Table 1S. Correlation weights for calculation of the optimal descriptor in CORAL model.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| SAk | CW(SAk) | ID | NSs | NSc | NSv | DEFECT[SAk] |
| #........... | -0.93886 | 1 | 7 | 3 | 5 | 0.0047 |
| (...(....... | 2.62523 | 2 | 19 | 17 | 17 | 0.0012 |
| (........... | -0.62449 | 3 | 28 | 33 | 26 | 0.0007 |
| +........... | -1.43618 | 4 | 3 | 3 | 0 | 1 |
| -........... | 2.74921 | 5 | 4 | 2 | 0 | 1 |
| 1...(....... | 1.1859 | 6 | 8 | 11 | 10 | 0.0039 |
| 1........... | -3.68312 | 7 | 23 | 27 | 26 | 0.0024 |
| 2...(....... | 1.18529 | 8 | 11 | 16 | 12 | 0.0018 |
| 2........... | -0.62745 | 9 | 17 | 22 | 16 | 0.0005 |
| 2...1....... | -11.7479 | 10 | 1 | 0 | 1 | 0.0005 |
| 3...(....... | -3.18416 | 11 | 3 | 7 | 2 | 0.0057 |
| 3........... | -1.80864 | 12 | 6 | 12 | 7 | 0.0028 |
| 4...(....... | 9.75433 | 13 | 1 | 4 | 1 | 0.0005 |
| 4........... | -1.18806 | 14 | 1 | 5 | 1 | 0.0005 |
| 4...3....... | 0 | 15 | 0 | 1 | 0 | 0 |
| 5...(....... | 0 | 16 | 0 | 3 | 0 | 0 |
| 5........... | 0 | 17 | 0 | 3 | 0 | 0 |
| 6...(....... | 0 | 18 | 0 | 2 | 0 | 0 |
| 6........... | 0 | 19 | 0 | 2 | 0 | 0 |
| =...(....... | 2.62382 | 20 | 13 | 17 | 14 | 0.0016 |
| =........... | -0.74913 | 21 | 26 | 27 | 24 | 0.0008 |
| =...1....... | 0 | 22 | 0 | 0 | 1 | 0 |
| =...2....... | 0 | 23 | 0 | 0 | 1 | 0 |
| C...#....... | 0.24647 | 24 | 7 | 3 | 5 | 0.0047 |
| C...(....... | 0.30804 | 25 | 26 | 32 | 25 | 0.0001 |
| C........... | -1.74985 | 26 | 33 | 33 | 31 | 0.0005 |
| C...1....... | -1.68798 | 27 | 9 | 10 | 6 | 0.0057 |
| C...2....... | -2.50445 | 28 | 5 | 5 | 4 | 0.0029 |
| C...3....... | 1.37123 | 29 | 1 | 2 | 1 | 0.0005 |
| C...4....... | 0 | 30 | 0 | 2 | 1 | 0 |
| C...5....... | 0 | 31 | 0 | 1 | 0 | 0 |
| C...=....... | -0.49878 | 32 | 20 | 23 | 17 | 0.002 |
| C...C....... | 0.18578 | 33 | 21 | 17 | 15 | 0.0047 |
| F...(....... | -0.62828 | 34 | 3 | 8 | 4 | 0.0049 |
| F........... | 0.30896 | 35 | 3 | 8 | 5 | 0.0082 |
| F...C....... | 2.99835 | 36 | 1 | 0 | 0 | 1 |
| H........... | 0 | 37 | 0 | 2 | 0 | 0 |
| Br..(....... | -2.49935 | 38 | 4 | 1 | 3 | 0.0039 |
| Br.......... | -3.00209 | 39 | 4 | 1 | 3 | 0.0039 |
| Br..1....... | -2.74951 | 40 | 1 | 1 | 0 | 1 |
| Br..2....... | 0 | 41 | 0 | 0 | 1 | 0 |
| Br..C....... | 8.99555 | 42 | 1 | 0 | 0 | 1 |
| I...(....... | 1.56171 | 43 | 1 | 1 | 0 | 1 |
| I........... | -0.12023 | 44 | 1 | 1 | 0 | 1 |
| Cl..(....... | -2.4969 | 45 | 7 | 10 | 10 | 0.0059 |
| Cl.......... | 0.87097 | 46 | 7 | 10 | 10 | 0.0059 |
| Cl..1....... | 1.30958 | 47 | 2 | 2 | 4 | 0.0107 |
| Cl..2....... | -2.00276 | 48 | 2 | 1 | 0 | 1 |
| Cl..3....... | 8.18999 | 49 | 1 | 0 | 1 | 0.0005 |
| N...#....... | -5.62023 | 50 | 5 | 3 | 5 | 0.0005 |
| N...(....... | 1.81619 | 51 | 15 | 13 | 11 | 0.0043 |
| N...+....... | -0.24936 | 52 | 3 | 3 | 0 | 1 |
| N...-....... | 6.62228 | 53 | 1 | 0 | 0 | 1 |
| N........... | -2.50133 | 54 | 21 | 21 | 17 | 0.0028 |
| N...1....... | 5.68503 | 55 | 5 | 2 | 2 | 0.0127 |
| N...2....... | 0 | 56 | 0 | 1 | 2 | 0 |
| N...4....... | 0 | 57 | 0 | 0 | 1 | 0 |
| N...=....... | -3.18413 | 58 | 3 | 4 | 2 | 0.0057 |
| N...C....... | -3.373 | 59 | 8 | 6 | 3 | 0.0135 |
| N...N....... | 13.75208 | 60 | 2 | 1 | 1 | 0.0098 |
| O...(....... | -0.62404 | 61 | 21 | 23 | 21 | 0.0005 |
| O...-....... | -1.99606 | 62 | 3 | 2 | 0 | 1 |
| O........... | 0.50075 | 63 | 29 | 31 | 29 | 0.0005 |
| O...1....... | 0.93388 | 64 | 1 | 4 | 0 | 1 |
| O...2....... | 18.87586 | 65 | 2 | 0 | 2 | 0.0005 |
| O...4....... | 0 | 66 | 0 | 0 | 1 | 0 |
| O...=....... | 1.99617 | 67 | 24 | 26 | 20 | 0.0023 |
| O...C....... | -0.37067 | 68 | 17 | 16 | 19 | 0.0022 |
| O...N....... | 1.99545 | 69 | 1 | 2 | 1 | 0.0005 |
| P...(....... | -3.87109 | 70 | 2 | 2 | 7 | 0.0176 |
| P........... | -5.74518 | 71 | 2 | 2 | 7 | 0.0176 |
| P...=....... | 0 | 72 | 0 | 1 | 1 | 0 |
| P...C....... | 0 | 73 | 0 | 0 | 1 | 0 |
| P...O....... | -3.37761 | 74 | 1 | 1 | 3 | 0.0159 |
| S...(....... | -3.43615 | 75 | 8 | 9 | 8 | 0.0005 |
| S........... | -5.12751 | 76 | 10 | 10 | 10 | 0.0005 |
| S...1....... | 2.44072 | 77 | 1 | 1 | 2 | 0.0107 |
| S...=....... | -2.37429 | 78 | 3 | 1 | 6 | 0.0107 |
| S...C....... | -3.93775 | 79 | 4 | 5 | 2 | 0.0098 |
| S...N....... | 6.74652 | 80 | 3 | 4 | 2 | 0.0057 |
| S...P....... | -12.5589 | 81 | 1 | 0 | 1 | 0.0005 |
| Sn.......... | 0 | 82 | 0 | 1 | 0 | 0 |
| [...(....... | 0.62329 | 83 | 4 | 6 | 0 | 1 |
| [...+....... | -2.43839 | 84 | 3 | 3 | 0 | 1 |
| [...-....... | 2.81333 | 85 | 4 | 2 | 0 | 1 |
| [........... | -1.74857 | 86 | 4 | 6 | 0 | 1 |
| [...2....... | 0 | 87 | 0 | 1 | 0 | 0 |
| [...=....... | 6.62529 | 88 | 2 | 2 | 0 | 1 |
| [...C....... | 0 | 89 | 0 | 1 | 0 | 0 |
| [...H....... | 0 | 90 | 0 | 2 | 0 | 0 |
| [...N....... | 0.74526 | 91 | 4 | 3 | 0 | 1 |
| [...O....... | -2.24634 | 92 | 3 | 2 | 0 | 1 |
| [...Sn...... | 0 | 93 | 0 | 1 | 0 | 0 |
| c...(....... | 0.00495 | 94 | 17 | 24 | 22 | 0.0044 |
| c........... | -1.50046 | 95 | 21 | 27 | 26 | 0.0037 |
| c...1....... | -2.50482 | 96 | 19 | 23 | 24 | 0.0041 |
| c...2....... | -0.75092 | 97 | 13 | 21 | 13 | 0.0005 |
| c...3....... | -0.56588 | 98 | 6 | 11 | 7 | 0.0028 |
| c...4....... | 1.18681 | 99 | 1 | 4 | 0 | 1 |
| c...5....... | 0 | 100 | 0 | 3 | 0 | 0 |
| c...6....... | 0 | 101 | 0 | 2 | 0 | 0 |
| c...C....... | 2.31308 | 102 | 5 | 6 | 4 | 0.0029 |
| c...F....... | 0 | 103 | 0 | 0 | 1 | 0 |
| c...N....... | -4.49634 | 104 | 3 | 6 | 3 | 0.0005 |
| c...O....... | -5.49518 | 105 | 7 | 11 | 8 | 0.0025 |
| c...S....... | 1.43933 | 106 | 1 | 0 | 0 | 1 |
| c...[....... | 0.37189 | 107 | 1 | 1 | 0 | 1 |
| c...c....... | 2.12393 | 108 | 18 | 26 | 25 | 0.0055 |
| n...(....... | 3.24543 | 109 | 8 | 3 | 6 | 0.0039 |
| n........... | 2.24867 | 110 | 13 | 6 | 8 | 0.0069 |
| n...1....... | 0.00216 | 111 | 8 | 3 | 5 | 0.0066 |
| n...2....... | 1.37765 | 112 | 4 | 1 | 1 | 0.018 |
| n...3....... | 0.68706 | 113 | 3 | 0 | 1 | 0.0149 |
| n...4....... | 1.50107 | 114 | 1 | 0 | 0 | 1 |
| n...H....... | 0 | 115 | 0 | 2 | 0 | 0 |
| n...[....... | 0 | 116 | 0 | 2 | 0 | 0 |
| n...c....... | 1.87504 | 117 | 11 | 3 | 6 | 0.0086 |
| n...n....... | 1.44054 | 118 | 4 | 1 | 1 | 0.018 |
| s........... | -3.80871 | 119 | 1 | 1 | 0 | 1 |
| s...1....... | 1.75455 | 120 | 1 | 0 | 0 | 1 |
| s...2....... | 4.37754 | 121 | 1 | 0 | 0 | 1 |
| s...c....... | 0 | 122 | 0 | 1 | 0 | 0 |

*SAk= descriptor, CW(SAk)= Correlation weight of descriptor, NSs= frequency of descriptor in training set, NSc= frequency of descriptor in Invisible set, NSv= frequency of descriptor in calibration set and DEFECT(SAk)= index of robustness of descriptors (lower is better)*

Table 2S. Data set of biocides with EC50 experimental value expressed as -log(mmol/l) (Target) and predictions made with LR, RF and CORAL models.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ID | CAS | SMILES (canonical SMILES) | Target | LR predictions | LR split | RF predictions | RF split | CORAL predictions | CORAL split |
| 1 | 112-53-8 | CCCCCCCCCCCCO | -0.23 | 1.03 | TS | 0.5 | TS | 1.51 | VS |
| 2 | 94-75-7 | OC(=O)COc1ccc(Cl)cc1Cl | 0.22 | 0.35 | TS | 0.77 | TS | 2.7 | ITS |
| 3 | 57960-19-7 | CC(=O)OC1C(C=CCCCCCCCCCC)C(=O)c2ccccc2C1=O | 4.99 | 4.63 | VS | 4.72 | TS | 3.56 | CS |
| 4 | 101007-06-1 | CC1(C)C(=C1CCC(=O)OC(C(F)(F)F)C(F)(F)F)C(=O)OC(C#N)c1cc(ccc1)Oc1ccccc1 | 7.39 | 6.7 | TS | 6.8 | TS | 6.15 | ITS |
| 6 | 348635-87-0 | CN(C)S(=O)(=O)[n]1c[n]c([n]1)S(=O)(=O)[n]1c2cc(F)ccc2c(Br)c1C | 4.1 | 3.85 | TS | 4.07 | TS | 2.24 | CS |
| 7 | 120162-55-2 | C[n]1[n][n]c([n]1)-c1c[n][n](C)c1S(=O)(=O)NC(=O)Nc1[n]c(cc([n]1)OC)OC | 0.05 | -0.07 | TS | 0.32 | TS | 0.09 | TS |
| 8 | 82560-54-1 | CN(SN(CCC(=O)OCC)C(C)C)C(=O)Oc1cccc2CC(C)(C)Oc12 | 4.61 | 5.41 | TS | 4.84 | VS | 4.3 | ITS |
| 11 | 56634-95-8 | CCCCCCC(=O)Oc1c(Br)cc(cc1Br)C#N | 4.1 | 4.55 | TS | 4.44 | TS | 5.42 | VS |
| 12 | 1689-99-2 | CCCCCCCC(=O)Oc1c(Br)cc(cc1Br)C#N | 3.96 | 4.68 | VS | 4.73 | VS | 5.59 | VS |
| 13 | 95465-99-9 | CC(CC)SP(=O)(OCC)SC(C)CC | 5.56 | 3.88 | VS | 4.77 | TS | 4.89 | ITS |
| 14 | 1563-66-2 | CC1(C)Cc2cccc(OC(=O)NC)c2O1 | 4.37 | 3.04 | TS | 3.58 | VS | 3.27 | TS |
| 15 | 55285-14-8 | CN(SN(CCCC)CCCC)C(=O)Oc1cccc2CC(C)(C)Oc21 | 5.4 | 4.77 | TS | 5.03 | TS | 4.49 | CS |
| 16 | 500008-45-7 | Cc1cc(Cl)cc(c1NC(=O)c1cc(Br)[n][n]1-c1[n]cccc1Cl)C(=O)NC | 4.62 | 3.81 | TS | 3.94 | TS | 4.71 | TS |
| 17 | 1698-60-8 | N=C1C=NN(C(=O)C1Cl)c1ccccc1 | 0.23 | 1.46 | TS | 0.86 | TS | 0.82 | TS |
| 18 | 1897-45-6 | N#Cc1c(Cl)c(Cl)c(Cl)c(C#N)c1Cl | 3.69 | 3.92 | TS | 3.79 | TS | 5.56 | CS |
| 19 | 2921-88-2 | CCOP(=S)(Oc1[n]c(Cl)c(Cl)cc1Cl)OCC | 6.54 | 4.67 | VS | 5.78 | TS | 5.41 | TS |
| 20 | 5598-13-0 | COP(=S)(Oc1[n]c(Cl)c(Cl)cc1Cl)OC | 5.73 | 5.07 | TS | 5.18 | TS | 5.07 | CS |
| 21 | 143807-66-3 | Cc1c(ccc2OCCCc12)C(=O)NN(C(=O)c1cc(C)cc(C)c1)C(C)(C)C | -0.12 | 1.13 | TS | 1.37 | TS | 0.99 | TS |
| 22 | 1031756-98-5 | CC(NC(=O)c1cc(Cl)cc(Br)c1NC(=O)c1cc(Br)[n][n]1-c1[n]cccc1Cl)C1CC1 | 3.87 | 4.19 | VS | 3.95 | TS | out of domain | TS |
| 25 | 39515-40-7 | CC(C)=CC1C(C(=O)OC(C#N)c2cccc(c2)Oc2ccccc2)C1(C)C | 5.94 | 4.69 | TS | 5.46 | TS | 5.44 | CS |
| 27 | 333-41-5 | Cc1cc([n]c([n]1)C(C)C)OP(=S)(OCC)OCC | 5.48 | 4.15 | TS | 5.22 | TS | 4.52 | CS |
| 28 | 104653-34-1 | O=C1C(C2CC(Cc3ccccc32)c2ccc(cc2)-c2ccc(Br)cc2)C(=O)Sc2ccccc12 | 5.09 | 4.79 | TS | 4.29 | TS | 5.21 | VS |
| 29 | 149961-52-4 | CON=C(C(=O)NC)c1ccccc1COc1cc(C)ccc1C | 3.92 | 3.44 | TS | 3.73 | TS | 4.87 | VS |
| 30 | 131-72-6 | CCCCCCC(C)c1cc(cc(c1OC(=O)CC=C)[N+]([O-])=O)[N+]([O-])=O | 4.94 | 4.26 | TS | 4.84 | TS | out of domain | TS |
| 32 | 66230-04-4 | CC(C)C(C(=O)OC(C#N)c1cc(ccc1)Oc1ccccc1)c1ccc(Cl)cc1 | 6.19 | 4.97 | TS | 5.08 | VS | 5.91 | ITS |
| 33 | 64-17-5 | CCO | -2.34 | -1.9 | TS | -0.79 | VS | -0.21 | TS |
| 34 | 126801-58-9 | CCOc1ccccc1OS(=O)(=O)NC(=O)Nc1[n]c(cc([n]1)OC)OC | 0.11 | 0.68 | VS | 0.89 | TS | 2.08 | ITS |
| 35 | 107-06-2 | ClCCCl | -0.4 | -0.34 | TS | 0.06 | TS | 0.25 | VS |
| 36 | 80844-07-1 | CCOc1ccc(cc1)C(C)(C)COCc1cc(ccc1)Oc1ccccc1 | 5.69 | 5.05 | TS | 5.16 | TS | 4.36 | VS |
| 37 | 153233-91-1 | CCOc1cc(ccc1C1COC(=N1)c1c(F)cccc1F)C(C)(C)C | 4.7 | 3.93 | TS | 4.71 | TS | 5.11 | VS |
| 38 | 131807-57-3 | CC1(OC(=O)N(Nc2ccccc2)C1=O)c1ccc(cc1)Oc1ccccc1 | 4.05 | 3.36 | VS | 3.76 | VS | 3.16 | CS |
| 39 | 22224-92-6 | Cc1cc(ccc1SC)OP(=O)(NC(C)C)OCC | 5.44 | 3.95 | TS | 5.07 | TS | 6.27 | CS |
| 40 | 120928-09-8 | CC(C)(C)c1ccc(CCOc2[n]c[n]c3ccccc32)cc1 | 4.87 | 3.99 | VS | 4.71 | TS | 2.51 | TS |
| 41 | 13356-08-6 | CC(C)(C[Sn](CC(C)(C)c1ccccc1)(CC(C)(C)c1ccccc1)O[Sn](CC(C)(C)c1ccccc1)(CC(C)(C)c1ccccc1)CC(C)(C)c1ccccc1)c1ccccc1 | 4.34 | 7.3 | VS | 4.47 | TS | out of domain | ITS |
| 42 | 122-14-5 | Cc1cc(ccc1[N+]([O-])=O)OP(=S)(OC)OC | 4.51 | 4.46 | TS | 4.41 | VS | out of domain | ITS |
| 43 | 39515-41-8 | CC1(C)C(C(=O)OC(C#N)c2cc(ccc2)Oc2ccccc2)C1(C)C | 5.82 | 4.81 | VS | 5.26 | TS | 4.64 | TS |
| 44 | 134098-61-6 | Cc1[n][n](C)c(Oc2ccccc2)c1C=NOCc1ccc(cc1)C(=O)OC(C)(C)C | 4.28 | 4.78 | TS | 4.3 | TS | 4.12 | ITS |
| 45 | 272451-65-7 | CC(C)(C=S(=C)(O)O)NC(=O)c1c(I)cccc1C(=O)Nc1ccc(cc1C)C(F)(C(F)(F)F)C(F)(F)F | 4.06 | 4.35 | TS | 4.22 | TS | 5.51 | ITS |
| 46 | 101463-69-8 | O=C(Nc1ccc(cc1F)Oc1ccc(cc1Cl)C(F)(F)F)NC(=O)c1c(F)cccc1F | 7.06 | 5.33 | TS | 6.5 | TS | 6.33 | ITS |
| 47 | 144740-54-5 | COC(=O)c1ccc([n]c1S(=O)(=O)NC(=O)[N-]c1[n]c(cc([n]1)OC)OC)C(F)(F)F | -0.17 | -0.32 | TS | 0.46 | TS | out of domain | TS |
| 49 | 22259-30-9 | CNC(=O)Oc1cc(ccc1)N=CN(C)C | 5.11 | 3 | VS | 4.27 | TS | 4.37 | ITS |
| 51 | 77182-82-2 | CP(O)(=O)CCC(N)C(O)=O | -0.57 | -0.17 | TS | -0.05 | TS | 1.02 | CS |
| 52 | 3861-47-0 | CCCCCCCC(=O)Oc1c(I)cc(cc1I)C#N | 4.66 | 4.13 | TS | 4.5 | TS | out of domain | TS |
| 53 | 881685-58-1 | CC(C)C1C2CCC1c1cccc(NC(=O)c3c[n](C)[n]c3C(F)F)c12 | 3.91 | 3.17 | TS | 3.28 | VS | 3.94 | ITS |
| 55 | 21609-90-5 | COP(=S)(Oc1cc(Cl)c(Br)cc1Cl)c1ccccc1 | 5.31 | 5.62 | TS | 5.12 | TS | 6 | CS |
| 56 | 121-75-5 | COP(=S)(OC)SC(=CC(=O)OCC)C(O)OCC | 5.67 | 6.18 | TS | 5.1 | TS | 5.06 | TS |
| 57 | 123-33-1 | Oc1ccc(O)[n][n]1 | 0.02 | -0.61 | TS | 0.39 | TS | -0.67 | VS |
| 58 | 2032-65-7 | CNC(=O)Oc1cc(C)c(SC)c(C)c1 | 4.45 | 3.96 | TS | 4.02 | TS | 5.3 | VS |
| 59 | 16752-77-5 | CC(=NOC(=O)NC)SC | 4.33 | 4.03 | TS | 3.58 | TS | 2.75 | TS |
| 60 | 4726-14-1 | CCCN(CCC)c1c(cc(cc1[N+]([O-])=O)[SH](=C)(O)=O)[N+]([O-])=O | 5.24 | 5.3 | TS | 4.89 | TS | out of domain | ITS |
| 62 | 116714-46-6 | O=C(NC(=O)Nc1cc(Cl)c(cc1)OC(F)(F)C(F)OC(F)(F)F)c1c(F)cccc1F | 3.93 | 5.78 | TS | 4.66 | TS | 5 | VS |
| 63 | 42874-03-3 | CCOc1cc(ccc1[N+]([O-])=O)Oc1ccc(cc1Cl)C(F)(F)F | 3.7 | 4.76 | TS | 4.37 | TS | out of domain | VS |
| 64 | 72-56-0 | CCc1ccc(cc1)C(C(Cl)Cl)c1ccc(CC)cc1 | 4.23 | 3.67 | TS | 3.6 | VS | 4.15 | CS |
| 65 | 2310-17-0 | CCOP(=S)(OCC)SCN1C(=O)Oc2cc(Cl)ccc12 | 5.7 | 5.65 | TS | 4.96 | VS | 5.92 | CS |
| 66 | 732-11-6 | COP(=S)(OC)SCN1C(=O)c2ccccc2C1=O | 5.2 | 6 | TS | 4.65 | VS | 5.73 | VS |
| 68 | 23103-98-2 | Cc1[n]c([n]c(OC(=O)N(C)C)c1C)N(C)C | 4.15 | 4.38 | TS | 4.09 | TS | 2.27 | TS |
| 69 | 29232-93-7 | Cc1cc([n]c([n]1)N(CC)CC)OP(=S)(OC)OC | 6.16 | 5.09 | TS | 5.33 | TS | 3.63 | CS |
| 71 | 23031-36-9 | CC(C)=CC1C(C(=O)OC2CC(=O)C(CC#C)C2=C)C1(C)C | 4.69 | 4.18 | VS | 4.55 | TS | 4.77 | TS |
| 72 | 2312-35-8 | CC(C)(C)c1ccc(cc1)OC1CCCCC1OS(=O)OCC#C | 4.4 | 4.78 | TS | 4.88 | VS | 6.34 | TS |
| 73 | 175013-18-0 | CON(C(=O)OC)c1ccccc1COc1cc[n]([n]1)-c1ccc(Cl)cc1 | 4.38 | 3.8 | TS | 4.58 | TS | 3.64 | VS |
| 74 | 96489-71-3 | CC(C)(C)[n]1[n]cc(SCc2ccc(cc2)C(C)(C)C)c(Cl)c1=O | 5.56 | 3.19 | TS | 5.14 | TS | 3.53 | ITS |
| 75 | 179101-81-6 | FC(F)(F)c1c[n]c(cc1)OCCCOc1c(Cl)cc(cc1Cl)OCC=C(Cl)Cl | 5.11 | 6.24 | TS | 4.96 | TS | 5.79 | TS |
| 76 | 124495-18-7 | Fc1ccc(cc1)Oc1cc[n]c2cc(Cl)cc(Cl)c21 | 3.59 | 4.37 | TS | 4.17 | VS | 5.43 | CS |
| 77 | 130561-48-7 | Cc1ccc(cc1)-[n]1[n]c(C(O)=O)c(=O)c2c1cccc2OCCOC | 0.17 | 0.15 | TS | 0.93 | TS | 3.55 | CS |
| 78 | 102851-06-9 | CC(C)C(=Nc1ccc(cc1Cl)C(F)(F)F)C(O)OC(C#N)c1cccc(c1)Oc1ccccc1 | 4.75 | 4.87 | TS | 4.66 | TS | 6.61 | CS |
| 79 | 119168-77-3 | CCc1[n][n](C)c(C(=O)NCc2ccc(cc2)C(C)(C)C)c1Cl | 3.86 | 3.31 | TS | 4 | VS | 3.22 | VS |
| 80 | 79538-32-2 | CC1(C)C(C=C(Cl)C(F)(F)F)C1C(=O)OCc1c(F)c(F)c(C)c(F)c1F | 6.78 | 5.54 | TS | 6.23 | TS | 6.22 | ITS |
| 81 | 7696-12-0 | CC(C)=CC1C(C(=O)OCN2C(=O)C3CCC=CC3C2=O)C1(C)C | 3.87 | 4.11 | TS | 4.39 | VS | 4.26 | VS |
| 82 | 59669-26-0 | CN(SN(C)C(=O)ON=C(C)SC)C(=O)ON=C(C)SC | 4.12 | 6.3 | VS | 4.41 | TS | 5.17 | ITS |
| 83 | 2303-17-5 | CC(C)N(C(C)C)C(=O)SCC(Cl)=C(Cl)Cl | 3.52 | 4.15 | TS | 4 | TS | 3.7 | ITS |
| 84 | 101200-48-0 | Cc1[n]c([n]c([n]1)OC)N(C)C(=O)NS(=O)(=O)c1ccccc1C(=O)OC | -0.35 | 0.4 | TS | 0.29 | TS | 0.87 | CS |
| 85 | 141517-21-7 | CC(=NOCc1ccccc1C(=NOC)C(=O)OC)c1cc(ccc1)C(F)(F)F | 4.57 | 6.01 | TS | 4.58 | VS | 4.57 | CS |
| 86 | 64628-44-0 | O=C(Nc1ccc(cc1)OC(F)(F)F)NC(=O)c1ccccc1Cl | 5.35 | 4.27 | TS | 5.01 | TS | 3.55 | ITS |
| 88 | 27519-02-4 | CCCCCCCCCCCCCC=CCCCCCCCC | 2.48 | 2.89 | TS | 3.18 | TS | 3.34 | VS |
| 89 | 57-06-7 | C=CCN=C=S | 2.13 | 1.71 | TS | 1.94 | TS | 1.86 | VS |
| 97 | 10222-01-2 | NC(=O)C(Br)(Br)C#N | 2.44 | 3.04 | TS | 2.37 | TS | 1.94 | VS |
| 131 | 131341-86-1 | N#Cc1c[nH]cc1-c1cccc2OC(F)(F)Oc21 | 2.53 | 2 | TS | 2.94 | TS | out of domain | VS |
| 136 | 122453-73-0 | CCOC[n]1c(c(C#N)c(Br)c1C(F)(F)F)-c1ccc(Cl)cc1 | 4.72 | 4.6 | TS | 4.79 | TS | 4.8 | CS |
| 142 | 35691-65-7 | N#CCCC(Br)(CBr)C#N | 2.08 | 3.13 | VS | 2.44 | TS | 2.38 | TS |
| 143 | 420-04-2 | NC#N | 1.12 | -0.34 | TS | 0.47 | TS | 1.25 | CS |
| 146 | 6317-18-6 | N#CSCSC#N | 3.33 | 3.03 | TS | 2.96 | TS | 4.81 | VS |
| 151 | 21564-17-0 | N#CSCSc1[n]c2ccccc2[s]1 | 3.89 | 4.09 | TS | 3.72 | TS | out of domain | TS |
| 155 | 66215-27-8 | Nc1[n]c(NC2CC2)[n]c(N)[n]1 | 1.19 | 2.3 | VS | 0.95 | TS | 1.06 | TS |
| 156 | 886-50-0 | CCNc1[n]c(NC(C)(C)C)[n]c([n]1)SC | 1.81 | 3.45 | VS | 2.66 | VS | 2.58 | TS |
| 158 | 95737-68-1 | CC(COc1ccc(cc1)Oc1ccccc1)Oc1cccc[n]1 | 2.9 | 4.82 | TS | 2.99 | TS | 3.43 | ITS |
| 161 | 60207-90-1 | CCCC1COC(C[n]2c[n]c[n]2)(O1)c1ccc(Cl)cc1Cl | 1.67 | 2.51 | TS | 2.43 | TS | -0.31 | CS |
| 166 | 148-79-8 | c1[n]c(c[s]1)-c1[nH]c2ccccc2[n]1 | 2.59 | 2.57 | TS | 2.61 | TS | out of domain | ITS |
| 170 | 52-51-7 | [O-][N+](=O)C(Br)(CO)CO | 2.1 | 1.31 | TS | 1.89 | TS | out of domain | TS |
| 182 | 50-00-0 | C=O | 0.02 | -2.56 | VS | -0.16 | VS | -0.5 | TS |
| 184 | 112-12-9 | CCCCCCCCCC(C)=O | 2.4 | 1.58 | TS | 2.29 | TS | 1.26 | TS |
| 186 | 134-62-3 | Cc1cc(ccc1)C(=O)N(CC)CC | 0.41 | 2.02 | TS | 1.21 | TS | 2.29 | ITS |
| 188 | 86479-06-3 | O=C(Nc1cc(Cl)c(OC(F)(F)C(F)F)c(Cl)c1)NC(=O)c1c(F)cccc1F | 6.6 | 5.22 | TS | 5.91 | TS | 5.41 | ITS |
| 203 | 34123-59-6 | CN(C)C(=O)Nc1ccc(cc1)C(C)C | 2.55 | 3.33 | TS | 2.2 | VS | 2.91 | CS |
| 204 | 79-33-4 | CC(=O)C(O)O | -0.92 | 0.13 | TS | 0.18 | VS | 0.19 | CS |
| 206 | 110-44-1 | CC=CC=CC(O)=O | 0.2 | -0.16 | TS | 0.36 | TS | 0.95 | VS |
| 207 | 65-85-0 | OC(=O)c1ccccc1 | -0.85 | 0.87 | TS | 0.49 | VS | 1.37 | CS |
| 212 | 124-07-2 | CCCCCCCC(O)=O | 0.36 | 0.7 | TS | 0.37 | TS | 0.87 | TS |
| 213 | 112-05-0 | CCCCCCCCC(O)=O | 0.22 | 0.83 | VS | 0.39 | TS | 1.04 | ITS |
| 214 | 143-07-7 | CCCCCCCCCCCC(O)=O | 1.75 | 1.64 | TS | 1.48 | TS | 1.56 | VS |
| 215 | 79-14-1 | OC(O)C=O | 0.24 | -0.47 | TS | 0 | TS | -0.17 | CS |
| 216 | 65733-16-6 | CC(C)OC(=O)CC(=C)C=CCC(C)CCCC(C)(C)OC | 2.94 | 3.9 | TS | 4.16 | VS | 3.21 | TS |
| 231 | 22781-23-3 | CNC(=O)Oc1cccc2OC(C)(C)Oc21 | 3.88 | 2.15 | TS | 3.65 | VS | 3.08 | TS |
| 237 | 72490-01-8 | CCOC(=O)NCCOc1ccc(cc1)Oc1ccccc1 | 2.84 | 4.47 | VS | 3.5 | TS | 4.37 | VS |
| 252 | 72963-72-5 | CC(C)=CC1C(C(=O)OCN2C(=O)CN(CC#C)C2=O)C1(C)C | 3.8 | 4.56 | TS | 4.14 | TS | 3.69 | VS |
| 258 | 26530-20-1 | CCCCCCCC[n]1[s]ccc1=O | 2.98 | 2.71 | TS | 2.66 | VS | 2.74 | TS |
| 263 | 81-81-2 | CC(=O)CC(C1C(=O)c2ccccc2OC1=O)c1ccccc1 | 0.48 | 2.34 | TS | 1.2 | TS | 3.49 | ITS |
| 266 | 28772-56-7 | OC(CC(C1C(=O)Oc2ccccc2C1=O)c1ccccc1)c1ccc(cc1)-c1ccc(Br)cc1 | 2.42 | 1.55 | TS | 2.65 | TS | out of domain | VS |
| 267 | 2527-66-4 | C[n]1[s]c2ccccc2c1=O | 2.25 | 2.29 | TS | 2.44 | TS | 1.98 | CS |
| 268 | 4299-07-04 | CCCC[n]1[s]c2ccccc2c1=O | 3.33 | 2.46 | TS | 3.09 | TS | 2.49 | ITS |
| 269 | 83-79-4 | CC(=C)C1Cc2c3OC4COc5cc(OC)c(cc5C4C(=O)c3ccc2O1)OC | 4.92 | 4.67 | TS | 4.55 | TS | 4.72 | ITS |
| 280 | 104-55-2 | O=CC=Cc1ccccc1 | 1.27 | 1.32 | TS | 1.14 | VS | 1.49 | CS |
| 281 | 111-30-8 | O=CCCCC=O | 1.06 | 0.25 | TS | 1.04 | VS | 0.05 | CS |
| 282 | 64-18-6 | OC=O | -0.52 | -1.47 | VS | -0.43 | TS | -0.52 | CS |
| 286 | 731-27-1 | CN(C)S(=O)(=O)N(SC(F)(Cl)Cl)c1ccc(C)cc1 | 3.26 | 4.02 | TS | 3.42 | TS | 4.92 | VS |
| 288 | 1085-98-9 | CN(C)S(=O)(=O)N(SC(F)(Cl)Cl)c1ccccc1 | 2.5 | 4.11 | TS | 3.05 | TS | 4.42 | VS |
| 290 | 67564-91-4 | CC(Cc1ccc(cc1)C(C)(C)C)CN1CC(C)OC(C)C1 | 2.11 | 3.5 | TS | 2.79 | TS | 3.96 | ITS |
| 295 | 75-21-8 | C1CO1 | -0.67 | -1.22 | TS | -0.27 | TS | 0.83 | VS |
| 299 | 7747-35-5 | CCC12COCN1COC2 | 0.53 | 1.12 | TS | 1.7 | VS | 0.34 | VS |
| 300 | 67-63-0 | CC(C)O | -2.23 | -1.24 | TS | -1.25 | TS | 0.01 | ITS |
| 301 | 94361-06-5 | CC(C1CC1)C(O)(C[n]1c[n]c[n]1)c1ccc(Cl)cc1 | 1.05 | 0.87 | TS | 1.41 | TS | 1.73 | VS |
| 302 | 59-50-7 | Cc1cc(O)ccc1Cl | 1.85 | 1.53 | VS | 1.47 | TS | 2.59 | CS |
| 311 | 120-32-1 | Oc1ccc(Cl)cc1Cc1ccccc1 | 2.57 | 2.22 | VS | 1.95 | VS | 2.66 | VS |
| 312 | 90-43-7 | Oc1ccccc1-c1ccccc1 | 1.9 | 1.49 | TS | 1.22 | VS | 2.4 | VS |
| 330 | 106-24-1 | CC(C)=CCCC(C)=CCO | 0.98 | 1.26 | TS | 0.87 | TS | 1.68 | ITS |
| 331 | 100-51-6 | OCc1ccccc1 | -0.33 | 0.58 | VS | 0.55 | VS | 1.06 | CS |
| 332 | 71-23-8 | CCCO | -2 | -1.61 | VS | -1.06 | VS | -0.04 | TS |
| 342 | 4719-04-04 | OCCN1CN(CN(C1)CCO)CCO | 0.92 | 0.49 | TS | 0.95 | TS | 3.24 | VS |
| 344 | 7173-51-5 | C[N+](C)(CCCCCCCCCC)CCCCCCCCCC | 4.3 | 3.37 | TS | 3.89 | TS | out of domain | ITS |
| 352 | 122454-29-9 | N#Cc1c(Br)c([nH]c1-c1ccc(Cl)cc1)C(F)(F)F | 5.37 | 3.58 | TS | 3.82 | VS | out of domain | ITS |
| 355 | 120068-37-3 | Nc1c(c(C#N)[n][n]1-c1c(Cl)cc(cc1Cl)C(F)(F)F)S(=O)C(F)(F)F | 3.36 | 4.64 | TS | 4.75 | VS | 4.34 | TS |
| 368 | 138261-41-3 | [O-][N+](=O)NC1=NCCN1Cc1ccc(Cl)[n]c1 | 0.48 | 1.65 | TS | 1.02 | TS | out of domain | TS |
| 390 | 3691-35-8 | O=C(C(c1ccc(Cl)cc1)c1ccccc1)C1C(=O)c2ccccc2C1=O | 2.94 | 4.17 | TS | 3.48 | TS | 2.4 | ITS |
| 392 | 56073-07-5 | O=C1C(C2CC(Cc3ccccc32)c2ccc(cc2)-c2ccccc2)C(=O)Oc2ccccc12 | 2.93 | 4.09 | TS | 2.74 | TS | out of domain | ITS |