=CC(CN4C5=C(C=CC([H])=C5)N=C4)=C3 | -9.3 |  |
| 185 |  | O=C(CC1=CC2=C(C=CC=C2)S1)NCC3=CC=CC(CN4C5=C(C=CC([H])=C5)N=C4)=C3 | -9.3 |  |
| 186 |  | O=C(CC1=CC2=C(C=CC=C2)N1)NCC3=CC=CC(CN4C5=C(C=CC([H])=C5)N=C4)=C3 | -8.8 |  |
| 187 |  | O=C(CC1=CC2=C(C=CC(C)=C2)N1)NCC3=CC=CC(CN4C5=C(C=CC([H])=C5)N=C4)=C3 | -9.6 |  |
| 188 |  | O=C(CC1=CC2=C(C=CC(O)=C2)N1)NCC3=CC=CC(CN4C5=C(C=CC([H])=C5)N=C4)=C3 | -9.2 |  |
| 189 |  | O=C(CC1=CC2=C(C=CC(OC)=C2)N1)NCC3=CC=CC(CN4C5=C(C=CC([H])=C5)N=C4)=C3 | -9.3 |  |
| 190 |  | O=C(CC1=NC2=C(C=CC=C2)N1)NCC3=CC=CC(CN4C5=C(C=CC([H])=C5)N=C4)=C3 | -8.9 |  |
| 191 |  | O=C(CCC1=CC=C(OCO2)C2=C1)NCC3=CC=CC(CN4C5=C(C=CC([H])=C5)N=C4)=C3 | -8.7 |  |
| 192 |  | O=C(CC1=CC=CC=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -9.4 |  |
| 193 |  | O=C(CC1=CC=C(C)C=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -9.1 |  |
| 194 |  | O=C(CC1=CC=C(C(F)(F)F)C=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -9.2 |  |
| 195 |  | O=C(CC1=CC=C(Br)C=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -9.0 |  |
| 196 |  | O=C(CC1=CC=C(Cl)C=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -9.0 |  |
| 197 |  | O=C(CC1=CC=C(F)C=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -9.0 |  |
| 198 |  | O=C(CC1=CC=C(C#N)C(C)=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -9.0 |  |
| 199 |  | O=C(CC1=C(F)C=C(C#N)C=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -8.9 |  |
| 200 |  | O=C(CC1=CC=C(C#N)C(F)=C1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -8.3 |  |
| 201 |  | O=C(CCCN1CCOCC1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -8.2 |  |
| 202 |  | O=C(CCCCN)NCC1=CC=CC(CN2C3=C(C=CC([H])=C3)N=C2)=C1 | -7.7 |  |
| 203 |  | O=C(CCNC(C)=O)NCC1=CC=CC(CN2C3=C(C=CC([H])=C3)N=C2)=C1 | -8.1 |  |
| 204 |  | O=C(CCNC(C1=CC=CC=C1)=O)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -9.2 |  |
| 205 |  | O=C(CC1=CC(Br)=CN1)NCC2=CC=CC(CN3C4=C(C=CC([H])=C4)N=C3)=C2 | -8.6 |  |
| 206 |  | NCC1=CC=CC(CN2C3=CC=CC=C3N=C2)=C1 | -7.2 |  |
| 207 |  | O=C(CC1=CC=CN1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -8.3 |  |
| 208 |  | O=C(CC1=CC=CO1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -8.8 |  |
| 209 |  | O=C(CC1=CC=CS1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -8.8 |  |
| 210 |  | O=C(CC1=CC(C=CC=C2)=C2N1)NCC3=CC=CC(CN4C5=C(C=CC=C5)N=C4)=C3 | -8.9 |  |
| 211 |  | O=C(CC1=CC(C=CC(C)=C2)=C2N1)NCC3=CC=CC(CN4C5=C(C=CC=C5)N=C4)=C3 | -9.4 |  |
| 212 |  | O=C(CC1=CC(C=CC=C2)=C2S1)NCC3=CC=CC(CN4C5=C(C=CC=C5)N=C4)=C3 | -9.4 |  |
| 213 |  | O=C(CC1=CC(C=CC=C2)=C2O1)NCC3=CC=CC(CN4C5=C(C=CC=C5)N=C4)=C3 | -8.8 |  |
| 214 |  | O=C(CC1=CC(C=CC(O)=C2)=C2N1)NCC3=CC=CC(CN4C5=C(C=CC=C5)N=C4)=C3 | -9.3 |  |
| 215 |  | O=C(CC1=CC(C=CC(OC)=C2)=C2N1)NCC3=CC=CC(CN4C5=C(C=CC=C5)N=C4)=C3 | -9.3 |  |
| 216 |  | O=C(CC1=CC=CC(C)=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -9.2 |  |
| 217 |  | O=C(CC1=NC(C=CC=C2)=C2N1)NCC3=CC=CC(CN4C5=C(C=CC=C5)N=C4)=C3 | -9.4 |  |
| 218 |  | O=C(CCC1=C(OCO2)C2=CC=C1)NCC3=CC=CC(CN4C5=C(C=CC=C5)N=C4)=C3 | -8.7 |  |
| 219 |  | O=C(CC1=CC=CC=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -9.1 |  |
| 220 |  | O=C(CC1=CC=CC(C(F)(F)F)=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -9.3 |  |
| 221 |  | O=C(CC1=CC=CC(Br)=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -8.5 |  |
| 222 |  | O=C(CC1=CC=CC(Cl)=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -8.5 |  |
| 223 |  | O=C(CC1=CC=CC(F)=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -8.3 |  |
| 224 |  | O=C(CC1=CC=CC(C#N)=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -9.0 |  |
| 225 |  | O=C(CC1=CC=C(C)C(C#N)=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -8.8 |  |
| 226 |  | O=C(CC1=CC(F)=CC(C#N)=C1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -9.0 |  |
| 227 |  | O=C(CC1=CC=CC(C#N)=C1F)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -8.9 |  |
| 228 |  | O=C(CC1COCCN1)NCC2=CC=CC(CN3C4=C(C=CC=C4)N=C3)=C2 | -6.7 |  |
| 229 |  | ClC1=CC=C2C(N=C(C3=CC=C(OCC4=CC=CC=C4)C=C3)N2C5CCCC5)=C1 | -6.8 | R1 |
| 230 |  | ClC1=C(Cl)C=C2C(N(C3CCCC3)C(Cl)=N2)=C1 | -8.5 |  |
| 231 |  | ClC1=C(Cl)C=C2C(N(C3CCCC3)C(Br)=N2)=C1 | -8.8 |  |
| 232 |  | ClC1=C(Cl)C=C2C(N(C3CCCC3)C(N)=N2)=C1 | -7.1 |  |
| 233 |  | ClC1=C(Cl)C=C2C(NC(C3=CC=C(F)C=C3)=N2)=C1 | -7.9 |  |
| 234 |  | ClC1=C(Cl)C=C2C(NC(C3=CC=C(Cl)C=C3)=N2)=C1 | -7.1 |  |
| 235 |  | ClC1=C(Cl)C=C2C(NC(C3=CC=C(C#C)C=C3)=N2)=C1.[HH] |  |  |
| 236 |  | CN1C(CCC2=NC3=CC=CC=C3N2)=CC=C1 | -7.0 | R2 |
| 237 |  | CN(CC1=NC(C([H])=CC=C2)=C2N1CCCCN)C3C4=CC=CC=C4CCC3 | -8.1 |  |
| 238 |  | CN(CC1=NC(C([H])=CC=C2)=C2N1CCCN)C3C4=CC=CC=C4CCC3 | -8.6 |  |
| 239 |  | CN(CC1=NC(C([H])=CC=C2)=C2N1CCCCN(C)C)C3C4=CC=CC=C4CCC3 | -8.3 |  |
| 240 |  | CN(CC1=NC(C(CCCCN)=CC=C2)=C2N1[H])C3C4=CC=CC=C4CCC3 | -8.2 |  |
| 241 |  | CN(CC1=NC(C(N2CCN(C)CC2)=CC=C3)=C3N1[H])C4C5=CC=CC=C5CCC4 | -8.5 |  |
| 242 |  | COC(C=C1)=CC=C1C2=NC3=CC=CC=C3N2 | -7.1 | R3 |
| 243 |  | CC1=CC=C2C(N=C(C3=CC=C(OC)C=C3)N2)=C1 | -6.9 |  |
| 244 |  | ClC1=CC=C2C(N=C(C3=CC=C(OC)C=C3)N2)=C1 | -7.0 |  |
| 245 |  | ClC1=CC=C2C(N=C(C3=CC=C(OC)C=C3)N2)=C1 | -7.6 |  |
| 246 |  | O=C(C1=CC=C2N(CCCN3C(CCC3)=O)C(C4=CC=C(N(C)C)C=C4)=NC2=C1)OCC | -8.7 | R4 |
| 247 |  | O=C(C1=CC=C2N(C3=CC=CC=C3)C(C4=CC=C(N(C)C)C=C4)=NC2=C1)OCC | -7.7 |  |
| 248 |  | O=C(C1=CC=C2N(C3=CC=CC=C3)C(C4=CC=C(C)C=C4)=NC2=C1)OCC | -8.3 |  |
| 249 250 |  | O=C(C1=CC=C2N(CCCN3C(CCC3)=O)C(C4=CC=CC=C4)=NC2=C1)OCCz | -8.1  -8.4 |  |
| 251 |  | c1(cccc2)c2[nH]cn1 | -5.7 | db |
| 252 |  | CCN1CCN(C2=C(Cl)C=C3N=C(S[C@]4(CC[C@H](N(C(C)=O)C)CC4)C)NC3=C2)CC1 | -7.7 |  |
| 253 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(S[C@]4(CC[C@H](NC(OC)=O)CC4)C)n3)CC1 | -7.8 |  |
| 254 |  | CCN1CCN(c(c2)c(C)cc3c2[nH]c(S[C@]4(CC[C@H](NC(OC)=O)CC4)C)n3)CC1 | -7.6 |  |
| 255 |  | Clc1c(c(n2)[nH]c3c2cccc3)cccc1 | -7.4 |  |
| 256 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(SC(C)(C)C)n3)[C@@H](C1)C | -6.9 |  |
| 257 |  | C[C@@H]1CN(CCN1c(c2)c(Cl)cc3c2[nH]c(SC(C)(C)C)n3)CC(n)F | -7.3 |  |
| 258 |  | C[C@@H]1CN(CCN1c(c2)c(Cl)cc3c2[nH]c(SC(C)(C)C)n3)CC(F)(F)F | -7.1 |  |
| 259 |  | C[C@@H]1CN(CCN1c(c2)c(Cl)cc3c2[nH]c(SC(C)(C)C)n3)CC#N | -7.3 |  |
| 260 |  | C[C@@H]1CN(CCN1c(c2)c(Cl)cc3c2[nH]c(SC(C)(C)C)n3)CC(C)=O | -6.9 |  |
| 261 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(SC(C)(C)C)n3)CC1 | -6.6 |  |
| 262 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(SC(C)(CCNC(OC)=O)C)n3)CC1 | -7.1 |  |
| 263 |  | CCOC(N1CCC(CC1)(Sc(n2)[nH]c3c2cc(Cl)c(N4CCN(CC4)CC)c3)C)=O | -7.9 |  |
| 264 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(S[C@@]4(CC[C@H](NC(OC)=O)CC4)C)n3)CC1 | -7.7 |  |
| 265 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(S[C@]4(CC[C@H](NC(C)=O)CC4)C)n3)CC1 | -7.6 |  |
| 266 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(S[C@]4(CC[C@H](N5CCCC5=O)CC4)C)n3)CC1 | -8.0 |  |
| 267 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(S[C@]4(CC[C@H](C(NC)=O)CC4)C)n3)CC1 | -7.6 |  |
| 268 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(S[C@]4(CC[C@H](C5=NN=NN5C)CC4)C)n3)CC1 | -8.5 |  |
| 269 |  | CCN1CCN(c(c2)c(Cl)cc3c2[nH]c(S[C@]4(CC[C@H](c5onc(C)n5)CC4)C)n3)CC1 | -8.4 |  |
| 270 |  | Clc(c(I)c1I)c(I)c2c1nc[nH]2 | -5.5 |  |
| 271 |  | Brc(c(I)c1I)c(I)c2c1[nH]cn2 | -5.4 |  |
| 272 |  | FC(F)(C(F)(c(n1)[nH]c2c1c(I)c(I)c(I)c2I)F)F | -6.9 |  |
| 273 |  | Clc(n1)[nH]c2c1c(I)c(I)c(I)c2I | -5.8 |  |
| 274 |  | Brc(n1)[nH]c2c1c(I)c(I)c(I)c2I | -5.3 |  |
| 275 |  | OCCNc(n1)[nH]c2c1c(I)c(I)c(I)c2I | -6.7 |  |
| 276 |  | Ic1c(I)c2c(NC(N2)=S)c(I)c1I | -5.9 |  |
| 277 |  | OC(CN1C=Nc2c1c(I)c(I)c(I)c2I)=O | -6.4 |  |
| 278 |  | CNC(CN1C=Nc2c1c(I)c(I)c(I)c2I)=O | -6.6 |  |
| 279 |  | NC(CN1C=Nc2c1c(Br)c(Br)c(Br)c2Br)=O | -6.5 |  |
| 280 |  | CNC(CN1C=Nc2c1c(Br)c(Br)c(Br)c2Br)=O | -6.7 |  |
| 281 |  | COc1c(O)ccc(c(cc2)cc3c2c(c(n4)[nH]c5c4c(N6CCN(CC6)C)ccc5)n[nH]3)c1 | -9.4 |  |
| 282 |  | CN1CCN(c(ccc2)c3c2[nH]c(c(n[nH]4)c5c4cc(c6ccc(O)cc6)cc5)n3)CC1 | -10.1 |  |
| 283 |  | CN1CCN(c(ccc2)c3c2[nH]c(c(n[nH]4)c5c4cc(c6ccc(CO)cc6)cc5)n3)CC1 | -9.7 |  |
| 284 |  | COc1cc(OC)c(c(cc2)cc3c2c(c(n4)[nH]c5c4c(N6CCN(CC6)C)ccc5)n[nH]3)cc1 | -9.0 |  |
| 285 |  | COc1c(c(cc2)cc3c2c(c(n4)[nH]c5c4c(N6CCN(CC6)C)ccc5)n[nH]3)cccc1 | -9.4 |  |
| 286 |  | COc1c(c(cc2)cc3c2c(c(n4)[nH]c5c4c(N6CCN(CC6)C)ccc5)n[nH]3)ccc(F)c1 | -10.4 |  |
| 287 |  | CN1CCN(c(ccc2)c3c2[nH]c(c(n[nH]4)c5c4cc(c6ccc(N)cc6)cc5)n3)CC1 | -10.1 |  |
| 288 |  | CN1CCN(c(ccc2)c3c2[nH]c(c(n[nH]4)c5c4cc(c6cc(N)ccc6)cc5)n3)CC1 | -9.6 |  |
| 289 |  | CN1CCN(c(ccc2)c3c2[nH]c(c(n[nH]4)c5c4cc(c6ccc(C(O)=O)cc6)cc5)n3)CC1 | -10.0 |  |
| 290 |  | CN1CCN(c(ccc2)c3c2[nH]c(c(n[nH]4)c5c4cc(c6ccc(C(O)=O)cc6)cc5)n3)CC1 | -10.0 |  |
| 291 |  | CN1CCN(c(ccc2)c3c2[nH]c(c(n[nH]4)c5c4cc(c6ccc(C(N)=O)cc6)cc5)n3)CC1 | -10.2 |  |
| 292 |  | CN1CCN(c(ccc2)c3c2[nH]c(c(n[nH]4)c5c4cc(c6ccc(S(N)(=O)=O)cc6)cc5)n3)CC1 | -9.9 |  |
| 293 |  | NC(c(cc1)cc2c1nc(c3nc[nH]c3)[nH]2)=[NH2+] | -7.3 |  |
| 294 |  | C1(c(cc2)cc3c2nc(c4nc[nH]c4)[nH]3)=[NH+]CCN1 | -8.2 |  |
| 295 |  | C1(c(cc2)cc3c2nc(/C=C/c4ccccc4)[nH]3)=[NH+]CCN1 | -7.9 |  |
| 296 |  | c1(/C=C/c(n2)[nH]c3c2cccc3)ccccc1 | -7.3 |  |
| 297 |  | CN(CCCN1C(c2c(c3ccccc3)n[nH]c2)=Nc4c1ccc(c5ccc(C(O)=O)cc5)c4)C | -9.1 |  |
| 298 |  | CN(CCCN1C(c2c(c3ccc(C(F)(F)F)cc3)n[nH]c2)=Nc4c1ccc(c5ccc(C(O)=O)cc5)c4)C | -9.8 |  |
| 299 |  | OC(c1ccc(c2cc3c(N(C(c4c(c5ccc(C(F)(F)F)cc5)n[nH]c4)=N3)CCCN6C=CN=C6)cc2)cc1)=O | -10.1 |  |
| 300 |  | OC(c1ccc(c2cc3c(N(C(c4c(c5cc(Cl)ccc5)n[nH]c4)=N3)CCCN6C=CN=C6)cc2)cc1)=O | -10.3 |  |
| 301 |  | OC(C1=CC=C(C2=CC=C3N(C(C4=CNN=C4C5=CC=C(C(F)(F)F)C=C5)=NC3=C2)CCCN6CCCCC6)C=C1)=O | -10.6 |  |
| 302 |  | OC(C1=CC=C(C2=CC=C3N(C(C4=CNN=C4C5=C(Cl)C(Cl)=CC=C5)=NC3=C2)CCCNC6CCCCC6)C=C1)=O | -10.5 |  |
| 303 |  | N#CCN1C[C@H](C)N(C2=C(Cl)C=C3N=C(SC(C)(C)C)NC3=C2)CC1 | -6.6 |  |
| 304 |  | ClC1=CC2=C(N=C(S[C@]3(C)CC[C@@H](NS(C)(=O)=O)CC3)N2)C=C1NN4CCN(CC)CC4 | -7.7 |  |
| 305 |  | ClC1=CC2=C(N=C(S[C@]3(C)CC[C@@H](S(C)(=O)=O)CC3)N2)C=C1NN4CCN(CC)CC4 | -8.1 |  |
| 306 |  | ClC1=CC2=C(N=C(S[C@]3(C)CC[C@@H](C4=NN(C)N=N4)CC3)N2)C=C1NN5CCN(CC)CC5 | -7.6 |  |
| 307 |  | ClC1=CC2=C(N=C(S[C@]3(C)CC[C@@H](C4=NN=CO4)CC3)N2)C=C1NN5CCN(CC)CC5 | -8.0 |  |
| 308 |  | ClC1=CC2=C(N=C(S[C@]3(C)CC[C@@H](C4=NN=C(C)O4)CC3)N2)C=C1NN5CCN(CC)CC5 | -7.9 |  |
| 309 |  | BrC1=C(Br)C(Br)=C(Br)C2=C1N=CN2CC(O)=O | -6.4 |  |
| 310 |  | COC1=CC(O)=CC=C1C2=CC3=C(C=C2)C(C(N4)=NC5=C4C=CC=C5N6CCN(C)CC6)=NN3 | -10.0 |  |
| 311 |  | NC(C=C1)=C(F)C=C1C2=CC3=C(C=C2)C(C(N4)=NC5=C4C=CC=C5N6CCN(C)CC6)=NN3 | -9.9 |  |
| 312 |  | COC1=CC(N)=CC=C1C2=CC3=C(C=C2)C(C(N4)=NC5=C4C=CC=C5N6CCN(C)CC6)=NN3 | -10.5 |  |
| 313 |  | CN(CC1)CCN1C2=CC=CC3=C2N=C(C4=NNC5=C4C=CC(C6=CC=C(CN)C=C6)=C5)N3 | -9.7 |  |
| 314 |  | CN(CC1)CCN1C2=CC=CC3=C2N=C(C4=NNC5=C4C=CC(C6=CC=C(NC(C)=O)C=C6)=C5)N3 | -10.3 |  |
| 315 |  | CN(CC1)CCN1C2=CC=CC3=C2N=C(C4=NNC5=C4C=CC(C6=CC=C(NC)C=C6)=C5)N3 | -9.7 |  |
| 316 |  | CN(CC1)CCN1C2=CC=CC3=C2N=C(C4=NNC5=C4C=CC(C6=CC=C(N(C)C)C=C6)=C5)N3 | -9.4 |  |
| 317 |  | COC1=CC(N)=CC=C1C2=CC3=C(C=C2)C(C(N4)=NC5=C4C=CC=C5N6CCN(C)CC6)=NN3 | -9.4 |  |
| 318 |  | CN(CC1)CCN1C2=CC=CC3=C2N=C(C4=NNC5=C4C=CC(C6=CC(C=CN7)=C7C=C6)=C5)N3 | -10.4 |  |
| 319 |  | CN(CC1)CCN1C2=CC=CC3=C2N=C(C4=NNC5=C4C=CC(C6=CC(N=CC=C7)=C7C=C6)=C5)N3 | -10.8 |  |
| 320 |  | CN(CC1)CCN1C2=CC=CC3=C2N=C(C4=NNC5=C4C=CC(C6=CC7=CNN=C7C=C6)=C5)N3 | -10.3 |  |
| 321 |  | CN(CC1)CCN1C2=CC=CC3=C2N=C(C4=NNC5=C4C=CC(C6=CC=C7C(OC=C7)=C6)=C5)N3 | -10.6 |  |
| 322 |  | IC1=C(I)C(I)=C(I)C2=C1N=C(C(F)(F)F)N2 | -5.9 |  |
| 323 |  | IC1=C(I)C(I)=C(I)C2=C1N=C(SCC(O)=O)N2 | -6.0 |  |
| 324 |  | IC1=C(I)C(I)=C(I)C2=C1NC(N2)=O | -6.0 |  |
| 325 |  | IC1=C(I)C(I)=C(I)C2=C1N=C(SCC(N)=O)N2 | -5.7 |  |
| 326 |  | IC1=C(I)C(I)=C(I)C2=C1N=C(SCC(NN)=O)N2 | -6.8 |  |
| 327 |  | IC1=C(Cl)C(Cl)=C(I)C2=C1N=CN2 | -5.8 |  |
| 328 |  | ClC1=C(I)C(Cl)=C(I)C2=C1N=CN2 | -5.8 |  |
| 329 |  | BrC1=C(I)C(Br)=C(I)C2=C1N=CN2 | -5.7 |  |
| 330 |  | IC1=C(I)C(I)=C(I)C2=C1N=C(C)N2 | -5.6 |  |
| 331 |  | IC1=C(I)C(I)=C(I)C2=C1N=C(CC)N2 | -6.2 |  |
| 332 |  | IC1=C(Cl)C(Cl)=C(I)C2=C1N=C(C)N2 | -6.0 |  |
| 333 |  | CCCOC1=CC=C(CSC2=NC3=CC=CC=C3N2)C=C1 | -7.9 |  |
| 334 |  | CC1=CC=C(CN2C(CC3=CC=CC=C3)=NC4=CC=CC=C24)C=C1 | -8.5 |  |
| 335 |  | CCN1CCN(C2=C(Cl)C=C3N=C(S[C@]4(CC[C@H](NC(OC)=O)C4)C)NC3=C2)CC1 | -7.7 |  |
| 336 |  | ClC1=CC=C2N=C(N3CCCCC3)NC2=C1 | -6.5 |  |
| 337 |  | BrC1=C(OCCCN2C=NC3=CC=CC=C23)C=CC=C1 | -6.7 |  |
| 338 |  | CCS(=O)(C1=NC2=CC=CC=C2N1CC3=CC=CC=N3)=O | -7.4 |  |
| 339 |  | ClC1=C(OCCN2C=NC3=CC=CC=C23)C=CC=C1 | -6.5 |  |
| 340 |  | CC(C)(CC1=NC2=CC=CC=C2N1CCC3=CC=CC=C3)C | -7.2 |  |
| 341 |  | CCN1C(/C=C/C2=CC=CC=C2)=NC3=CC=CC=C13 | -7.0 |  |
| 342 |  | ON1C2=CC=CC(C2=NC13CCCCC3)=N | -7.1 |  |
| 343 |  | CC(SC1=NC2=CC=C(C=C2N1)Br)C | -5.8 |  |
| 344 |  | CC(C1=NC2=CC=CC=C2N1CC3=CC=CC=C3)N4CCCCC4 | -8.1 |  |
| 345 |  | FC1=C2C=CC=CC2=C(CSC3=NC4=CC=CC=C4N3)C=C1 | -8.5 |  |
| 346 |  | CC1=CC=C(C2=NC3=CC=CC=C3N2)S1 | -7.0 |  |
| 347 |  | ClC1=CC=C(C=C1)OCCSCC2=NC3=CC=CC=C3N2 | -7.5 |  |
| 348 |  | C[C@@H]1CN(CCN1C2=C(Cl)C=C3N=C(SC(C)(C)C)NC3=C2)CCO | -7.5 |  |
| 349 |  | CC1=CC=C2N=CNC2=C1 | -5.7 |  |
| 350 |  | O=C1C2=C(C(C3=C1C=CC=C3)=O)NC=N2 | -8.0 |  |
| 351 |  | COc1cc2c(N=C(c3ccccc3)N2)cc1 | -7.0 |  |
| 352 |  | COc1cc2c(N=C(c3ccccc3)N2)cc1 | -7.2 |  |
| 353 |  | CC1=C(NC(N1CC2=CC=C(OC)C=C2)=S)C=C | -6.1 |  |
| 354 |  | SC(N1SCCCCOC2=CC=CC=C2)NC3=C1C=CC(C)=C3 | -6.8 |  |
| 355 |  | O=C1N(C)C2=C(C=CC=C2)C31N=C4C=CC=CC4=N3 | -7.9 |  |
| 356 |  | ClC(C=C1Cl)=CC=C1/C=C/C2=NC3=CC=CC=C3N2 | -7.5 |  |
| 357 |  | ClC1=CC=CC(Cl)=C1/C=C/C2=NC3=CC=CC=C3N2 | -8.0 |  |
| 358 |  | O=[N+](C1=CC=C(C=C1)CSC2=NC3=CC(C)=CC=C3N2)[O-] | -8.7 |  |
| 359 |  | FC1=CC=CC(F)=C1CSC2=NC3=CC=CC=C3N2 | -7.5 |  |
| 360 |  | CN1C(C2=NC3=CC=CC=C3N2)=CC4=C1C=CC=C4 | -7.9 |  |
| 361 |  | COC(C=C1)=CC=C1CSC2=NC3=CC=CC=C3N2 | -7.6 |  |
| 362 |  | O=C(NNC(C1=CC=C(Br)C=C1)=O)C2=NC3=CC=CC=C3N2 | -8.3 |  |
| 363 |  | CC(C=C1)=CC=C1OCCCCN2C=NC3=CC=CC=C32 | -6.2 |  |
| 364 |  | BrC1=C2C(N(CCCCl)C=N2)=C(Br)C(Br)=C1Br | -6.1 |  |
| 365 |  | CCC1=NC2=CC(Cl)=C(C=C2N1)Cl | -6.2 |  |
| 366 |  | CC1=C(C)C=C2N(CCCCOC3=CC=CC=C3)C=NC2=C1 | -5.0 |  |
| 367 |  | CS(=O)(C1=CC([N+]([O-])=O)=C(SC2=NC3=CC=CC=C3N2)C([N+]([O-])=O)=C1)=O | -8.1 |  |
| 368 |  | FC(F)(OC1=CC=C(NC(C2=CC=C3N=CNC3=C2)=O)C=C1)F | -7.8 |  |
| 369 |  | FC1=C(F)C=C2NC(C3=CC=NC=C3)=NC2=C1 | -7.0 |  |
| 370 |  | [O-][N+](C1=C(OCCCN2C=NC3=CC=CC=C23)C=CC=C1)=O | -6.5 |  |
| 371 |  | COC1=CC=C(C2=NC3=CC=C([N+]([O-])=O)C=C3N2)C=C1 | -7.4 |  |
| 372 |  | CC1=NC2=CC=C(C(O)=O)C=C2N1 | -6.4 |  |
| 373 |  | CC1=C(NC(C2=NC3=CC=CC=C3N2)=S)C=CC=C1 | -7.8 |  |
| 374 |  | CC1=CC=C(C2=NC3=CC=C([N+]([O-])=O)C=C3N2)C=C1 | -8.0 |  |
| 375 |  | CC1=CC=C2N=C(N3CCN(S(=O)(C4CC4)=O)CC3)NC2=C1 | -7.5 |  |
| 376 |  | CC1=CC=C2N=C(N3CCN(S(C)(=O)=O)CC3)NC2=C1 | -6.9 |  |
| 377 |  | N#C/C(C#N)=C1C=CC2=NC3(NC2=C\1)CCCCC3 | -7.3 |  |
| 378 |  | C1(/C=C/C2=CC=CO2)=NC3=CC=CC=C3N1 | -7.1 |  |
| 379 |  | ClC1=CC(Cl)=C(/C=N/NC(C2=CC=C3N=CNC3=C2)=O)C=C1 | -8.3 |  |
| 380 |  | O=C(c1cc2c(N=CN2)cc1)Nc3c(N4CCOCC4)cccc3 | -8.0 |  |
| 381 |  | [O-][N+](C1=CC(S(=O)(C(F)(F)F)=O)=CC=C1SC2=NC3=CC=CC=C3N2)=O | -8.4 |  |
| 382 |  | COC1=CC=CC(C2=NC3=CC=C(N4CCN(CC4)C)C=C3N2)=C1 | -8.0 |  |
| 383 |  | ClC1=CC=C(OCCN2C(C3=CC=CO3)=NC4=CC=CC=C24)C=C1 | -8.3 |  |
| 384 |  | ClC1=CC=C(C=C1)CON2C(C3=CC=C(Cl)C=C3)=NC4=CC=CC=C24 | -8.1 |  |
| 385 |  | CC1=NC=CC(C2=CC=C(N3C=NC4=CC=CC=C34)C=C2)=N1 | -8.1 |  |
| 386 |  | C12=CC=CC=C1N(C3=CC=C(C4=NC(C5=CC=CC=C5)=NC=C4)C=C3)C=N2 | -9.2 |  |
| 387 |  | CCCN1C(/C=C/C2=CC=CC=C2)=NC3=CC=CC=C13 | -7.1 |  |
| 388 |  | CC1=NC2C(N1C3CCCCC3)C(C4=CC=CC=C4C2=O)=O | -7.7 |  |
| 389 |  | CC1=C(C)C=C2N(C3=NN=NN3C4=CC=CC=C4)C=NC2=C1 | -8.5 |  |
| 390 |  | CC1=NC2=CC=CC=C2N1CC3=CC=C(Br)C=C3 | -7.2 |  |
| 391 |  | ClC1=CC=C(S(=O)(CCC2=NC3=CC=CC=C3N2)=O)C=C1 | -7.1 |  |
| 392 |  | ClC1=CC=C(C=C1)CNC(C2=CC=C3N=CNC3=C2)=O | -8.3 |  |
| 393 |  | CC1=CC(OCCN2C(C3=CC=CO3)=NC4=CC=CC=C24)=CC=C1 | -7.6 |  |
| 394 |  | C1(OCCCN2C=NC3=CC=CC=C23)=CC=C4CCCC4=C1 | -8.4 |  |
| 395 |  | CC1=C2NC=NC2=C(Br)C(Br)=C1Br | -5.7 |  |
| 396 |  | OS(=O)(C1=CC=C2NC(C3=CCCC=C3)=NC2=C1)=O | -7.7 |  |
| 397 |  | ClCC1=NC2=CC=CC=C2N1CC3=CC=CC=C3 | -7.1 |  |
| 398 |  | CN1C=CC=C1C2=NC3=CC=CC=C3N2C | -6.5 |  |
| 399 |  | C1(SCCOC2=CC=CC=C2)=NC3=CC=CC=C3N1 | -7.4 |  |
| 400 |  | CC(CN1C(C2=CC=CS2)=NC3=CC=CC=C13)C | -6.5 |  |
| 401 |  | COC1=CC=C(C2=NC3=CC=CC=C3N2CC=C)C=C1 | -6.8 |  |
| 402 |  | CC1=CC=CC(OCCCSC2=NC3=C(N2)C=C(C)C=C3)=C1 | -7.7 |  |
| 403 |  | CCCC#C/C=C1CN2C(S/1)=NC3=CC=CC=C23 | -6.5 |  |
| 404 |  |  | -8.9 |  |
| 405 |  | CC1=CC(OCC(NNC(C2=CC=C3N=CNC3=C2)=O)=O)=CC=C1 | -9.1 |  |
| 406 |  | C12=CC=CC=C1N(C3=CC=C(C4=CC=NC(C5=CC=CC=N5)=N4)C=C3)C=N2 | -9.3 |  |
| 407 |  | CCN1CCN(C2=CC(SC3=NC4=CC=CC=C4N3)=C([N+]([O-])=O)C=C2)CC1 | -7.9 |  |
| 408 |  | COCCOCCN1C(/C=C/C2=CC=CC=C2)=NC3=CC=CC=C13 | -6.9 |  |
| 409 |  | FC1=CC=C(C=C1)CN2C3=NCCCN3C4=C2C=CC=C4 | -8.1 |  |
| 410 |  | [O-][N+](C1=CC=CC(/C=C/C2=NC3=CC=C([N+]([O-])=O)C=C3N2)=C1)=O | -8.3 |  |
| 411 |  | CON1C(C2=CC=CC=C2)=NC3=CC=C(C=C13)Cl | -6.8 |  |
| 412 |  | Brc1c(Br)c2c(NC=N2)c(Br)c1Br | -5.6 |  |
| 413 |  | N1(C(C2CC2)=Nc3c1cccc3)CCc4ccccc4 | -7.4 |  |
| 414 |  | CN1C(C2=CC=CO2)=Nc(c3)c1cc4c3cccc4 | -7.8 |  |
| 415 |  | COc1ccc(Nc(c([N+]([O-])=O)cc2)c3c2=NC4(N=3)CCCCC4)cc1 | -8.5 |  |
| 416 |  | Cc1c(C#N)c2n(c3c(N=2)cccc3)c(Cl)c1 | -7.4 |  |
| 417 |  | CCN1C(SCc2c(Cl)cccc2)=Nc3c1cccc3 | -7.4 |  |
| 418 |  | Cc1c(CS(C2=Nc3c(N2)cccc3)=O)nccc1OCC(F)(F)F | -7.5 |  |
| 419 |  | CC1CCC2(N=C(NC3=Nc4c(N23)cccc4)N)CC1 | -9.2 |  |
| 420 |  | COc1cc(CN2C=Nc3c2cc(C)c(C)c3[N+]([O-])=O)ccc1 | -8.1 |  |
| 421 |  | OCC[N-]c1c([N+]([O-])=O)ccc2c1NC3([N+]2=O)CCCCC3 | -7.6 |  |
| 422 |  | [O-][N+](c1c([N-]CCc2ccccc2)c(NC3([N+]4=O)CCCCC3)c4cc1)=O | -8.7 |  |
| 423 |  | CC1=Nc2c(N1Cc3c(C)cccc3)cccc2 | -7.3 |  |
| 424 |  | [O-][N+](c1c(NC([C-]2C3=Nc4c([N+]3=CCC2=O)cccc4)=O)cccc1)=O | -8.4 |  |
| 425 |  | CCCCC1=NC2=C(N1CCN3CCCC3)C=CC(C(NC(NCCCCCC(NO)=O)=O)=O)=C2 | -8.0 |  |
| 426 |  | CC(C1=C(C#N)C2=NC3=C(C=CC=C3)N2C(N4CCN(C(C5=CC=CO5)=O)CC4)=C1)C | -8.8 |  |
| 427 |  | CCCC1=C(C#N)C2=NC3=C(C=CC=C3)N2C(NCCOCCO)=C1 | -6.8 |  |
| 428 |  | O=C(C1=CC=C2C(N=C(C)N2C3=CC=C(Br)C=C3)=C1)NCC4=CC=C(OCO5)C5=C4 | -9.8 |  |
| 429 |  | O=S(C1=C(C)C=C(N2CC)C(N(CC)C2=O)=C1)(NC3=CC=CC=C3C)=O | -8.3 |  |
| 430 |  | CC1=C(C)C=C2N=C(C3CCN(CC4=NN=NN4CC5=CC=CS5)CC3)NC2=C1 | -8.8 |  |
| 431 |  | N#CC1C(C2=CC=C(Br)C=C2)C(C#N)C3=NC4=CC=CC=C4N3C1=N | -7.6 |  |
| 432 |  | [O-][N+](c1cc2c(N=C(N2OCc3ccc(Cl)cc3)c4ccccc4)cc1)=O | -8.6 |  |
| 433 |  | COc1c(CN2C(S(C)(=O)=O)=Nc3c2cccc3)cc(C)cc1 | -7.9 |  |
| 434 |  | Cc1ccc(S(=O)(CC2CSC3=Nc4c(N23)cccc4)=O)cc1 | -8.3 |  |
| 435 |  | CC1(N2CCC(N3C=Nc4c3cccc4)CC2)CCCCCCC1 | -8.2 |  |
| 436 |  | C1(Cc(ccc2)c3c2cccc3)=Nc4c(N1)cccc4N5CCNCC5 | -9.0 |  |
| 437 |  | NC(c1c2c(NC(c3ccc(C4CCNCC4)cc3)=N2)ccc1)=O | -8.6 |  |
| 438 |  | CN1CCN(c2cc3c(N=C(N3)Cc4ccccc4)cc2)CC1 | -8.6 |  |
| 439 |  | COc1ccc(c2cc3c(N(c4ccccc4)CN3)cc2)cc1 | -7.9 |  |
| 440 |  | CC(c1c(OC(NS(=O)(NC2=Nc3c(N2)cccc3)=O)=O)c(C(C)C)ccc1)C | -8.5 |  |
| 441 |  | N#CC(C(C)=C1CC)=C2NC3=CC=CC=C3N2C1=S | -7.6 |  |
| 442 |  | O=C(C1=CC=C2C(N=C(CSC3=NC=CN3C)N2CC)=C1)O | -7.3 |  |
| 443 |  | N#CC1C(C2=CC=CC(Br)=C2)C(C#N)C3=NC4=CC=CC=C4N3C1=N | -8.3 |  |
| 444 |  | O=[N+](C1=CC=C2C(N=C([N+]3=C(C4=CC=CC=C4)C=C(C5=CC=CC=C5)C=C3C6=CC=CC=C6)N2C)=C1)[O-] | -9.2 |  |
| 445 |  | O=C(C1=C(OCC2=CC=CC(C)=C2)C=C(N3C=NC4=CC=CC=C34)S1)N | -9.0 |  |
| 446 |  | O=C(C1=C(OCC2CCCCC2)C=C(N3C4=CC(OC)=C(OC)C=C4N=C3)S1)N | -8.4 |  |
| 447 |  | O=C(C1=C(OCC2=CC=C(Cl)C=C2)C=C(N3C=NC4=CC=CC=C34)S1)N | -8.8 |  |
| 448 |  | O=C(C1=C(OCC2=CC=CC(OC)=C2)C=C(N3C=NC4=CC=CC=C34)S1)N | -9.1 |  |
| 449 |  | Cc1ccc(c2c(C#N)c3n(c4c(N=3)cccc4)c(N)c2C#N)cc1 | -8.1 |  |
| 450 |  | Cc1cc(/C=C(S(=O)(c2ccccc2)=O)\c(n3)[nH]c4c3cccc4)ccc1 | -8.7 |  |
| 451 |  | COc(cc1)cc2c1nc(c3ncccc3)[nH]2 | -6.9 |  |
| 452 |  | COc1ccc(NS(=O)(c(cc2)cc3c2nc(COc(ccc4)c5c4cccc5)[nH]3)=O)cc1 | -9.0 |  |
| 453 |  | Brc1c(Br)c2c(N(C=N2)CCN=[N+]=[N-])c(Br)c1Br | -7.0 |  |
| 454 |  | Brc1c(Br)c2c(N(C=N2)CCCN=[N+]=[N-])c(Br)c1Br | -5.9 |  |
| 455 |  | COc1ccc(c(n2)[nH]c3c2cccc3)cc1 | -7.4 |  |
| 456 |  | C1(/NCCN1)=N/N2C=Nc3c2cccc3 | -7.5 |  |
| 457 |  | COCN1C(COc2ccccc2)=Nc3c1cccc3 | -6.9 |  |
| 458 |  | COCCN1C=Nc2c1cc(C)c(C)c2 | -6.0 |  |
| 459 |  | Cc1ccc(S(=O)(n(c(ccc(C)c2)c2[nH]3)c3=S)=O)cc1 | -8.2 |  |
| 460 |  | c1(cc([nH]c(c2cnccc2)n3)c3c4)c4cccc1 | -8.7 |  |
| 461 |  | Cc1c(C)c(NS(=O)(c(cc2)cc3c2nc(c4ccccc4)[nH]3)=O)ccc1 | -9.5 |  |
| 462 |  | Cc(n1)[nH]c2c1cc(nc(C(F)(F)F)[nH]3)c3c2 | -7.8 |  |
| 463 |  | c1(c(n2)[nH]c3c2cc(cccc4)c4c3)ncccc1 | -8.5 |  |
| 464 |  | c1(c2[nH]c3ccc(cccc4)c4c3n2)ncccc1 | -8.5 |  |
| 465 |  | CSc(n1)[nH]c2c1cc(Cl)c(Oc3c(Cl)c(Cl)ccc3)c2 | -6.4 |  |
| 466 |  | COc1ccc(NS(=O)(c(cc2)cc3c2nc(COc(cc4)cc5c4cccc5)[nH]3)=O)cc1 | -9.2 |  |
| 467 |  | COc1c([N+]([O-])=O)cc(CN2C(SC)=Nc3c2cccc3)cc1 | -7.7 |  |
| 468 |  | Cc(n1)[nH]c2c1ccc(C(C(F)(F)F)(C(F)(F)F)C(F)(F)F)c2 | -7.7 |  |
| 469 |  | NC1=NC2(N3C(N1)=Nc4c3cccc4)CCN(CC2)Cc5ccccc5 | -9.1 |  |
| 470 |  | CC(c1ccccc1)C(c(n2)[nH]c3c2cccc3)Cc(n4)[nH]c5c4cccc5 | -9.2 |  |
| 471 |  | Cc(c1)c(C)cc2c1nc(c3cnc(SCc4ncccc4)cc3)[nH]2 | -8.1 |  |
| 472 |  | CN1C(c2sccc2)=Nc3c1cccc3 | -6.5 |  |
| 473 |  | CCS(=O)(C1=Nc2c(N1Cc3c(Cl)cccc3)cccc2)=O | -7.8 |  |
| 474 |  | Brc(cc1c2nc[nH]1)c3c2cccc3 | -6.7 |  |
| 475 |  | CON1C(c2ccc(Cl)cc2)=Nc3c1cc(Cl)cc3 | -8.1 |  |
| 476 |  | FC(F)(c1ccc(/C=C(S(=O)(c2ccccc2)=O)\c(n3)[nH]c4c3cccc4)cc1)F | -8.8 |  |
| 477 |  | FC(F)(c1ccc(/C=C(S(=O)(c2ccccc2)=O)/c(n3)[nH]c4c3cccc4)cc1)F | -9.0 |  |
| 478 |  | O=C1C2NC(NC2C(c3c1cccc3)=O)=O | -7.8 |  |
| 479 |  | c(Cc1ccccc1)(n2)[nH]c3c2c(N4CCNCC4)ccc3 | -8.4 |  |
| 480 |  | CCc(n1)[nH]c2c1cc([N+]([O-])=O)c([N+]([O-])=O)c2 | -6.6 |  |
| 481 |  | COc(cc1)cc2c1nc(N3CCCCC3)[nH]2 | -6.9 |  |
| 482 |  | CC1=Nc2c(N1S(=O)(c3ccc(C)cc3)=O)cccc2 | -7.3 |  |
| 483 |  | c1(OCCCN2CCOCC2)ccc(C3=Nc4c(N3C/C=C/CN5C(c6ccc(OCCCN7CCOCC7)cc6)=Nc8c5cccc8)cccc4)cc1 | -9.5 |  |
| 484 |  | c1(OCCCN2CCN(c3ccccc3)CC2)ccc(C4=Nc5c(N4C/C=C/CN6C(c7ccc(OCCCN8CCN(c9ccccc9)CC8)cc7)=Nc%10c6cccc%10)cccc5)cc1 | -9.7 |  |
| 485 |  | CCc(c1)c(C#N)c2[nH]c(cccc3)c3n2c1=S | -7.2 |  |
| 486 |  | CCSC1=Nc2c(N1CCOc3ccccc3)cccc2 | -6.9 |  |
| 487 |  | COc1ccc(NC(N2CCN3C2=Nc4c3cccc4)=O)cc1 | -7.8 |  |
| 488 |  | CN1C(SCc2c(Cl)cccc2)=Nc3c1cccc3 | -7.1 |  |
| 489 |  | Cc1c(C#N)c2n(c(cccc3)c3=N2)c(Cl)c1 | -7.0 |  |
| 490 |  | CCN1C(SCc2c(Cl)cccc2)=Nc3c1cccc3 | -7.4 |  |
| 491 |  | [O-][N+](c1cc2c(N=C(N2OCc3ccc(Cl)cc3)c4ccccc4)cc1)=O | -8.6 |  |
| 492 |  | CC1CCC2(N=C(NC3=Nc4c(N23)cccc4)N)CC1 | -8.3 |  |
| 493 |  | Cc1c(CS(c(n2)[nH]c3c2cccc3)=O)nccc1OCC(F)(F)F | -7.5 |  |
| 494 |  | CC1=Nc2c(N1Cc3c(C)cccc3)cccc2 | -7.3 |  |
| 495 |  | OCC[N-]c1c([N+]([O-])=O)ccc2c1NC3([N+]2=O)CCCCC3 | -7.6 |  |
| 496 |  | COc1c(CN2C(S(C)(=O)=O)=Nc3c2cccc3)cc(C)cc1 | -7.9 |  |
| 497 |  | Cc1ccc(S(=O)(CC2CSC3=Nc4c(N23)cccc4)=O)cc1 | -8.3 |  |
| 498 |  | CC1(N2CCC(N3C=Nc4c3cccc4)CC2)CCCCCCC1 | -8.1 |  |
| 499 |  | [O-][N+](c1c(NC([C-]2c([nH]3)[n+](CCC2=O)c4c3cccc4)=O)cccc1)=O | -9.5 |  |
| 500 |  | [O-][N+](c1c([N-]CCc2ccccc2)c(NC3([N+]4=O)CCCCC3)c4cc1)=O | -8.8 |  |
| 501 |  | COc1cc(CN2C=Nc3c2cc(C)c(C)c3[N+]([O-])=O)ccc1 | -8.0 |  |
| 502 |  | c(Cc(ccc1)c2c1cccc2)(n3)[nH]c4c3c(N5CCNCC5)ccc4 | -9.0 |  |
| 503 |  | NC(c(ccc1)c2c1[nH]c(c3ccc(C4CCNCC4)cc3)n2)=O | -8.6 |  |
| 504 |  | CN1CCN(c(cc2)cc3c2nc(Cc4ccccc4)[nH]3)CC1 | -8.1 |  |
| 505 |  | COc1ccc(c2cc3c(N(c4ccccc4)C=N3)cc2)cc1 | -8.0 |  |
| 506 |  | CC(c1c(OC(NS(=O)(Nc(n2)[nH]c3c2cccc3)=O)=O)c(C(C)C)ccc1)C | -8.8 |  |
| 507 |  | CN1CCN(c(ccc2)c3c2[nH]c(Cc4ccccc4)n3)CC1 | -8.2 |  |
| 508 |  | c(Cc(ccc1)c2c1cccc2)(n3)[nH]c4c3ccc(N5CCNCC5)c4 | -9.2 |  |
| 509 |  | NC(c(ccc1)c2c1[nH]c(c3ccc(C4CCNC4)cc3)n2)=O | -8.2 |  |
| 510 |  | NC(c(ccc1)c2c1[nH]c(c3ccc(C4CCCN4)cc3)n2)=O | -7.9 |  |
| 511 |  | NC(c(ccc1)c2c1[nH]c(c3ccc(C4CCCCN4)cc3)n2)=O | -8.8 |  |
| 512 |  | c(Cc(cc1)cc2c1cccc2)(n3)[nH]c4c3ccc(N5CCNCC5)c4 | -9.4 |  |
| 513 |  | Clc1ccc(NC(c(n2)[nH]c3c2cccc3)=S)cc1 | -7.7 |  |
| 514 |  | S=C1Nc(cc2)c(N1)c3c2cccc3 | -7.1 |  |
| 515 |  | NS(=O)(c1cc(NC(c(cc2)cc3c2nc[nH]3)=O)ccc1)=O | -8.1 |  |
| 516 |  | Cc1cc(C)c(NC(c(n2)[nH]c3c2cccc3)=S)cc1 | -7.7 |  |
| 517 |  | COc1ccc(CCCc(n2)[nH]c3c2cccc3)cc1 | -7.9 |  |
| 518 |  | CCOCCN1C(c2ccc(OC)cc2)=Nc3c1cccc3 | -6.5 |  |
| 519 |  | Cc1cc(C(c2cn3c(N=c4c3cccc4)c(C#N)c2)=O)c(O)cc1 | -8.7 |  |
| 520 |  | CN(C(c(cc1)cc2c1nc[nH]2)=O)CC(Nc3c(C)cccc3C)=O | -8.0 |  |
| 521 |  | CN1C(COc2ccccc2)=NN=C1SCc(n3)[nH]c4c3cccc4 | -8.5 |  |
| 522 |  | Cc1cc(OCCCSc(n2)[nH]c3c2cccc3)ccc1 | -7.5 |  |
| 523 |  | CC(c(n1)[nH]c2c1c(C(N)=O)ccc2)NS(=O)(N(C)C)=O | -7.6 |  |
| 524 |  | CC1=Nc2c(N1CCOc3ccc([N+]([O-])=O)cc3)cccc2 | -7.9 |  |
| 525 |  | NC(c(ccc1)c2c1nc[nH]2)=O | -7.0 |  |
| 526 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)Cc4ccccc4)ccc1 | -8.1 |  |
| 527 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC4CCCC4)ccc1 | -7.3 |  |
| 528 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1cccc3N)C | -7.6 |  |
| 529 |  | C[C@]1(c(n2)[nH]c3c2c(C(N)=O)ccc3)CCCN1 | -8.1 |  |
| 530 |  | CCN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1cccc3N | -7.2 |  |
| 531 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC4CC4)ccc1 | -7.1 |  |
| 532 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC4CCC4)ccc1 | -7.4 |  |
| 533 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC4CCCCC4)ccc1 |  |  |
| 534 |  | c(Cc(cc1)cc2c1cccc2)(n3)[nH]c4c3c(N5CCNCC5)ccc4 | -9.1 |  |
| 535 |  | CN1CCN(c(cc2)cc3c2nc(Cc(ccc4)c5c4cccc5)[nH]3)CC1 | -9.2 |  |
| 536 |  | CN1CCN(c(cc2)cc3c2nc(Cc(cc4)cc5c4cccc5)[nH]3)CC1 | -9.9 |  |
| 537 |  | CN1CCN(c(ccc2)c3c2[nH]c(Cc(ccc4)c5c4cccc5)n3)CC1 | -9.4 |  |
| 538 |  | CCCN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1cccc3N | -7.2 |  |
| 539 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC45CCC(C5)CC4)ccc1 | -7.7 |  |
| 540 |  | CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1cccc3N | -7.2 |  |
| 541 |  | Cc(c1)c(C)cc2c1nc[nH]2 | -6.6 |  |
| 542 |  | [O-][N+](c(cc1)cc2c1n(c3ccccc3)c(=S)[nH]2)=O | -7.4 |  |
| 543 |  | NC(c(ccc1)c2c1[nH]c(c3c(F)cc([C@@H]4CCCCN4)cc3)n2)=O | -8.5 |  |
| 544 |  | CC(C)(c1ccc(c2c(c3ccccc3)[nH]nc2c(n4)[nH]c5c4cccc5)cc1)C | -8.8 |  |
| 545 |  | ON1[C@H]2CCCC[C@H]2N(C1c3c(Cl)cc(Cl)cc3)O | -7.2 |  |
| 546 |  | CCN1C(N2CCN(S(=O)(c3ccc(OC)cc3)=O)CC2)=Nc4c1cccc4 | -8.6 |  |
| 547 |  | CCCc(c1)c(C#N)c2[nH]c(cccc3)c3n2c1=O | -8.5 |  |
| 548 |  | COc1ccc(CNC(CCCCCNC(N2CCN3C2=Nc4c3cccc4)=O)=O)cc1 | -7.4 |  |
| 549 |  | CC(Cc(c(C)c(C#N)c([nH]1)n2c3c1cccc3)c2=O)=C | -8.0 |  |
| 550 |  | CN(CCNC(c(ccc1)c2c1nc(c3ccncc3)[nH]2)=O)C | -7.0 |  |
| 551 |  | COc1ccc(S(=O)(N2CCC(N3C=Nc4c3ccc(C(F)(F)F)c4)CC2)=O)cc1 | -8.9 |  |
| 552 |  | CCOC(C1C(N2C(N=C1C)=Nc3c2cccc3)c4ccncc4)=O | -7.7 |  |
| 553 |  | Cc(cc(Cl)n12)c(C#N)c1=Nc3c2cc(F)c(F)c3 | -7.4 |  |
| 554 |  | Fc1c(F)cc(c(cc2)cc3c2[nH]c(=S)n3C4CCCC4)cc1 | -8.5 |  |
| 555 |  | NC(c(ccc1)c2c1[nH]c(c3c(F)cc(C4CCCCN4)cc3)n2)=O | -8.9 |  |
| 556 |  | COc1c(OC)c(OC)cc(c(n2)[nH]c3c2ccc(N4CCN(CC4)C)c3)c1 | -7.8 |  |
| 557 |  | ONC(c(cc1)cc2c1nc(c3cc(Br)ccc3)[nH]2)=O | -8.0 |  |
| 558 |  | CN1CCCCC1c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2 | -8.3 |  |
| 559 |  | CCCCc1ccc(c(n2)[nH]c3c2ccc(C(NO)=O)c3)cc1 | -7.9 |  |
| 560 |  | [O-][N+](c1c(N2CCN(CC2)CCCSc(n3)[nH]c4c3cccc4)cccc1)=O | -7.7 |  |
| 561 |  | CCc1ccc(c(n2)[nH]c3c2ccc(C(NO)=O)c3)cc1 | -8.0 |  |
| 562 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)Cc4cc(O)ccc4)ccc1 | -8.1 |  |
| 563 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)Cc4ccc(C(F)(F)F)cc4)ccc1 | -9.0 |  |
| 564 |  | N#Cc1cc(N=c2n3cccc2)c3cc1 | -7.1 |  |
| 565 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)Cc4cocc4)ccc1 | -7.4 |  |
| 566 |  | NC(c(ccc1)c2c1nc(C3CCCCN3)[nH]2)=O | -8.0 |  |
| 567 |  | ONC(c(cc1)cc2c1nc(c3ccc(Br)cc3)[nH]2)=O | -8.0 |  |
| 568 |  | ONC(c(cc1)cc2c1nc(c3ccc(C#C)cc3)[nH]2)=O | -8.0 |  |
| 569 |  | COc1c(N2CCN(CC2)CCSc(n3)[nH]c4c3cccc4)cccc1 | -7.8 |  |
| 570 |  | COc1c(N2CCN(CC2)CCCSc(n3)[nH]c4c3cccc4)cccc1 | -7.5 |  |
| 571 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)Cc4cscc4)ccc1 | -7.9 |  |
| 572 |  | Brc(cc(CCN1CCN(c2ccccc2)CC1)c3)c4c3[nH]cn4 | -8.3 |  |
| 573 |  | NC(c(cc(F)c1)c2c1[nH]c(c3ccc(C4CCCN4)cc3)n2)=O | -8.4 |  |
| 574 |  | Clc(cc(CCN1CCN(c2ccccc2)CC1)c3)c4c3[nH]cn4 | -7.8 |  |
| 575 |  | CC(N1CCCC1c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2)C | -8.3 |  |
| 576 |  | CC(N1CCC(c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2)C1)C | -8.4 |  |
| 577 |  | CCCCCCCN1C2=NCCCN2c3c1cccc3 | -6.8 |  |
| 578 |  | NC(c(cc(F)c1)c2c1[nH]c(c3ccc(C4CCCCN4)cc3)n2)=O | -8.9 |  |
| 579 |  | CN1CCC(c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2)C1 | -8.5 |  |
| 580 |  | NC(c(cc(Cl)c1)c2c1[nH]c(c3ccc(C4CCCN4)cc3)n2)=O | -8.2 |  |
| 581 |  | CN1CCCC1c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2 | -8.6 |  |
| 582 |  | COc1ccc(c(n2)[nH]c3c2c(C(N)=O)ccc3)cc1 | -8.2 |  |
| 583 |  | [O-][N+](c1c(N2CCN(CC2)CCSc(n3)[nH]c4c3cccc4)cccc1)=O | -7.9 |  |
| 584 |  | Cc1cc(CC(c(n2)[nH]c3c2cccc3)Cc(n4)[nH]c5c4cccc5)ccc1 | -9.3 |  |
| 585 |  | S=c([nH]1)n(Cc2ccccc2)c3c1cccc3 | -6.3 |  |
| 586 |  | COc1ccc(/C=C/C2=Nc3c(N2C)cccc3)cc1 | -7.3 |  |
| 587 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)Cc4ccc(c5ccccc5)cc4)ccc1 | -8.6 |  |
| 588 |  | Cc(c1)c(C)cc2c1nc(/C=C/c(n3)[nH]c4c3cc(C)c(C)c4)[nH]2 | -8.6 |  |
| 589 |  | Cc1cc(CC(c(n2)[nH]c3c2cccc3)Cc(n4)[nH]c5c4cccc5)cc(C)c1 | -9.3 |  |
| 590 |  | C[N-]c1c([N+]([O-])=O)ccc2c1NC3([N+]2=O)CCCCC3 | -7.3 |  |
| 591 |  | Brc1oc(CN2C(c3oc(Br)cc3)=Nc4c2cccc4)cc1 | -8.0 |  |
| 592 |  | CC(C)(c1ccc(S(=O)(N2CCC(c(n3)[nH]c4c3ccc(Cl)c4)CC2)=O)cc1)C | -9.0 |  |
| 593 |  | CCOC(C1C(N2C(NC1=O)=Nc3c2cccc3)C(C)C)=O | -7.9 |  |
| 594 |  | Fc1c(Cl)cc(NC(C2CC(N3C(N2)=Nc4c3cccc4)=O)=O)cc1 | -8.8 |  |
| 595 |  | CSCC[C@@H](C(NC1CC1)=O)NC(N2CCN3C2=Nc4c3cccc4)=O | -7.6 |  |
| 596 |  | CCCC[N-]c1c([N+]([O-])=O)ccc2c1NC3([N+]2=O)CCCCC3 | -7.6 |  |
| 597 |  | CCOc1c(N2C(C)=Nc3c2ccc(C(O)=O)c3)cccc1 | -7.6 |  |
| 598 |  | Cc(cc(N1CCN(C2CCCC2)CC1)n34)c(C#N)c3=Nc5c4cccc5 | -8.1 |  |
| 599 |  | Clc1cc(C2=NN=C(N2Cc3occc3)SCc(n4)[nH]c5c4cccc5)ccc1 | -8.5 |  |
| 600 |  | Cc1cc(C2=NN=C(N2Cc3occc3)SCc(n4)[nH]c5c4cccc5)ccc1 | -9.0 |  |
| 601 |  | CCN1C(SCc(n2)[nH]c3c2cccc3)=NN=C1c4c(OC)cccc4 | -7.3 |  |
| 602 |  | CC(CCc(n1)[nH]c2c1ccc(C(O)=O)c2)O | -6.8 |  |
| 603 |  | CCOc1ccc(S(=O)(N2C=Nc3c2cc(C)c(C)c3)=O)cc1 | -8.4 |  |
| 604 |  | CC1=Nc2c(N1Cc3ccc(Cl)cc3)cccc2 | -6.7 |  |
| 605 |  | CN1CCCC1c(n2)[nH]c3c2cccc3C(N)=O | -7.6 |  |
| 606 |  | ClCc1oc(CN2C(CN3CCOCC3)=Nc4c2cccc4)nn1 | -7.7 |  |
| 607 |  | Cc1oc(CN2C(CN3CCOCC3)=Nc4c2cccc4)nn1 | -7.7 |  |
| 608 |  | CC1(N2CCC(N3C([C@H]4CCCNC4)=Nc5c3cccc5)CC2)CCCCCCC1 | -8.3 |  |
| 609 |  | CCC1(c(n2)[nH]c3c2cccc3C(N)=O)CCCN1 | -7.9 |  |
| 610 |  | CN1CCCC(c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2)C1 | -8.4 |  |
| 611 |  | CN1CCC(c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2)CC1 | -8.6 |  |
| 612 |  | CC(N1CCCCC1c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2)C | -9.1 |  |
| 613 |  | COC1CCC(c(n2)[nH]c3c2cccc3C(N)=O)CC1 | -7.6 |  |
| 614 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CCCNCC1 | -8.0 |  |
| 615 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CCNCC1 | -7.8 |  |
| 616 |  | CC(C)(c1ccc(c(n2)[nH]c3c2ccc(C(NO)=O)c3)cc1)C | -8.2 |  |
| 617 |  | ONC(c(cc1)cc2c1nc(c3c(c4ccccc4)cccc3)[nH]2)=O | -8.4 |  |
| 618 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1ccc(Cl)c3N)C | -7.7 |  |
| 619 |  | CCc1c(N)c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC(C)C)cc1 | -7.3 |  |
| 620 |  | Nc1c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC4CC4)ccc1F | -7.4 |  |
| 621 |  | COc1c(N)c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC(C)C)cc1 | -7.5 |  |
| 622 |  | CCCc1c(N)c2c(N(C(c3oc(P(O)(O)=O)cc3)=N2)CC(C)C)cc1 | -7.8 |  |
| 623 |  | Cc(ccc1)c2c1[nH]c(c(cn3)nc4c3cccc4)n2 | -7.3 |  |
| 624 |  | CCc1oc(CN2C(CN3CCOCC3)=Nc4c2cccc4)nn1 | -8.2 |  |
| 625 |  | N1(CCOCC1)CC2=Nc3c(N2Cc4oc(c5ccccc5)nn4)cccc3 | -8.4 |  |
| 626 |  | NC(c(ccc1)c2c1nc(c3ccccc3)[nH]2)=O | -7.9 |  |
| 627 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CCNC1 | -7.8 |  |
| 628 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CCCCN1 | -8.2 |  |
| 629 |  | CCCN1CCCCC1c(n2)[nH]c3c2cccc3C(N)=O | -8.1 |  |
| 630 |  | CN1CCC(C1)(c(n2)[nH]c3c2cccc3C(N)=O)C | -7.7 |  |
| 631 |  | ONC(c(cc1)cc2c1nc(c3c(C(F)(F)F)cccc3)[nH]2)=O | -8.1 |  |
| 632 |  | ONC(c(cc1)cc2c1nc(c3ccc(c4ccccc4)cc3)[nH]2)=O | -8.9 |  |
| 633 |  | ONC(c(cc1)cc2c1nc(c3sccc3)[nH]2)=O | -7.3 |  |
| 634 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1c(Cl)ccc3N)C | -7.8 |  |
| 635 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1ccc(Br)c3N)C | -7.8 |  |
| 636 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1c(Br)ccc3N)C | -7.0 |  |
| 637 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1c(Br)cc(Br)c3N)C | -7.2 |  |
| 638 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1c(Cl)c(Cl)c(Br)c3N)C | -8.0 |  |
| 639 |  | CC(N1CCCC(c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2)C1)C | -8.9 |  |
| 640 |  | CC(N1CCC(c2ccc(c(n3)[nH]c4c3c(C(N)=O)ccc4)cc2)CC1)C | -8.9 |  |
| 641 |  | Cc1c(C#N)c2n(c3c(N=2)cccc3)cc1C(Nc4ccc(F)cc4)=O | -8.4 |  |
| 642 |  | Oc1ccc(C2=Nc3c(N2Cc4ccc(OCCN5CCCCC5)cc4)cccc3)cc1 | -8.6 |  |
| 643 |  | ONC(CCCCCNC(NC(c1cc2c(N(C=N2)CCc3ccccc3)cc1)=O)=O)=O | -8.8 |  |
| 644 |  | CC1(N2CCC(N3C([C@@H]4CCCNC4)=Nc5c3cccc5)CC2)CCCCCCC1 | -9.2 |  |
| 645 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1c(Cl)cc(Cl)c3N)C | -8.0 |  |
| 646 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1ccc(F)c3N)C | -7.8 |  |
| 647 |  | CC(C)(c1ccc(CN2C(c3oc(P(O)(O)=O)cc3)=Nc4c2cccc4N)cc1)C | -8.3 |  |
| 648 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CCN1 | -7.9 |  |
| 649 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CCCN1 | -7.9 |  |
| 650 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CNC1 | -7.3 |  |
| 651 |  | CN1CCCC1(c(n2)[nH]c3c2cccc3C(N)=O)C | -8.0 |  |
| 652 |  | COc1ccc(CN2C(/C=C/c3ccccc3)=Nc4c2cccc4)cc1 | -8.4 |  |
| 653 |  | Clc1ccc(CN2C(/C=C/c3occc3)=Nc4c2cccc4)cc1 | -8.4 |  |
| 654 |  | Clc1ccc(OCC2=NN=C(N2Cc3occc3)SCc(n4)[nH]c5c4cccc5)cc1 | -8.0 |  |
| 655 |  | CC(C)([N-]c1c([N+]([O-])=O)ccc2c1NC3([N+]2=O)CCCCC3)C | -7.8 |  |
| 656 |  | CC(C[C@@H](C(NCc1ccccc1)=O)NC(N2CCN3C2=Nc4c3cccc4)=O)C | -8.5 |  |
| 657 |  | COc1c(OC)c(OC)cc(c(c2)c(C#N)c(N)n3c2=Nc4c3cccc4)c1 | -8.0 |  |
| 658 |  | COc1ccc(c(c2)c(C#N)c(N)n3c2=Nc4c3cccc4)cc1 | -7.8 |  |
| 659 |  | CCN1C(C)=Nc2c1ccc(S(=O)(Nc3ccc(C)cc3)=O)c2 | -7.9 |  |
| 660 |  | [O-][N+](c1c(/C=N/NC(c(cc2)cc3c2nc[nH]3)=O)cccc1)=O | -8.6 |  |
| 661 |  | Cc1ccc(OCC2=NN=C(N2Cc3occc3)SCc(n4)[nH]c5c4cccc5)cc1 | -9.2 |  |
| 662 |  | CCCCc(c(C)c(C#N)c([nH]1)n2c3c1cccc3)c2=O | -7.7 |  |
| 663 |  | COc1cc(OC)cc(NC([C@@H](NC(N2CCN3C2=Nc4c3cccc4)=O)C)=O)c1 | -8.3 |  |
| 664 |  | NC(c(ccc1)c2c1[nH]c(c3c(F)cc([C@H]4CCCN4)cc3)n2)=O | -8.2 |  |
| 665 |  | NC(c(ccc1)c2c1[nH]c(c3c(F)cc([C@H]4CCCCN4)cc3)n2)=O | -8.9 |  |
| 666 |  | Clc1ccc(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cc1 | -8.5 |  |
| 667 |  | Fc1ccc(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cc1 | -8.7 |  |
| 668 |  | COc1ccc(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cc1 | -9.0 |  |
| 669 |  | CC1(N2CCC(N3C(c4cc(S(C)(=O)=O)ccc4)=Nc5c3cccc5)CC2)CCCCCCC1 | -9.0 |  |
| 670 |  | Nc(c1)c(N)cc2c1nc[nH]2 | -6.3 |  |
| 671 |  | ONC(c(cc1)cc2c1nc(c3ccc(c4c(F)cccc4)cc3)[nH]2)=O | -8.9 |  |
| 672 |  | Fc1c(CN2C(c3c(F)cccc3F)=Nc4c2cccc4)c(F)ccc1 | -8.3 |  |
| 673 |  | [O-][N+](c1c(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cccc1)=O | -8.3 |  |
| 674 |  | [O-][N+](c1ccc(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cc1)=O | -9.7 |  |
| 675 |  | Cc1ccc(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cc1 | -9.4 |  |
| 676 |  | C[C@@]1(c(n2)[nH]c3c2cccc3C(N)=O)CCCN1 | -8.0 |  |
| 677 |  | COc1c(N2CCN(CC2)CCCSC3=Nc4c(N3C)cccc4)cccc1 | -7.7 |  |
| 678 |  | N1(CCCCC1)CCOc2ccc(Oc(n3)[nH]c4c3cccc4)cc2 | -7.5 |  |
| 679 |  | CC(Nc1cc(C2CCN(CC2)CCCCN3C(c4ccccc4)=Nc5c3cccc5)ccc1)=O | -8.6 |  |
| 680 |  | CC(Nc1cc(C2CCN(CC2)CCCCCN3C(c4ccccc4)=Nc5c3cccc5)ccc1)=O | -9.1 |  |
| 681 |  | CCC(N1C(c2oc(P(O)(O)=O)cc2)=Nc3c1ccc(F)c3N)CC | -7.7 |  |
| 682 |  | COc1c(N2CCN(CC2)CCc(cc3Br)cc4c3nc[nH]4)cccc1 | -7.6 |  |
| 683 |  | Clc1c(N2CCN(CC2)CCc(cc3Cl)cc4c3nc[nH]4)cccc1 | -7.6 |  |
| 684 |  | NC(c(cc(F)c1)c2c1[nH]c(c3c(F)cc(C4CCCCN4)cc3)n2)=O | -9.3 |  |
| 685 |  | NC(c(cc(F)c1)c2c1[nH]c(c3c(F)cc(C4CCCN4)cc3)n2)=O | -8.6 |  |
| 686 |  | Oc1cc2c(N=C(N2Cc3ccc(OCCN4CCCCC4)cc3)c5ccccc5)cc1 | -8.1 |  |
| 687 |  | ClCCc1oc(CN2C(CN3CCOCC3)=Nc4c2cccc4)nn1 | -7.7 |  |
| 688 |  | Clc1c(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cccc1 | -8.3 |  |
| 689 |  | Fc1c(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cccc1 | -9.1 |  |
| 690 |  | Cc1c(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cccc1 | -8.9 |  |
| 691 |  | COc1c(c2oc(CN3C(CN4CCOCC4)=Nc5c3cccc5)nn2)cccc1 | -8.5 |  |
| 692 |  | Cc1c(c(n2)[nH]c3c2ccc(C(NO)=O)c3)c(C)cc(O)c1 | -8.2 |  |
| 693 |  | COc1c(O)c(c(n2)[nH]c3c2ccc(C(NO)=O)c3)ccc1 | -8.4 |  |
| 694 |  | ONC(c(cc1)cc2c1nc(c3c(O)ccc(Cl)c3)[nH]2)=O | -8.5 |  |
| 695 |  | ONC(c(cc1)cc2c1nc(c3cc(OCCOc4ccccc4)ccc3)[nH]2)=O | -8.3 |  |
| 696 |  | CC1(N2CCC(N3C(c4cc(C(F)(F)F)ccc4)=Nc5c3cccc5)CC2)CCCCCCC1 | -9.9 |  |
| 697 |  | COc1c(N2CCN(CC2)CCc(cc3Cl)cc4c3nc[nH]4)cccc1 | -7.6 |  |
| 698 |  | Clc(cc(CCN1CCN(c2ncccn2)CC1)c3)c4c3[nH]cn4 | -8.1 |  |
| 699 |  | NC(c(ccc1)c2c1[nH]c(c3c(F)cc([C@@H]4CCCN4)cc3)n2)=O | -8.2 |  |
| 700 |  | N1(CCCC1)CCOc2ccc(Oc(n3)[nH]c4c3cccc4)cc2 | -7.2 |  |
| 701 |  | Clc1c(N2CCN(CC2)CCc(cc3Br)cc4c3nc[nH]4)cccc1 | -7.5 |  |
| 702 |  | N1(CCOCC1)CCOc2ccc(Oc(n3)[nH]c4c3cccc4)cc2 | -7.8 |  |
| 703 |  | c1(OCCCN2CCCCC2)ccc(Oc(n3)[nH]c4c3cccc4)cc1 | -8.1 |  |
| 704 |  | N1(CCCCCC1)CCOc2ccc(Oc(n3)[nH]c4c3cccc4)cc2 | -8.6 |  |
| 705 |  | CN(CCN1C=Nc2c1ccc(C(NC(NCCCCCC(NO)=O)=O)=O)c2)C | -7.8 |  |
| 706 |  | CC(Nc1cc(C2CCN(CC2)CCN3C(c4ccccc4)=Nc5c3cccc5)ccc1)=O | -9.3 |  |
| 707 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4ccccc4)=Nc5c3cccc5)ccc1)=O | -8.8 |  |
| 708 |  | Fc1c(Cl)cc(c(cc2)cc3c2[nH]c(=S)n3C4CCCC4)cc1 | -8.5 |  |
| 709 |  | Cc1oc(c2cc3c(N=CN3c4ccc(S(C)=O)cc4)cc2)cc1 | -8.2 |  |
| 710 |  | COc1ccc(OCc(n2)[nH]c3c2ccc(S(=O)(Nc4c(Cl)cccc4)=O)c3)cc1 | -9.4 |  |
| 711 |  | ONC(c(cc1)cc2c1nc(c3sc(c4ccccc4)cc3)[nH]2)=O | -8.6 |  |
| 712 |  | CC(Oc1ccc(c(n2)[nH]c3c2ccc(C(NO)=O)c3)cc1)C | -8.2 |  |
| 713 |  | CC(c1ccc(c(n2)[nH]c3c2ccc(C(NO)=O)c3)cc1)C | -8.4 |  |
| 714 |  | COc1ccc(Oc2cc(c(n3)[nH]c4c3ccc(C(NO)=O)c4)ccc2)cc1 | -9.8 |  |
| 715 |  | ONC(c(cc1)cc2c1nc(c(ccn3)c4c3cccc4)[nH]2)=O | -8.9 |  |
| 716 |  | c1(c(n2)[nH]c3c2cccc3)n[nH]cc1 | -6.9 |  |
| 717 |  | ONC(c(cc1)cc2c1nc(c3cc(F)c(c4ccccc4)cc3)[nH]2)=O | -8.8 |  |
| 718 |  | [O-][N+](c1ccc(/C=C/c(n2)[nH]c3c2ccc([N+]([O-])=O)c3)cc1)=O | -8.0 |  |
| 719 |  | CCCc(cc(N1CCN=C1)n23)c(C#N)c2=Nc4c3cccc4 | -7.5 |  |
| 720 |  | Clc(cc1)cc2c1nc(C3CCN(CC3)CC4N(C)N(C)N(C(C)C)N4C5CCCCC5)[nH]2 | -8.9 |  |
| 721 |  | CCOc1c(S(=O)(N2C=Nc3c2cc(C)c(C)c3)=O)cc(Cl)cc1 | -7.9 |  |
| 722 |  | CC(c1c(C#N)c2n(c3c(N=2)cccc3)c(NCCCN4CCOCC4)c1)C | -8.2 |  |
| 723 |  | CN1C(CN2CCN(c3cc(Cl)ccc3)CC2)=Nc4c1cccc4 | -8.4 |  |
| 724 |  | Cc(cc(NCCCCO)n12)c(C#N)c1=Nc3c2cccc3 | -6.8 |  |
| 725 |  | CCC([C@@H](C(NCc1ccc(OC)cc1)=O)NC(N2CCN3C2=Nc4c3cccc4)=O)C | -8.7 |  |
| 726 |  | CC1(CC(N2C(Nc3ccc(OC(F)(F)F)cc3)=Nc4c2ccc(C#N)c4)CC(C)(C1)C)C | -9.1 |  |
| 727 |  | CSCC[C@@H](C(NCc1ccc(F)cc1)=O)NC(N2CCN3C2=Nc4c3cccc4)=O | -8.5 |  |
| 728 |  | CN1CCC[C@@H](C2=Nc3c(N2C4CCN(C5(CCCCCCC5)C)CC4)cccc3)C1 | -8.5 |  |
| 729 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4c(C(F)(F)F)cccc4)=Nc5c3cccc5)ccc1)=O | -8.8 |  |
| 730 |  | COc1cc(C2=Nc3c(N2CCCN4CCC(c5cc(NC(C)=O)ccc5)CC4)cccc3)ccc1 | -9.6 |  |
| 731 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4cc(C(F)(F)F)ccc4)=Nc5c3cccc5)ccc1)=O | -9.9 |  |
| 732 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4ccc(F)cc4)=Nc5c3cccc5)ccc1)=O | -9.6 |  |
| 733 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4ccc(c5ccccc5)cc4)=Nc6c3cccc6)ccc1)=O | -9.0 |  |
| 734 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4ccc(Br)cc4)=Nc5c3cccc5)ccc1)=O | -10.1 |  |
| 735 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4ccc(Cl)cc4)=Nc5c3cccc5)ccc1)=O | -9.5 |  |
| 736 |  | Clc1ccc(C2=Nc3c(N2CCCN4CCC(c5cc(NC(c6ccccc6)=O)ccc5)CC4)cccc3)cc1 | -10.4 |  |
| 737 |  | CC(C(Nc1cc(C2CCN(CC2)CCCN3C(c4ccc(Cl)cc4)=Nc5c3cccc5)ccc1)=O)C | -10.0 |  |
| 738 |  | CC(Nc1c(C2CCN(CC2)CCCN3C(c4ccc(Cl)cc4)=Nc5c3cccc5)cccc1)=O | -8.3 |  |
| 739 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4ccc(C#N)cc4)=Nc5c3cccc5)ccc1)=O | -9.1 |  |
| 740 |  | CC(c1ccc(C2=Nc3c(N2CCCN4CCC(c5cc(NC(C)=O)ccc5)CC4)cccc3)cc1)C | -9.4 |  |
| 741 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4ccc(Oc5ccccc5)cc4)=Nc6c3cccc6)ccc1)=O | -10.7 |  |
| 742 |  | NC(c(ccc1)c2c1nc(C3CCN3)[nH]2)=O | -7.8 |  |
| 743 |  | CN(C(c1cc(c2ccc(c(n3)[nH]c4c3ccc(C(NO)=O)c4)cc2)ccc1)=O)C | -9.7 |  |
| 744 |  | CCN(CCOc1ccc(c(n2)[nH]c3c2ccc(C(NO)=O)c3)cc1)CC | -9.6 |  |
| 745 |  | OC(c1cc2c(N(C(c3ccc(OCc4c(c5ccc(Cl)cc5)ccc(Cl)c4)cc3)=N2)C6CCCCC6)cc1)=O | -11.1 |  |
| 746 |  | OC(c1cc2c(N(C(c3ccc(OCc4c(c5ccccc5)ccc(Cl)c4)cc3)=N2)C6CCCCC6)cc1)=O | -9.5 |  |
| 747 |  | CCC(n(c(cc(c1cc(Cl)c(F)cc1)cc2)c2[nH]3)c3=S)CC | -7.1 |  |
| 748 |  | FC(F)(c1cc(N2CCN(CC2)CCc(cc3Br)cc4c3nc[nH]4)ccc1)F | -8.8 |  |
| 749 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1cc(Cl)c(F)c3N)C | -7.8 |  |
| 750 |  | CCN(CCN1C=Nc2c1ccc(C(NC(NCCCCCC(NO)=O)=O)=O)c2)CC | -7.7 |  |
| 751 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4c(Cl)cccc4)=Nc5c3cccc5)ccc1)=O | -9.5 |  |
| 752 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4cc(Cl)ccc4)=Nc5c3cccc5)ccc1)=O | -8.2 |  |
| 753 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4ccc(C(F)(F)F)cc4)=Nc5c3cccc5)ccc1)=O | -10.4 |  |
| 754 |  | Clc1cc(Nc2nc(N3C=Nc4c3cccc4)ccn2)ccc1 | -7.9 |  |
| 755 |  | COc1c(C2=Nc3c(N2CCCN4CCC(c5cc(NC(C)=O)ccc5)CC4)cccc3)cccc1 | -9.1 |  |
| 756 |  | CCc1ccc(C2=Nc3c(N2CCCN4CCC(c5cc(NC(C)=O)ccc5)CC4)cccc3)cc1 | -9.5 |  |
| 757 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4c(Cl)cc(Cl)cc4)=Nc5c3cccc5)ccc1)=O | -9.0 |  |
| 758 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4cc(Cl)c(Cl)cc4)=Nc5c3cccc5)ccc1)=O | -9.2 |  |
| 759 |  | ONC(CCCCCNC(NC(c1cc2c(N(C=N2)CCCc3ccccc3)cc1)=O)=O)=O | -8.1 |  |
| 760 |  | Oc1ccc(C2=Nc3c(N2Cc4ccc(OCCN5CCCCC5)cc4)ccc(O)c3)cc1 | -8.6 |  |
| 761 |  | COc1ccc(C2=Nc3c(N2CCCN4CCC(c5cc(NC(C)=O)ccc5)CC4)cccc3)cc1 | -9.1 |  |
| 762 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4cc(F)c(F)cc4)=Nc5c3cccc5)ccc1)=O | -9.6 |  |
| 763 |  |  |  |  |
| 764 |  | OC(c1cc2c(N(C(c3ccc(OCc4c(c5cc(Cl)ccc5)ccc(Cl)c4)cc3)=N2)C6CCCCC6)cc1)=O | -9.9 |  |
| 765 |  | [C@H]1(c(c[nH]2)c3c2cccc3)CC[C@H](N4CCN(c(ccc5)c6c5[nH]cn6)CC4)CC1 | -9.2 |  |
| 766 |  | CC1(N2CCC(N3C(c4cc(Cl)c(F)cc4)=Nc5c3cccc5)CC2)CCCCCCC1 | -9.5 |  |
| 767 |  | C[C@]1(c(n2)[nH]c3c2cccc3C(N)=O)CCCN1 | -8.2 |  |
| 768 |  | Cc(c1)c(C)cc2c1nc(CS)[nH]2 | -5.6 |  |
| 769 |  | CC1(N2CCC(N3C(c(c4)oc5c4cccc5)=Nc6c3cccc6)CC2)CCCCCCC1 | -10.0 |  |
| 770 |  | CN1CCC[C@H](C2=Nc3c(N2C4CCN(C5(CCCCCCC5)C)CC4)cccc3)C1 | -8.7 |  |
| 771 |  | CC1CN(C2=Nc3c(N2C4CCN(C5(CCCCCCC5)C)CC4)cccc3)CC(N1)C | -8.9 |  |
| 772 |  | CC1(c(n2)[nH]c3c2c(C(N)=O)cc(C(F)(F)F)c3)CCCN1 | -8.1 |  |
| 773 |  | NC(c(ccc1)c2c1nc(C3CNCCN3)[nH]2)=O | -7.9 |  |
| 774 |  | COc1ccc(c2c(c(n3)[nH]c4c3cccc4)c(c5ccccc5)n[nH]2)cc1 | -8.6 |  |
| 775 |  | CCc1c(/N=C/c(c(C)c(C#N)c([nH]2)n3c4c2cccc4)c3=O)cccc1 | -8.3 |  |
| 776 |  | CCN1C(C)=Nc2c1ccc(C(N/N=C/c3ccc([N+]([O-])=O)cc3)=O)c2 | -8.0 |  |
| 777 |  | CC1(CC(N2C(Nc3ccc(OC(F)(F)F)cc3)=Nc4c2ccc(S(N)(=O)=O)c4)CC(C)(C1)C)C | -9.6 |  |
| 778 |  | COc1c(/N=C/c(c(C)c(C#N)c([nH]2)n3c4c2cccc4)c3=O)cccc1 | -8.3 |  |
| 779 |  | CC(CCc(c(C)c(C#N)c([nH]1)n2c3c1cccc3)c2=O)C | -7.4 |  |
| 780 |  | CCc(c(C)c1C#N)c(Cl)n2c1=Nc3c2cccc3 | -7.5 |  |
| 781 |  | O=C(C1C2=Nc3c(N2CCC1=O)cccc3)Nc4ccc(c5ccccc5)cc4 | -9.2 |  |
| 782 |  | CCCc1c(C#N)c2n(c3c(N=2)cccc3)c(NCC4CCCO4)c1 | -7.0 |  |
| 783 |  | CCOC(N1c2c(N(C1=O)Cc3c(Cl)cccc3)cccc2)=O | -7.7 |  |
| 784 |  | Cc(cc(c1occc1)c2C#N)n3c2=Nc4c3cccc4 | -8.1 |  |
| 785 |  | Cc1cc(C)c(NC(C2CC(NC3=Nc4c(N23)cccc4)=O)=O)cc1 | -9.1 |  |
| 786 |  | CCC([C@@H](C(NCCc1cc(OC)c(OC)cc1)=O)NC(N2CCN3C2=Nc4c3cccc4)=O)C | -8.3 |  |
| 787 |  | CC1=Nc2c(N1C3CCN(CC3)CC4=NN=NN4CCc5ccccc5)cccc2 | -9.1 |  |
| 788 |  | COc(cc1)cc2c1nc(SC3C([N+]([O-])=O)N=C(N3Cc4ccccc4)C)[nH]2 | -8.3 |  |
| 789 |  | COc1ccc(CN2CNC3=Nc4c(N3C2)cccc4)cc1 | -8.0 |  |
| 790 |  | COc1ccc(/C=C/C2=Nc3c(N2Cc4cc(OC)c(OC)cc4)cccc3)cc1 | -8.5 |  |
| 791 |  | CCOC(c1cc2c(N(C(COc3ccc(OC)cc3)=N2)CC)cc1)=O | -7.4 |  |
| 792 |  | CCCCOc1ccc(S(=O)(N2C(C)=Nc3c2cccc3)=O)cc1 | -7.3 |  |
| 793 |  | CCCN1c2c(c3c1ccc(C4=Nc5c(N4CC6CC6)ccc(C(O)=O)c5)c3)cccc2 | -8.8 |  |
| 794 |  | CCCN1CCC(c(n2)[nH]c3c2cccc3C(N)=O)C1 | -7.7 |  |
| 795 |  | NC(c(ccc1)c2c1nc(C3CCN(C4CCCC4)C3)[nH]2)=O | -8.9 |  |
| 796 |  | CCCN1CC(c(n2)[nH]c3c2cccc3C(N)=O)C1 | -7.2 |  |
| 797 |  | CC(NC(c(ccc1)c2c1nc(C3=CC(C)(NC3(C)C)C)[nH]2)=O)C | -7.9 |  |
| 798 |  | Nc1c2c(N(C(c3c(F)cccc3F)=N2)Cc4c(F)cccc4F)ccc1 | -8.2 |  |
| 799 |  | CCc1c2c(N(C(c3c(F)cccc3F)=N2)Cc4c(F)cccc4F)ccc1 | -8.4 |  |
| 800 |  | [O-][N+](c1c2c(N(C(c3c(F)cccc3F)=N2)Cc4c(F)cccc4F)ccc1)=O | -8.9 |  |
| 801 |  | CCNc1c(N2CCN(c(n3)[nH]c4c3c(C(N)=O)ccc4)CC2)nccc1 | -8.3 |  |
| 802 |  | CC(Nc1cnc(N2CCN(c(n3)[nH]c4c3c(C(N)=O)ccc4)CC2)nc1)=O | -8.8 |  |
| 803 |  | NC(c(ccc1)c2c1[nH]c(N3CCN(c4ncnc(C(F)(F)F)c4)CC3)n2)=O | -8.6 |  |
| 804 |  | OC(c1cc2c(N(C(c3cc4c(N(c5c4cccc5)CC=C)cc3)=N2)CC6CC6)cc1)=O | -8.3 |  |
| 805 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CCOC)ccc(C#N)c5)c3)cccc2 | -6.0 |  |
| 806 |  | CN(c(n1)[nH]c2c1c(Br)c(Br)c(Br)c2Br)C | -8.1 |  |
| 807 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CCOC)ccc(C(N)=O)c5)c3)cccc2 | -8.6 |  |
| 808 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4C(C)C)ccc(C(O)=O)c5)c3)cccc2 | -9.1 |  |
| 809 |  | CC1(CC(N2C(Nc3ccc(OC(F)(F)F)cc3)=Nc4c2ccc(C(O)=O)c4)CC(C)(C1)C)C | -7.9 |  |
| 810 |  | CN1CCN(c(ccc2)c3c2[nH]cn3)CC1 | -9.2 |  |
| 811 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1c(CCCCCl)cc(F)c3N)C | -6.6 |  |
| 812 |  | CC(CCCc1c2c(N=C(N2CC(C)C)c3oc(P(O)(O)=O)cc3)c(N)c(F)c1)C | -8.0 |  |
| 813 |  | CC(CCCc1c2c(N=C(N2CC(C)C)c3oc(P(O)(O)=O)cc3)c(N)c(F)c1)C | -8.0 |  |
| 814 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1c(c4ccc(F)cc4)cc(F)c3N)C | -6.8 |  |
| 815 |  | COc1c(OC)cc2c(N=CN2c3sc(C#N)c(O)c3)c1 | -8.9 |  |
| 816 |  | CCS(=O)(c1ccc(Oc(c2)c(CN3C=CN=C3)cc4c2[nH]c(c5ncccc5)n4)cc1)=O | -8.2 |  |
| 817 |  | Cc1c2c(N(C(c3c(F)cccc3F)=N2)Cc4c(F)cccc4F)ccc1 | -8.2 |  |
| 818 |  | Fc1c(CN2C(c3c(F)cccc3F)=Nc4c2cccc4Cl)c(F)ccc1 | -8.7 |  |
| 819 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CC=C)ccc(C(OC)=O)c5)c3)cccc2 | -8.7 |  |
| 820 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4C)ccc(C(NC)=O)c5)c3)cccc2 | -8.0 |  |
| 821 |  | CCOC(c1cc2c(N(C(c3cc4c(N(c5c4cccc5)CC)cc3)=N2)C(C)C)cc1)=O | -8.3 |  |
| 822 |  | CCN1C(c2cc3c(N(c4c3cccc4)CC)cc2)=Nc5c1ccc(C(OC)=C)c5 | -8.5 |  |
| 823 |  | NC(c(ccc1)c2c1nc([C@H]3CCCCN3)[nH]2)=O | -8.0 |  |
| 824 |  | NC(c(ccc1)c2c1nc([C@@H]3CCCCN3)[nH]2)=O | -8.0 |  |
| 825 |  | CN1CCCCC1c(n2)[nH]c3c2cccc3C(N)=O | -7.4 |  |
| 826 |  | CC.NC(c(ccc1)c2c1nc(C3CCN(C4CCCC4)CC3)[nH]2)=O |  |  |
| 827 |  | CN1CCN(C(c(n2)[nH]c3c2cccc3C(N)=O)C1)C | -8.1 |  |
| 828 |  | C[C@]1(c(n2)[nH]c3c2cccc3C(N)=O)CCC(N1)=O | -8.4 |  |
| 829 |  | COc1cnc(N2CCN(c(n3)[nH]c4c3c(C(N)=O)ccc4)CC2)nc1 | -8.0 |  |
| 830 |  | NC(c(ccc1)c2c1[nH]c(N3CCN(c4ncc(N)cn4)CC3)n2)=O | -8.4 |  |
| 831 |  | NC(c(ccc1)c2c1[nH]c(N3CCN(c4nc(C(F)(F)F)ccn4)CC3)n2)=O | -8.7 |  |
| 832 |  | ONC(c(cc1)cc2c1nc(c3cc4c(OCC4)cc3)[nH]2)=O | -8.6 |  |
| 833 |  | NC(c1cnc(N2CCN(c(n3)[nH]c4c3c(C(N)=O)ccc4)CC2)cc1)=O | -9.1 |  |
| 834 |  | NC(c(ccc1)c2c1[nH]c(N3CCN(c4cc(C(F)(F)F)ncc4)CC3)n2)=O | -9.0 |  |
| 835 |  | ONC(c(cc1)cc2c1nc(c3sc(c4c(F)cccc4)cc3)[nH]2)=O | -8.6 |  |
| 836 |  | CN(C(c1cnc(N2CCN(c(n3)[nH]c4c3c(C(N)=O)ccc4)CC2)cc1)=O)C | -9.5 |  |
| 837 |  | CC1(C=C(C(C)(N1O)C)CN2C=Nc3c2cccc3C(N)=O)C | -8.4 |  |
| 838 |  | CC(CN1C(c2oc(P(O)(O)=O)cc2)=Nc3c1c(CCCO)cc(F)c3N)C | -8.1 |  |
| 839 |  | CS(=O)(Nc1ccc(c2ccc(c(n3)[nH]c4c3ccc(C(NO)=O)c4)cc2)cc1)=O | -9.3 |  |
| 840 |  | C[C@@H]1[C@@H]([C@@]1(C(O)=O)NS(=O)(N2CCN3C(C2)=Nc4c3cccc4)=O)c5ccccc5 | -8.8 |  |
| 841 |  | N1(CCCCC1)CCOc2ccc(c3cc4c(N(c5ccccc5)C=N4)cc3)cc2 | -9.1 |  |
| 842 |  | CCCCC1=Nc2c(N1CC(c3cc(S(N)(=O)=O)c(Cl)cc3)=O)cccc2 | -8.0 |  |
| 843 |  | COc1c2c(N(C(c3c(F)cccc3F)=N2)Cc4c(F)cccc4F)ccc1 | -8.5 |  |
| 844 |  | CCCc1c2c(N=C(N2CC(C)C)c3oc(P(O)(O)=O)cc3)c(N)c(F)c1 | -7.0 |  |
| 845 |  | CC(CN1C(C2=CC=C(P(O)(O)=O)O2)=Nc3c1c(c4ccc(Cl)cc4)cc(F)c3N)C | -7.8 |  |
| 846 |  | Fc1c(CN2C(c3c(F)cccc3F)=Nc4c2cccc4Br)c(F)ccc1 | -8.6 |  |
| 847 |  | CC1(Cc2c(O1)cc(N3CCOCC3)c(NC(c(ccc4)c5c4[nH]cn5)=O)c2)C | -8.2 |  |
| 848 |  | CC(c1ccc(C2=Nc3c(N2C)ccc(C(NO)=O)c3)cc1)C | -8.9 |  |
| 849 |  | COc1c(OC)cc(c2oc(c(n3)[nH]c4c3ccc(C(NO)=O)c4)cc2)cc1 | -8.8 |  |
| 850 |  | OC(c1cc2c(N(C(c3cc4c(N(c5c4cccc5)CC6CCC6)cc3)=N2)CC7CC7)cc1)=O | -9.2 |  |
| 851 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CCOC)ccc(S(N)(=O)=O)c5)c3)cccc2 | -8.7 |  |
| 852 |  | CN(C(c1ccc(N(c2c3cccc2)CC)c3c1)=N4)c5c4cc(S(=O)(NC)=O)cc5 | -9.1 |  |
| 853 |  | CN1c2c(c3c1ccc(C4=Nc5c(N4CC6CC6)ccc(C(O)=O)c5)c3)cccc2 | -9.6 |  |
| 854 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CC6CC6)ccc(C(OC)=O)c5)c3)cccc2 | -9.3 |  |
| 855 |  | C[C@]1(c(n2)[nH]c3c2c(C(N)=O)cc(F)c3)CCCN1 | -8.5 |  |
| 856 |  | C[C@]1(c(n2)[nH]c3c2c(C(N)=O)cc(Cl)c3)CCCN1 | -8.0 |  |
| 857 |  | COC(Nc(n1)[nH]c2c1ccc(Oc3ccc(NC(Nc4ccccc4)=O)cc3)c2)=O | -10.3 |  |
| 858 |  | [O-][N+](c(cc1)cc2c1nc(CCCc(n3)[nH]c4c3ccc([N+]([O-])=O)c4)[nH]2)=O | -9.4 |  |
| 859 |  | CN1CCC(c(n2)[nH]c3c2cccc3C(N)=O)CC1 | -7.8 |  |
| 860 |  | CC(N1CCC(c(n2)[nH]c3c2cccc3C(N)=O)CC1)=O | -8.1 |  |
| 861 |  | NC(c(ccc1)c2c1nc(C3CCCN(C4CCCC4)CC3)[nH]2)=O | -8.4 |  |
| 862 |  | NC(c(ccc1)c2c1nc(C3CCN3C4CCCC4)[nH]2)=O | -8.0 |  |
| 863 |  | NC(c(ccc1)c2c1nc(C3CN(C4CCCC4)C3)[nH]2)=OSSS | -7.3 |  |
| 864 |  | CN1CCCC(c(n2)[nH]c3c2cccc3C(N)=O)C1 | -7.8 |  |
| 865 |  | COc1ccc(/C=C/C2=Nc3c(N2Cc4c(OC)cccc4)cccc3)cc1 | -8.4 |  |
| 866 |  | CC(c(cc(NCc1ncccc1)n23)c(C#N)c2=Nc4c3cccc4)C | -8.5 |  |
| 867 |  | COCCN(c(cc(C)c1C#N)n2c1=Nc3c2cccc3)CCOC | -7.0 |  |
| 868 |  | CCCCN1C(SCc2c(C)onc2C)=Nc3c1ccc(S(N)(=O)=O)c3 | -8.1 |  |
| 869 |  | CCN(c1cc(O)c(/C=N/NC(c(cc2)cc3c2nc[nH]3)=O)cc1)CC | -7.6 |  |
| 870 |  | OC[C@H]1O[C@@H](c(n2)[nH]c3c2ccc(C(NCc4cc(Cl)cc(Cl)c4)=O)c3)C[C@@H]1O | -8.7 |  |
| 871 |  | CN(CCNc(c(CC=C)c(C)c1C#N)n2c1=Nc3c2cccc3)C | -6.5 |  |
| 872 |  | CCN(S(=O)(c1cc2c(N(C(SCn(nnc3c4cccc3)c4=O)=N2)CC)cc1)=O)CC | -8.1 |  |
| 873 |  | CCN1C(COc2ccc(Cl)cc2)=NN=C1SCc(n3)[nH]c4c3cccc4 | -8.4 |  |
| 874 |  | CCOC(N1c2c(N(C1=O)Cc3c(Cl)cccc3Cl)cccc2)=O | -7.8 |  |
| 875 |  | CC(c1c(OCCn(c(cccc2)c2[nH]3)c3=S)ccc(C)c1)C | -8.2 |  |
| 876 |  | CC(C)(c1ccc(CN2C3=NCCCN3c4c2cccc4)cc1)C | -8.9 |  |
| 877 |  | Cc(c1)c(C)cc2c1nc(C3CCN(CC3)CC4COc5c(O4)cccc5)[nH]2 | -9.7 |  |
| 878 |  | C[C@@H]1[C@](c2ccccc2)([C@@]1(C(O)=O)NS(=O)(N3CCN4C(C3)=Nc5c4ccc(F)c5)=O)C | -8.7 |  |
| 879 |  | C[C@@H]1[C@@H]([C@@]1(C(O)=O)NS(=O)(N2CCN3C(C2)=Nc4c3ccc(C)c4)=O)c5ccccc5 | -9.2 |  |
| 880 |  | COc1cc(N2C(C)=Nc3c2ccc(C(O)=O)c3)c(OC)cc1 | -7.7 |  |
| 881 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CCC6CC6)ccc(C(O)=O)c5)c3)cccc2 | -9.0 |  |
| 882 |  | CCN1C(COc2cc(C)ccc2)=Nc3c1cccc3 | -7.3 |  |
| 883 |  | CCN1C(COc2c(C)cccc2)=Nc3c1cccc3 | -7.4 |  |
| 884 |  | CCNC(Nc(n1)[nH]c2c1c(c3cnccc3)cc(c4cnccc4)c2)=O | -8.0 |  |
| 885 |  | c1([nH]c(c(cn2)nc3c2cccc3)n4)c4cccc1 | -8.1 |  |
| 886 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4c(Cl)cc(F)cc4)=Nc5c3cccc5)ccc1)=O | -9.3 |  |
| 887 |  | CC(Nc1cc(C2CCN(CC2)CCCN3C(c4c(F)cc(Cl)cc4)=Nc5c3cccc5)ccc1)=O | -9.2 |  |
| 888 |  | OC(c(cc1)cc2c1nc(C(F)(F)F)[nH]2)=O | -8.1 |  |
| 889 |  | Cc1ccc(C(Nc2cc(C3CCN(CC3)CCCN4C(c5ccc(Cl)cc5)=Nc6c4cccc6)ccc2)=O)cc1 | -10.2 |  |
| 889 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CCO)ccc(C(O)=O)c5)c3)cccc2 |  |  |
| 890 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CCCOC)ccc(C(O)=O)c5)c3)cccc2 | -9.0 |  |
| 891 |  | CN1CCC[C@@H]1c(n2)[nH]c3c2cccc3C(N)=O | -7.5 |  |
| 892 |  | CN1CCC[C@H]1c(n2)[nH]c3c2cccc3C(N)=O | -7.9 |  |
| 893 |  | NC(c(ccc1)c2c1nc([C@@H]3CCC(N3)=O)[nH]2)=O | -7.8 |  |
| 894 |  | CC(CC1=Nc2c(N1CC(c3cc(S(N)(=O)=O)c(Cl)cc3)=O)cccc2)C | -8.4 |  |
| 895 |  | NC(c(ccc1)c2c1[nH]c(C3CCN(S(=O)(c4ccccc4)=O)CC3)n2)=O | -8.3 |  |
| 896 |  | CN(S(=O)(N1CCC(c(n2)[nH]c3c2cccc3C(N)=O)CC1)=O)C | -8.0 |  |
| 897 |  | CN(S(=O)(c1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)=O)C | -9.3 |  |
| 898 |  | CN(C(c1cc(c2ccc(Cl)cc2)c(COc3ccc(C4=Nc5c(N4C6CCCCC6)ccc(C(O)=O)c5)cc3)cc1)=O)C | -9.6 |  |
| 899 |  | CC(c1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)=O | -9.8 |  |
| 900 |  | CC(Nc1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)=O | -9.4 |  |
| 901 |  | OC(c1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)=O | -9.7 |  |
| 902 |  | COc1ccc(c2c(COc3ccc(C4=Nc5c(N4C6CCCCC6)ccc(C(O)=O)c5)cc3)cc(Cl)cc2)cc1 | -8.4 |  |
| 903 |  | Cc1ccc(c2c(COc3ccc(C4=Nc5c(N4C6CCCCC6)ccc(C(O)=O)c5)cc3)cc(Cl)cc2)cc1 | -10.4 |  |
| 904 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CCN(C1)Cc4c(F)cccc4 | -9.6 |  |
| 905 |  | CCNC(Nc(n1)[nH]c2c1ccc(c3cnccc3)c2)=O | -7.6 |  |
| 906 |  | OC(c1cc2c(N(C(c3ccc(OCc4c(c5ccc(Cl)cc5)nccc4)cc3)=N2)C6CCCCC6)cc1)=O | -9.8 |  |
| 907 |  | COc1c(OC)cc2c(N=CN2c3sc(C#N)c(OCC4CC4)c3)c1 | -6.6 |  |
| 908 |  | CCNC(Nc(n1)[nH]c2c1cc(c3cncnc3)cc2)=O | -7.6 |  |
| 909 |  | Cc1c2c(N(C(Nc3ccc(OC(F)(F)F)cc3)=N2)C4CC(C)(CC(C)(C4)C)C)ccc1C(N)=O | -9.8 |  |
| 910 |  | Cc(n1)[nH]c2c1c(N3CCN([C@H]4CC[C@H](c(c[nH]5)c6c5cccc6)CC4)CC3)ccc2 | -9.2 |  |
| 911 |  | CC(N)(C(N[C@H](C(N1CCC[C@H]1c(n2)[nH]c3c2cc(Cl)c(Cl)c3)=O)Cc4ccc(Cl)cc4)=O)C | -8.8 |  |
| 912 |  | COc1ccc(C[C@@H](C(N2CC[C@H]2c(n3)[nH]c4c3cc(Cl)c(Cl)c4)=O)NC(C(C)(N)C)=O)cc1 | -9.6 |  |
| 913 |  | COc1c(COc2c(C(N)=O)sc(N3C=Nc4c3cccc4)c2)cccc1 | -9.1 |  |
| 914 |  | Cc1c(COc2c(C(N)=O)sc(N3C=Nc4c3cccc4)c2)cccc1 | -9.0 |  |
| 915 |  | NC(c1c(OCc2cc(Cl)ccc2)cc(N3C=Nc4c3cccc4)s1)=O | -8.7 |  |
| 916 |  | Cc1c(C(N)=O)cc2c(N(C(Nc3ccc(OC(F)(F)F)cc3)=N2)C4CC(C)(CC(C)(C4)C)C)c1 | -9.5 |  |
| 917 |  | CN(CCN(c(cc1c(cc2)cc3c2scn3)c(C(N)=O)c4c1nc[nH]4)C)C | -7.6 |  |
| 918 |  | OC(Cc1cc(c2cc([N+]([O-])=O)ccc2)c(O)c(c(n3)[nH]c4c3cccc4)c1)=O | -8.6 |  |
| 919 |  | COc(cc1)cc2c1[nH]c(C(N3CCC(N4C=Nc5c4cccc5)CC3)=O)c2 | -9.2 |  |
| 920 |  | CCNC(Nc(n1)[nH]c2c1c(C(OC)=O)cc(c3cnccc3)c2)=O | -7.2 |  |
| 921 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CC=C)ccc(C(NC)=O)c5)c3)cccc2 | -8.9 |  |
| 922 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4C)ccc(C(O)=O)c5)c3)cccc2 | -9.1 |  |
| 923 |  | CCOC(c1cc2c(N(C(c3cc4c(N(c5c4cccc5)CC)cc3)=N2)CCCOC)cc1)=O | -7.4 |  |
| 924 |  | CCCN1c2c(c3c1ccc(C4=Nc5c(N4CCOC)ccc(C(O)=O)c5)c3)cccc2 | -8.9 |  |
| 925 |  | CC(Nc1c(c(n2)[nH]c3c2cccc3)n[nH]c1)=O | -7.8 |  |
| 926 |  | O=C(c1ccccc1)Nc2c(c(n3)[nH]c4c3cccc4)n[nH]c2 | -8.8 |  |
| 927 |  | CC1(c(n2)[nH]c3c2cccc3C(N)=O)CCN(C1)CCc4ccccc4 | -9.1 |  |
| 928 |  | NC(c1c(OCc2c(Cl)cccc2)cc(N3C=Nc4c3cccc4)s1)=O | -8.4 |  |
| 929 |  | COc1ccc(COc2c(C(N)=O)sc(N3C=Nc4c3cccc4)c2)cc1 | -9.0 |  |
| 930 |  | NC(c1c(OCc2c(F)cccc2)cc(N3C=Nc4c3cccc4)s1)=OS | -8.5 |  |
| 931 |  | NC(c1c(OCc2c(Br)cccc2)cc(N3C=Nc4c3cccc4)s1)=O | -8.9 |  |
| 932 |  | COc1c(OC)cc2c(N=CN2c3sc(C(N)=O)c(OCc4ccccc4)c3)c1 | -8.3 |  |
| 933 |  | COc1c(OC)cc2c(N=CN2c3sc(C(N)=O)c(OCC4CCCC4)c3)c1 | -8.3 |  |
| 934 |  | CN1CCN(CC1)Cc2ccc(c(n3)[nH]c4c3ccc(C(NO)=O)c4)cc2 | -8.8 |  |
| 935 |  | CN1CCN(CC1)Cc2ccc(c(n3)[nH]c4c3ccc(C(NO)=O)c4)cc2 | -8.7 |  |
| 936 |  | COc1cc(c(n2)[nH]c3c2c(C(N)=O)ccc3)ccc1 | -7.6 |  |
| 937 |  | NC(c1ccc(c2c(COc3ccc(C4=Nc5c(N4C6CCCCC6)ccc(C(O)=O)c5)cc3)cc(Cl)cc2)cc1)=O | -9.8 |  |
| 938 |  | OC(c1cc2c(N(C(c3ccc(OCc4c(c5ccc(Cl)cc5)cccn4)cc3)=N2)C6CCCCC6)cc1)=O | -10.0 |  |
| 939 |  | CN(C(c1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)=O)C | -9.7 |  |
| 940 |  | OC(c1ccc(c2c(COc3ccc(C4=Nc5c(N4C6CCCCC6)ccc(C(O)=O)c5)cc3)cc(Cl)cc2)cc1)=O | -9.7 |  |
| 941 |  | CNC(c1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)=O | -9.1 |  |
| 942 |  | CN(c1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)C | -9.3 |  |
| 943 |  | CC(C1=Nc2c(N1CC(c3cc(S(N)(=O)=O)c(Cl)cc3)=O)cccc2)C | -8.1 |  |
| 944 |  | CSC1=Nc2c(N1CC(c3cc(S(N)(=O)=O)c(Cl)cc3)=O)cccc2 | -7.7 |  |
| 945 |  | Clc1ccc(C2=Nc3c(N2CCCN4CCC(c5cc(NC(c6cc(Cl)ccc6)=O)ccc5)CC4)cccc3)cc1 | -10.5 |  |
| 946 |  | C[C@@H]1[C@@H]([C@@]1(C(O)=O)NS(=O)(N2CCN3C(C2)=Nc4c3ccc(F)c4)=O)c5ccccc5 | -9.0 |  |
| 947 |  | C[C@@H]1[C@@H]([C@@]1(C(O)=O)NS(=O)(N2CCN3C(C2)=Nc4c3ccc(C#N)c4)=O)c5ccccc5 | -8.6 |  |
| 948 |  | COc1cc2c(N3CCN(S(=O)(N[C@@]4(C(O)=O)[C@@H]([C@@H]4c5ccccc5)C)=O)CC3=N2)cc1 | -8.9 |  |
| 949 |  | CC1=Nc2c(N1CC(c3cc(S(N)(=O)=O)c(Cl)cc3)=O)cccc2 | -7.7 |  |
| 950 |  | NS(=O)(c1c(Cl)ccc(C(CN2C(CO)=Nc3c2cccc3)=O)c1)=O | -7.7 |  |
| 951 |  | CCCC1=Nc2c(N1CC(c3cc(S(N)(=O)=O)c(Cl)cc3)=O)cccc2 | -7.5 |  |
| 952 |  | C[C@@H]1[C@@H]([C@@]1(C(O)=O)NS(=O)(N2CCN3C(C2)=Nc4c3cc(F)cc4)=O)c5ccccc5 | -8.8 |  |
| 953 |  | OC(c1cc2c(N(C(c3ccc(OCc4c(c5ccc(C#N)cc5)ccc(Cl)c4)cc3)=N2)C6CCCCC6)cc1)=O | -9.5 |  |
| 954 |  | OC(c1cc2c(N(C(c3ccc(OCc4c(c5ccc(Cl)cc5)ccc(C(NCc6ccccc6)=O)c4)cc3)=N2)C7CCCCC7)cc1)=O | -9.6 |  |
| 955 |  | OC(c1cc2c(N(C(c3ccc(OCc4c(c5ccc(Cl)cc5)ccc(C#N)c4)cc3)=N2)C6CCCCC6)cc1)=O | -9.1 |  |
| 956 |  | NS(=O)(c1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)=O | -9.7 |  |
| 957 |  | NC(c1cc(COc2ccc(C3=Nc4c(N3C5CCCCC5)ccc(C(O)=O)c4)cc2)c(c6ccc(Cl)cc6)cc1)=O | -9.5 |  |
| 958 |  | Cc(n1)[nH]c2c1c(N3CCN([C@H]4CC[C@@H](c(c[nH]5)c6c5cccc6)CC4)CC3)ccc2 | -10.1 |  |
| 959 |  | FC(F)(c(n1)[nH]c2c1c(N3CCN([C@H]4CC[C@@H](c(c[nH]5)c6c5cccc6)CC4)CC3)ccc2)F | -9.8 |  |
| 960 |  | FC(F)(c(n1)[nH]c2c1c(N3CCN([C@H]4CC[C@H](c(c[nH]5)c6c5cccc6)CC4)CC3)ccc2)F | -9.7 |  |
| 961 |  | CCS(=O)(c1ccc(Oc(c2)c(CN3CCCS3(=O)=O)cc4c2[nH]c(c5ncccc5)n4)cc1)=O | -9.7 |  |
| 962 |  | CCN1c2c(c3c1ccc(C4=Nc5c(N4CCOC)ccc(C(OC)=O)c5)c3)cccc2 | -8.5 |  |
| 963 |  | CCC1=Nc2c(N1CC(c3cc(S(N)(=O)=O)c(Cl)cc3)=O)cccc2 | -8.3 |  |
| 964 |  | CN1C=Nc2c1ccc(S(=O)(N3CCN=C3N4CCN(C5CCC5)CC4)=O)c2 | -7.8 |  |
| 965 |  | ONC(c(cc1)cc2c1nc(c3ccc(c4ccc(/C=N/O)cc4)cc3)[nH]2)=O | -9.1 |  |
| 966 |  | CCN1c2c(c3c1cncc3)cc(C4=Nc5c(N4CC6CC6)ccc(C(O)=O)c5)cc2 | -9.1 |  |
| 967 |  | COCCN1C(c2cc3c(N(c4c3cccc4)CC5CCC5)cc2)=Nc6c1ccc(C(O)=O)c6 | -9.1 |  |
| 968 |  | COCCN1C(c2cc3c(N(c4c3cccc4)CC5CC5)cc2)=Nc6c1ccc(C(O)=O)c6 | -8.9 |  |
| 969 |  | C[C@@H]1C[C@H](N2C(Nc3ccc(OC(F)(F)F)cc3)=Nc4c2ccc(S(O)(=O)=O)c4)CC(C)(C1)C | -9.3 |  |
| 970 |  | COCCN1C(c2cc3c(N(c4c3cccc4)CC=C)cc2)=Nc5c1ccc(C(O)=O)c5 | -8.8 |  |
| 971 |  | COC(c1cc2c(N(C(Nc3ccc(OC(F)F)cc3)=N2)[C@@H]4C[C@@H](CC(C)(C4)C)C)cc1)=O | -8.3 |  |
| 972 |  | COc1c(C(O)=O)cc2c(N(C(Nc3ccc(OC(F)(F)F)cc3)=N2)C4CC(C)(CC(C)(C4)C)C)c1 | -8.5 |  |
| 973 |  | C[C@@H]1C[C@H](N2C(Nc3ccc(OC(F)(F)F)cc3)=Nc4c2ccc(C(O)=O)c4)CC(C)(C1)C | -9.0 |  |
| 974 |  | COC(c1cc2c(N(C(Nc3ccc(OC(F)(F)F)cc3)=N2)[C@H]4C[C@H](CC(C)(C4)C)C)cc1)=O | -8.9 |  |
| 975 |  | NC(c1c(OCc2ccc(Cl)cc2)cc(N3C=Nc4c3cccc4)s1)=O | -8.6 |  |
| 976 |  | COc1cc(COc2c(C(N)=O)sc(N3C=Nc4c3cccc4)c2)ccc1 | -8.9 |  |
| 977 |  | COc1c(OC)cc2c(N=CN2c3sc(C(N)=O)c(OCC4CCCCC4)c3)c1 | -8.4 |  |
| 978 |  | Cc1cc(COc2c(C(N)=O)sc(N3C=Nc4c3cccc4)c2)ccc1 | -9.3 |  |
| 979 |  | CN1C([n+]2c(c3ccccc3)cc(c4ccccc4)cc2c5ccccc5)=Nc6c1ccc([N+]([O-])=O)c6 | -9.3 |  |
| 980 |  | Brc1cc(C2C(C3=Nc4c(N3C(C2C#N)=N)cccc4)C#N)ccc1 | -8.2 |  |
| 981 |  | CCN1C(CSC2=NC=CN2C)=Nc3c1ccc(C(O)=O)c3 | -7.2 |  |
| 982 |  | CCc(c(C)c(C#N)c([nH]1)n2c3c1cccc3)c2=S | -7.2 |  |
| 983 |  | Brc1ccc(C2C(C3=Nc4c(N3C(C2C#N)=N)cccc4)C#N)cc1 | -8.2 |  |
| 984 |  | Cc(c1)c(C)cc2c1nc(C3CCN(CC3)CC4=NN=NN4Cc5sccc5)[nH]2 | -8.5 |  |
| 985 |  | CCN1c2c(N(C1=O)CC)cc(S(=O)(Nc3c(C)cccc3)=O)c(C)c2 | -7.1 |  |
| 986 |  | CC1=Nc2c(N1c3ccc(Br)cc3)ccc(C(NCc4cc5c(OCO5)cc4)=O)c2 | -9.7 |  |
| 987 |  | CCCc1c(C#N)c2n(c3c(N=2)cccc3)c(NCCOCCO)c1 | -6.9 |  |
| 988 |  | CC(c1c(C#N)c2n(c3c(N=2)cccc3)c(N4CCN(C(c5occc5)=O)CC4)c1)C | -8.1 |  |
| 989 |  | CCCCC1=Nc2c(N1CCN3CCCC3)ccc(C(NC(NCCCCCC(NO)=O)=O)=O)c2 | -8.3 |  |
| 990 |  | ClC(C=C1)=CC=C1C2=CC=C(N=C(C3=NC4=C(C=C(OC)C(OC)=C4)N3)C=C5N6C=C(C7=CC(OC)=C(OC)C(OC)=C7)N=N6)C5=C2 | -9.8 |  |
| 991 |  | SC1=NC2=CC=CC=C2N1 | -5.7 |  |
| 992 |  | O=C(NN)CCN1C2=CC=CC=C2N=C1SC3=NN=NN3C4=CC=CC=C4 | -8.9 |  |
| 993 |  | O=C(OCC)CCN1C2=CC=CC=C2N=C1SC3=NN=NN3C4=CC=CC=C4 | -7.8 |  |
| 994 |  | SC1=NN=C(CCN2C3=CC=CC=C3N=C2SC4=NN=NN4C5=CC=CC=C5)O1 | -8.7 |  |
| 995 |  | SC1=NN=C(CCN2C3=CC=CC=C3N=C2SC4=NN=NN4C5=CC=CC=C5)N1C6=CC=CC=C6 | -9.3 |  |
| 996 |  | O=C(N[C@@]([H])(C(O)=O)CC1C2=CC([H])=C(NC(C(O)=O)=O)C=C2N([H])C1)C3=CC(N=C(C4=COC=C4)N5C6CCCCC6)=C5C=C3 | -8.7 |  |
| 997 |  | O=C(N[C@@]([H])(C(O)=O)CC1C2=CC([H])=C(NC(C(O)=O)=O)C=C2N([H])C1)C3=CC(N=C(C4=COC=C4)N5C6CCCCC6)=C5C=C3 | -9.0 |  |
| 998 |  | O=C(N[C@@]([H])(C(O)=O)CC1C2=CC([H])=C(NC(C(O)=O)=O)C=C2N([H])C1)C3=CC(N=C(C4=COC=C4)N5C6CCCCC6)=C5C=C3 | -8.8 |  |
| 999 |  | O=C(N[C@@]([H])(C(O)=O)CC1C2=CC([H])=C(NC(C(O)=O)=O)C=C2N(C(C)=O)C1)C3=CC(N=C(C4=COC=C4)N5C6CCCCC6)=C5C=C3 | -9.6 |  |
| 1000 |  | O=C(N[C@@]([H])(C(O)=O)CC1C2=CC(O)=C(NC(C(N)=O)=O)C=C2N(C(C)=O)C1)C3=CC(N=C(C4=COC=C4)N5C6CCCCC6)=C5C=C3 | -9.8 |  |