

SUPPLEMENTARY INFORMATION

A STRUCTURE-ACTIVITY RELATIONSHIP STUDY OF THE TOXICITY OF IONIC LIQUIDS USING AN ADAPTED FERREIRA-KIRALJ
HYDROPHOBICITY PARAMETER.

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Table S1. SMILES strings, Chemical Abstracts Service (CAS) code and LogEC₅₀ for each sample of dataset

| Samples | SMILES | CAS | LogEC ₅₀ |
|---------|--|-------------|---------------------|
| 1 | [Cl-].CCCCCCCC[N+]1=CN(C)C=C1 | 64697-40-1 | 2 |
| 2 | CCCCN1C=C[N+](=C1)C.[Cl-] | 79917-90-1 | 3.55 |
| 3 | [Cl-].C[n+]1ccn(CCCCCCCCCCCCCC)c1 | 61546-01-8 | -0.24 |
| 4 | [N+]1(C)=CN(C=C1)CCCC.[Cl-] | 171058-22-3 | 3.16 |
| 5 | [N+]1(C)=CN(C=C1)CCCCCC.[Cl-] | 581101-92-0 | 2.53 |
| 6 | [N+]1(C)=CN(C=C1)CCCCCCCC.[Cl-] | 171058-20-1 | 1.4 |
| 7 | [N+]1(C)=CN(C=C1)CCCC.[Br-] | 85100-77-2 | 3.43 |
| 8 | [N+]1(CC)=CN(C=C1)CCCC.[Br-] | 547719-00-6 | 2 |
| 9 | [N+]1(C)=CN(C=C1)CCCC.[I-] | 65039-05-6 | 3.48 |
| 10 | [N+]1(CC)=CN(C=C1)CCCC.[B-](F)(F)(F)F | 393550-29-3 | 2.26 |
| 11 | [N+]1(C)=CN(C=C1)CC.[B-](F)(F)(F)F | 143314-16-3 | 3.44 |
| 12 | [N+]1(C)=CN(C=C1)CCCCCC.[B-](F)(F)(F)F | 244193-52-0 | 1.59 |
| 13 | [N+]1(C)=CN(C=C1)CCC.[B-](F)(F)(F)F | 244193-48-4 | 3.45 |
| 14 | [N+]1(C)=CN(C=C1)CCCCCCCCO.[Br-] | 952429-65-1 | 2.36 |
| 15 | [N+]1(C)=CN(C=C1)Cc1ccc(cc1)C.[Cl-] | 637348-60-8 | 2.64 |
| 16 | [N+]1(C)=C(C)N(C=C1)CCCC.[B-](F)(F)(F)F | 384347-21-1 | 1.9 |
| 17 | [N+]1(C)=CN(C=C1)Cc1cccc1.[B-](F)(F)(F)F | 500996-04-3 | 2.97 |
| 18 | [N+]1(C)=CN(C=C1)COCC.[Cl-] | 945996-02-1 | 3.6 |
| 19 | [N+]1(C)=CN(C=C1)CC.[O-]C(=O)C | 143314-17-4 | 4.23 |
| 20 | [N+]1(C)=CN(C=C1)CCCC.[O-]S(=O)(=O)OCCOCCOC | 595565-54-1 | 3.15 |
| 21 | [N+]1(C)=CN(C=C1)CC.[O-]S(=O)(=O)C(F)(F)F | 145022-44-2 | 4.09 |
| 22 | [N+]1(C)=CN(C=C1)CCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 174899-83-3 | 2.68 |
| 23 | [N+]1(C)=CN(C=C1)CCCCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 178631-04-4 | 1.64 |
| 24 | [N+]1(C)=CN(C=C1)CC.[O-]C(=O)C(F)(F)F | 174899-65-1 | 4 |
| 25 | [N+]1(C)=CN(C=C1)CC.[O-]S(=O)(=O)C | 145022-45-3 | 3.97 |
| 26 | [n+]1(ccccc1)CCCC.[B-](F)(F)(F)F | 203389-28-0 | 3.16 |
| 27 | [n+]1(ccc(C)cc1)CCCC.[Cl-] | 112400-86-9 | 3.32 |
| 28 | [N+]1(C)(CCCC1)CCCC.[Cl-] | 909398-59-0 | 2.93 |
| 29 | [N+]1(C)(CCCC1)CCCCCCCC.[Cl-] | 909398-60-3 | 2.59 |
| 30 | [N+]1(C)(CCCC1)CCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 380497-19-8 | 2.56 |
| 31 | [n+]1(ccccc1)CCCC.[O-]S(=O)(=O)OC | 885456-20-2 | 3.92 |
| 32 | [n+]1(ccccc1)CCCC.[Br-] | 874-80-6 | 3.9 |

| | | | |
|----|---|--------------|------|
| 33 | [n+]1(cc(C)ccc1)CCCC.[B-](F)(F)(F)F | 597581-48-1 | 3.3 |
| 34 | [n+]1(ccccc1)CCCC.[O-]S(=O)(=O)C(F)(F)F | 390423-43-5 | 3.66 |
| 35 | [n+]1(ccccc1)CCCCC.[O-]S(=O)(=O)C(F)(F)F | 623167-81-7 | 2.54 |
| 36 | [n+]1(ccccc1)CCCC.[Cl-] | 1124-64-7 | 3.77 |
| 37 | [n+]1(cc(C)ccc1)CCCCC.[Cl-] | 916730-40-0 | 2.4 |
| 38 | [n+]1(ccc(C)cc1)CCCCC.[Cl-] | 62409-49-8 | 2.67 |
| 39 | [n+]1(ccc(C)cc1)CCCCC.[B-](F)(F)(F)F | 952429-73-1 | 2.17 |
| 40 | [n+]1(ccccc1)CCO.[I-] | 69095-13-2 | 4.16 |
| 41 | [n+]1(ccccc1)COCC.[Cl-] | 21379-36-2 | 3.32 |
| 42 | [n+]1(c(C)cccc1)CCCC.[B-](F)(F)(F)F | 286453-46-1 | 3.25 |
| 43 | [n+]1(ccc(C)cc1)CCCCC.[B-](F)(F)(F)F | 936239-96-2 | 1.49 |
| 44 | [n+]1(cc(C)c(C)cc1)CCCC.[B-](F)(F)(F)F | 952429-71-9 | 3.02 |
| 45 | [n+]1(ccccc1)CCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 890532-45-3 | 2.85 |
| 46 | [n+]1(ccccc1)CCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1104525-90-7 | 3.2 |
| 47 | [n+]1(ccccc1)CCCC.[Br-] | 53385-72-1 | 3.15 |
| 48 | [n+]1(c(C)cccc1)CCCC.[Cl-] | 112400-85-8 | 3.75 |
| 49 | [N+]1(C)(CCCC1)CC(=O)OCC.[Br-] | 129412-64-2 | 3.83 |
| 50 | [N+]1(C)(CCCC1)CC(=O)OCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1107545-20-9 | 3.59 |
| 51 | [n+]1(ccccc1)CCCOC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1049752-00-2 | 3.38 |
| 52 | [N+]1(C)(CCCC1)CCCO.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1049751-96-3 | 3.62 |
| 53 | [N+]1(C)(CCCC1)CCCOC.[Cl-] | 1012794-04-5 | 4.4 |
| 54 | [n+]1(ccccc1)CCOCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 849418-12-8 | 3.26 |
| 55 | [N+](C)(C)(Cc1cccc1)CCCCCCCCCCCC.[Cl-] | 139-08-2 | 0.16 |
| 56 | [n+]1(cccc2cccc12)CCCC.[B-](F)(F)(F)F | 952429-68-4 | 2.16 |
| 57 | [n+]1(cccc2cccc12)CCCC.[Br-] | 31537-79-8 | 2.32 |
| 58 | [N+]1(C)(CCOCC1)CC.[O-]S(=O)(=O)c1ccc(C)cc1 | 445497-25-6 | 3.81 |
| 59 | [N+]1(C)(CCOCC1)COCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1049751-90-7 | 3.36 |
| 60 | [N+]1(C)(CCOCC1)CCOC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 796039-07-1 | 3.81 |
| 61 | [N+]1(C)(CCOCC1)CCCOC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1049751-91-8 | 3.77 |
| 62 | [N+]1(C)(CCOCC1)CCCO.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1026019-24-8 | 3.53 |
| 63 | [N+]1(C)(CCOCC1)CCOCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 663628-48-6 | 3.69 |
| 64 | [N+]1(C)(CCOCC1)CCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 324574-95-0 | 3.43 |
| 65 | [N+]1(C)(CCCC1)CCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 608140-12-1 | 3.16 |
| 66 | [N+]1(C)(CCCC1)CCCOC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1049751-95-2 | 3.27 |

| | | | |
|-----|---|----------------|------|
| 67 | [N+]1(C)(CCCCC1)CCOC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 873583-83-6 | 3.25 |
| 68 | [N+]1(C)(CCCCC1)CCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 623580-02-9 | 3.41 |
| 69 | [N+]1(C)(CCCCC1)COCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1049751-93-0 | 3.41 |
| 70 | [N+]1(C)(CCCCC1)CCCO.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1049751-96-3 | 3.6 |
| 71 | [N+]1(C)(CCCCC1)CCOCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 663628-45-3 | 3.34 |
| 72 | [N+]1(C)(CCCCC1)CCO.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 757212-03-6 | 3.65 |
| 73 | N#CC[N+]1(C)CCCCC1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F | sem CAS | 3.95 |
| 74 | [N+]1(C)(CCCCC1)COCC.[Cl-] | 1012794-08-9 | 4.24 |
| 75 | [N+]1(C)(CCCCC1)CCCOC.[Cl-] | 1012794-04-5 | 4.4 |
| 76 | [N+]1(C)(CCCCC1)CCO.[I-] | 67889-35-4 | 4.58 |
| 77 | [n+]1(ccccc1)CCCCC.[Cl-] | 6220-15-1 | 2.8 |
| 78 | [n+]1(ccccc1)CC#N.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1017553-46-6 | 3.51 |
| 79 | [n+]1(ccccc1)CC#N.[Cl-] | 17281-59-3 | 3.79 |
| 80 | [N+]1(C)(CCCCC1)CCCC.[Br-] | 94280-72-5 | 4.03 |
| 81 | [N+]1(C)=CN(C=C1)CCCCCCCC.[Cl-] | 171058-18-7 | 1.34 |
| 82 | [N+]1(C)=CN(C=C1)CCCCC.[Cl-] | 171058-17-6 | 2.82 |
| 83 | [N+]1(C)=CN(C=C1)CC.[Cl-] | 65039-09-0 | 3.86 |
| 84 | [N+]1(C)=CN(C=C1)CCCCCCCC.[B-](F)(F)(F)F | 244193-55-3 | 1.65 |
| 85 | [N+]1(C)=CN(C=C1)CCCC.[B-](F)(F)(F)F | 244193-49-5 | 3.09 |
| 86 | [N+]1(CC)=CN(C=C1)CCCC.[B-](F)(F)(F)F | 581101-91-9 | 3.26 |
| 87 | [N+]1(C)=CN(C=C1)CCCC.[O-]S(=O)(=O)C(F)(F)F | 174899-66-2 | 3 |
| 88 | [N+]1(C)=CN(C=C1)CCCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 382150-50-7 | 2.24 |
| 89 | [N+]1(C)=CN(C=C1)CCCC.[N-](C(F)(F)F)C(F)(F)F | 710336-91-7 | 2.18 |
| 90 | [N+]1(C)=CN(C=C1)CC.[O-]S(=O)(=O)OC | 516474-01-4 | 4.2 |
| 91 | [n+]1(ccc(C)cc1)CCCCCCC.[Cl-] | 141645-91-2 | 2.97 |
| 92 | [n+]1(ccccc1)CC.[Cl-] | 2294-38-4 | 4.22 |
| 93 | [N+]1(C)(CCCCC1)CC#N.[Cl-] | 194986-67-9 | 4.58 |
| 94 | [N+](C)(C)(Cc1cccc1)CCCCCCCC.[Cl-] | 965-32-2 | 0.65 |
| 95 | [n+]1(cccc2cccc12)CCCCC.[B-](F)(F)(F)F | 952429-69-5 | 1.07 |
| 96 | [N+]1(C)(CCOCC1)CC#N.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1040381-03-0 | 3.53 |
| 97 | [N+]1(C)=CN(C=C1)CCCOC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1015254-36-0 | 3.34 |
| 98 | [N+]1(C)(CCCC1)CC#N.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F | 1017553-47-7 | 3.81 |
| 99 | [N+]1(C)(CCCC1)CCCCC.[Cl-] | 909398-59-0 | 1.63 |
| 100 | [N+]1(C)=CN(C=C1)CCCC.[B-](F)(F)(F)F | 174501-65-6 | 3.11 |

Table S2. Molecular descriptors used in this study.

| Sample | apol | nAromBond | nAtom | nHeavyAtom | nH | nC | nO | nS | nBonds | nBonds2 | nBondsS | nBondsS2 | C2SP2 | C1SP3 | C2SP3 | CrippenMR | fragC | nHBAcc | nHBAcc_ Lipinski | nAtomLC | nAtomLAC | nRotB | TopoPSA | VABC | VAdjMat |
|--------|--------|-----------|-------|------------|----|----|----|----|--------|---------|---------|----------|-------|-------|-------|-----------|-------|--------|---------------------|---------|----------|-------|---------|---------|---------|
| 1 | 40.836 | 5 | 38 | 15 | 23 | 12 | 0 | 0 | 14 | 37 | 37 | 32 | 0 | 2 | 6 | 63.268 | 14.03 | 1 | 2 | 8 | 8 | 7 | 8.81 | 233.34 | 4.907 |
| 2 | 28.462 | 5 | 26 | 11 | 15 | 8 | 0 | 0 | 10 | 25 | 25 | 20 | 0 | 2 | 2 | 44.8 | 10.03 | 1 | 2 | 4 | 4 | 3 | 8.81 | 164.156 | 4.459 |
| 3 | 66.252 | 0 | 63 | 23 | 40 | 20 | 0 | 0 | 22 | 62 | 60 | 60 | 0 | 2 | 14 | 99.428 | 22.03 | 1 | 2 | 16 | 16 | 15 | 4.44 | 383.926 | 5.524 |
| 4 | 31.555 | 5 | 29 | 12 | 17 | 9 | 0 | 0 | 11 | 28 | 28 | 23 | 0 | 2 | 3 | 49.417 | 11.03 | 1 | 2 | 5 | 5 | 4 | 8.81 | 181.452 | 4.585 |
| 5 | 37.743 | 5 | 35 | 14 | 21 | 11 | 0 | 0 | 13 | 34 | 34 | 29 | 0 | 2 | 5 | 58.651 | 13.03 | 1 | 2 | 7 | 7 | 6 | 8.81 | 216.044 | 4.807 |
| 6 | 43.93 | 5 | 41 | 16 | 25 | 13 | 0 | 0 | 15 | 40 | 40 | 35 | 0 | 2 | 7 | 67.885 | 15.03 | 1 | 2 | 9 | 9 | 8 | 8.81 | 250.636 | 5 |
| 7 | 29.332 | 5 | 26 | 11 | 15 | 8 | 0 | 0 | 10 | 25 | 25 | 20 | 0 | 2 | 2 | 44.8 | 10.03 | 1 | 2 | 4 | 4 | 3 | 8.81 | 168.229 | 4.459 |
| 8 | 38.613 | 5 | 35 | 14 | 21 | 11 | 0 | 0 | 13 | 34 | 34 | 29 | 0 | 4 | 4 | 58.727 | 13.03 | 1 | 2 | 6 | 6 | 6 | 8.81 | 220.117 | 4.807 |
| 9 | 31.632 | 5 | 26 | 11 | 15 | 8 | 0 | 0 | 10 | 25 | 25 | 20 | 0 | 2 | 2 | 44.8 | 10.03 | 1 | 2 | 4 | 4 | 3 | 8.81 | 174.222 | 4.459 |
| 10 | 40.821 | 5 | 39 | 18 | 21 | 11 | 0 | 0 | 17 | 38 | 38 | 33 | 0 | 4 | 4 | 68.913 | 17.07 | 1 | 2 | 6 | 6 | 6 | 8.81 | 263.618 | 5.17 |
| 11 | 25.353 | 5 | 24 | 13 | 11 | 6 | 0 | 0 | 12 | 23 | 23 | 18 | 0 | 2 | 0 | 45.752 | 12.07 | 1 | 2 | 5 | 0 | 1 | 8.81 | 177.138 | 4.7 |
| 12 | 43.914 | 5 | 42 | 19 | 23 | 12 | 0 | 0 | 18 | 41 | 41 | 36 | 0 | 2 | 6 | 73.454 | 18.07 | 1 | 2 | 8 | 8 | 7 | 8.81 | 280.914 | 5.248 |
| 13 | 28.446 | 5 | 27 | 14 | 13 | 7 | 0 | 0 | 13 | 26 | 26 | 21 | 0 | 2 | 1 | 50.369 | 13.07 | 1 | 2 | 5 | 3 | 2 | 8.81 | 194.434 | 4.807 |
| 14 | 42.508 | 5 | 39 | 16 | 23 | 12 | 1 | 0 | 15 | 38 | 38 | 33 | 0 | 2 | 6 | 63.639 | 15.04 | 2 | 3 | 9 | 8 | 8 | 29.04 | 246.203 | 5 |
| 15 | 35.502 | 11 | 30 | 15 | 15 | 12 | 0 | 0 | 15 | 30 | 30 | 19 | 4 | 2 | 0 | 57.014 | 15.03 | 1 | 2 | 0 | 0 | 2 | 8.81 | 202.174 | 4.907 |
| 16 | 40.821 | 5 | 39 | 18 | 21 | 11 | 0 | 0 | 17 | 38 | 38 | 33 | 0 | 3 | 4 | 67.86 | 17.07 | 1 | 2 | 6 | 6 | 5 | 8.81 | 263.618 | 5.17 |
| 17 | 35.486 | 11 | 31 | 18 | 13 | 11 | 0 | 0 | 18 | 31 | 31 | 20 | 5 | 1 | 0 | 63.56 | 18.07 | 1 | 2 | 5 | 0 | 2 | 8.81 | 232.452 | 5.17 |
| 18 | 26.17 | 5 | 24 | 11 | 13 | 7 | 1 | 0 | 10 | 23 | 23 | 18 | 0 | 2 | 0 | 41.028 | 10.04 | 2 | 3 | 4 | 0 | 3 | 18.04 | 155.65 | 4.459 |
| 19 | 27.219 | 5 | 26 | 12 | 14 | 8 | 2 | 0 | 11 | 25 | 24 | 19 | 0 | 3 | 0 | 49.49 | 11.04 | 3 | 4 | 4 | 0 | 1 | 48.94 | 163.889 | 4.585 |
| 20 | 50.129 | 5 | 48 | 22 | 26 | 13 | 6 | 1 | 21 | 47 | 45 | 40 | 0 | 6 | 2 | 76.284 | 21.09 | 7 | 8 | 12 | 4 | 10 | 102.08 | 306.675 | 5.459 |
| 21 | 28.832 | 5 | 27 | 16 | 11 | 7 | 3 | 1 | 15 | 26 | 24 | 19 | 0 | 2 | 0 | 44.458 | 15.09 | 4 | 5 | 8 | 0 | 2 | 74.39 | 194.731 | 5 |
| 22 | 43.252 | 5 | 40 | 25 | 15 | 10 | 4 | 2 | 24 | 39 | 35 | 30 | 0 | 2 | 2 | 78.197 | 24.15 | 6 | 7 | 15 | 4 | 7 | 93.85 | 303.118 | 5.644 |
| 23 | 55.626 | 5 | 52 | 29 | 23 | 14 | 4 | 2 | 28 | 51 | 47 | 42 | 0 | 2 | 6 | 96.665 | 28.15 | 6 | 7 | 15 | 8 | 11 | 93.85 | 372.302 | 5.858 |
| 24 | 26.89 | 5 | 26 | 15 | 11 | 8 | 2 | 0 | 14 | 25 | 24 | 19 | 0 | 3 | 0 | 49.871 | 14.07 | 3 | 4 | 7 | 2 | 2 | 48.94 | 182.092 | 4.907 |
| 25 | 29.161 | 5 | 27 | 13 | 14 | 7 | 3 | 1 | 12 | 26 | 24 | 19 | 0 | 2 | 0 | 44.327 | 12.06 | 4 | 5 | 5 | 0 | 1 | 74.39 | 176.529 | 4.7 |
| 26 | 31.533 | 6 | 29 | 15 | 14 | 9 | 0 | 0 | 14 | 28 | 28 | 22 | 3 | 2 | 2 | 54.974 | 14.06 | 0 | 1 | 5 | 4 | 3 | 3.88 | 215.393 | 4.907 |
| 27 | 31.549 | 6 | 28 | 12 | 16 | 10 | 0 | 0 | 11 | 27 | 27 | 21 | 2 | 3 | 2 | 48.428 | 11.02 | 0 | 1 | 4 | 4 | 3 | 3.88 | 185.115 | 4.585 |
| 28 | 38.643 | 0 | 37 | 13 | 24 | 11 | 0 | 0 | 12 | 36 | 36 | 36 | 0 | 4 | 6 | 54.161 | 12.02 | 0 | 1 | 6 | 6 | 5 | 0 | 221.22 | 4.7 |
| 29 | 44.83 | 0 | 43 | 15 | 28 | 13 | 0 | 0 | 14 | 42 | 42 | 42 | 0 | 4 | 8 | 63.395 | 14.02 | 0 | 1 | 8 | 8 | 7 | 0 | 255.812 | 4.907 |
| 30 | 53.433 | 0 | 51 | 27 | 24 | 13 | 4 | 2 | 26 | 50 | 46 | 46 | 0 | 4 | 6 | 87.558 | 26.14 | 5 | 6 | 15 | 6 | 9 | 85.04 | 360.182 | 5.755 |

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|----|--------|----|----|----|----|----|---|---|----|----|----|----|---|---|----|---------|-------|---|---|----|----|----|--------|---------|-------|
| 31 | 36.143 | 6 | 33 | 16 | 17 | 10 | 4 | 1 | 15 | 32 | 30 | 24 | 3 | 2 | 2 | 54.634 | 15.06 | 4 | 5 | 6 | 4 | 4 | 78.69 | 223.574 | 5 |
| 32 | 29.325 | 6 | 25 | 11 | 14 | 9 | 0 | 0 | 10 | 24 | 24 | 18 | 3 | 2 | 2 | 44.788 | 10.02 | 0 | 1 | 4 | 4 | 3 | 3.88 | 171.891 | 4.459 |
| 33 | 34.627 | 6 | 32 | 16 | 16 | 10 | 0 | 0 | 15 | 31 | 31 | 25 | 2 | 3 | 2 | 58.614 | 15.06 | 0 | 1 | 5 | 4 | 3 | 3.88 | 232.689 | 5 |
| 34 | 35.012 | 6 | 32 | 18 | 14 | 10 | 3 | 1 | 17 | 31 | 29 | 23 | 3 | 2 | 2 | 53.68 | 17.08 | 3 | 4 | 8 | 4 | 4 | 69.46 | 232.986 | 5.17 |
| 35 | 41.199 | 6 | 38 | 20 | 18 | 12 | 3 | 1 | 19 | 37 | 35 | 29 | 3 | 2 | 4 | 62.914 | 19.08 | 3 | 4 | 8 | 6 | 6 | 69.46 | 267.578 | 5.322 |
| 36 | 28.455 | 6 | 25 | 11 | 14 | 9 | 0 | 0 | 10 | 24 | 24 | 18 | 3 | 2 | 2 | 44.788 | 10.02 | 0 | 1 | 4 | 4 | 3 | 3.88 | 167.819 | 4.459 |
| 37 | 37.736 | 6 | 34 | 14 | 20 | 12 | 0 | 0 | 13 | 33 | 33 | 27 | 2 | 3 | 4 | 57.662 | 13.02 | 0 | 1 | 6 | 6 | 5 | 3.88 | 219.707 | 4.807 |
| 38 | 37.736 | 6 | 34 | 14 | 20 | 12 | 0 | 0 | 13 | 33 | 33 | 27 | 2 | 3 | 4 | 57.662 | 13.02 | 0 | 1 | 6 | 6 | 5 | 3.88 | 219.707 | 4.807 |
| 39 | 40.814 | 6 | 38 | 18 | 20 | 12 | 0 | 0 | 17 | 37 | 37 | 31 | 2 | 3 | 4 | 67.848 | 17.06 | 0 | 1 | 6 | 6 | 5 | 3.88 | 267.281 | 5.17 |
| 40 | 26.24 | 6 | 20 | 10 | 10 | 7 | 1 | 0 | 9 | 19 | 19 | 13 | 3 | 2 | 0 | 33.723 | 9.03 | 1 | 2 | 3 | 2 | 2 | 24.11 | 152.083 | 4.322 |
| 41 | 26.164 | 6 | 23 | 11 | 12 | 8 | 1 | 0 | 10 | 22 | 22 | 16 | 3 | 2 | 0 | 41.016 | 10.03 | 1 | 2 | 4 | 0 | 3 | 13.11 | 159.313 | 4.459 |
| 42 | 34.627 | 6 | 32 | 16 | 16 | 10 | 0 | 0 | 15 | 31 | 31 | 25 | 4 | 3 | 2 | 58.614 | 15.06 | 0 | 1 | 5 | 4 | 3 | 3.88 | 232.689 | 5 |
| 43 | 47.001 | 6 | 44 | 20 | 24 | 14 | 0 | 0 | 19 | 43 | 43 | 37 | 2 | 3 | 6 | 77.082 | 19.06 | 0 | 1 | 8 | 8 | 7 | 3.88 | 301.873 | 5.322 |
| 44 | 37.72 | 6 | 35 | 17 | 18 | 11 | 0 | 0 | 16 | 34 | 34 | 28 | 1 | 4 | 2 | 62.254 | 16.06 | 0 | 1 | 5 | 4 | 3 | 3.88 | 249.985 | 5.087 |
| 45 | 46.339 | 6 | 42 | 26 | 16 | 12 | 4 | 2 | 25 | 41 | 37 | 31 | 3 | 2 | 3 | 82.802 | 25.14 | 5 | 6 | 15 | 5 | 8 | 88.92 | 324.077 | 5.7 |
| 46 | 40.152 | 6 | 36 | 24 | 12 | 10 | 4 | 2 | 23 | 35 | 31 | 25 | 3 | 2 | 1 | 73.568 | 23.14 | 5 | 6 | 15 | 3 | 6 | 88.92 | 289.485 | 5.585 |
| 47 | 32.419 | 6 | 28 | 12 | 16 | 10 | 0 | 0 | 11 | 27 | 27 | 21 | 3 | 2 | 3 | 49.405 | 11.02 | 0 | 1 | 5 | 5 | 4 | 3.88 | 189.187 | 4.585 |
| 48 | 31.549 | 6 | 28 | 12 | 16 | 10 | 0 | 0 | 11 | 27 | 27 | 21 | 4 | 3 | 2 | 48.428 | 11.02 | 0 | 1 | 4 | 4 | 3 | 3.88 | 185.115 | 4.585 |
| 49 | 33.596 | 0 | 31 | 13 | 18 | 9 | 2 | 0 | 12 | 30 | 29 | 29 | 0 | 5 | 2 | 49.895 | 12.04 | 2 | 3 | 6 | 2 | 4 | 26.3 | 205.645 | 4.7 |
| 50 | 47.516 | 0 | 45 | 27 | 18 | 11 | 6 | 2 | 26 | 44 | 39 | 39 | 0 | 5 | 2 | 83.292 | 26.16 | 7 | 8 | 15 | 2 | 8 | 111.34 | 340.534 | 5.755 |
| 51 | 44.047 | 6 | 40 | 26 | 14 | 11 | 5 | 2 | 25 | 39 | 35 | 29 | 3 | 2 | 1 | 76.527 | 25.15 | 6 | 7 | 15 | 3 | 8 | 98.15 | 315.571 | 5.7 |
| 52 | 48.048 | 0 | 46 | 26 | 20 | 11 | 5 | 2 | 25 | 45 | 41 | 41 | 0 | 4 | 4 | 79.736 | 25.15 | 6 | 7 | 15 | 3 | 7 | 105.27 | 334.38 | 5.7 |
| 53 | 36.351 | 0 | 35 | 13 | 22 | 10 | 1 | 0 | 12 | 34 | 34 | 34 | 0 | 4 | 4 | 51.129 | 12.03 | 1 | 2 | 5 | 3 | 4 | 9.23 | 212.714 | 4.7 |
| 54 | 44.047 | 6 | 40 | 26 | 14 | 11 | 5 | 2 | 25 | 39 | 35 | 29 | 3 | 4 | 0 | 76.527 | 25.15 | 6 | 7 | 15 | 2 | 8 | 98.15 | 315.571 | 5.7 |
| 55 | 71.765 | 6 | 67 | 25 | 42 | 23 | 0 | 0 | 24 | 66 | 66 | 60 | 5 | 3 | 12 | 107.443 | 24.02 | 0 | 1 | 18 | 14 | 15 | 0 | 409.963 | 5.644 |
| 56 | 39.907 | 11 | 35 | 19 | 16 | 13 | 0 | 0 | 19 | 35 | 35 | 24 | 7 | 2 | 2 | 72.48 | 19.06 | 0 | 1 | 5 | 4 | 3 | 3.88 | 256.047 | 5.248 |
| 57 | 37.699 | 11 | 31 | 15 | 16 | 13 | 0 | 0 | 15 | 31 | 31 | 20 | 7 | 2 | 2 | 62.294 | 15.02 | 0 | 1 | 4 | 4 | 3 | 3.88 | 212.546 | 4.907 |
| 58 | 47.184 | 6 | 43 | 20 | 23 | 14 | 4 | 1 | 20 | 43 | 41 | 35 | 5 | 7 | 0 | 71.02 | 20.06 | 4 | 5 | 4 | 0 | 2 | 74.81 | 280.401 | 5.322 |
| 59 | 45.756 | 0 | 44 | 26 | 18 | 10 | 6 | 2 | 25 | 43 | 39 | 39 | 0 | 6 | 0 | 76.627 | 25.16 | 7 | 8 | 15 | 0 | 7 | 103.5 | 325.875 | 5.7 |
| 60 | 45.756 | 0 | 44 | 26 | 18 | 10 | 6 | 2 | 25 | 43 | 39 | 39 | 0 | 6 | 0 | 76.877 | 25.16 | 7 | 8 | 15 | 2 | 7 | 103.5 | 325.875 | 5.7 |
| 61 | 48.85 | 0 | 47 | 27 | 20 | 11 | 6 | 2 | 26 | 46 | 42 | 42 | 0 | 6 | 1 | 81.494 | 26.16 | 7 | 8 | 15 | 3 | 8 | 103.5 | 343.171 | 5.755 |
| 62 | 45.756 | 0 | 44 | 26 | 18 | 10 | 6 | 2 | 25 | 43 | 39 | 39 | 0 | 6 | 1 | 76.704 | 25.16 | 7 | 8 | 15 | 3 | 7 | 114.5 | 325.875 | 5.7 |
| 63 | 48.85 | 0 | 47 | 27 | 20 | 11 | 6 | 2 | 26 | 46 | 42 | 42 | 0 | 8 | 0 | 81.494 | 26.16 | 7 | 8 | 15 | 2 | 8 | 103.5 | 343.171 | 5.755 |
| 64 | 48.048 | 0 | 46 | 26 | 20 | 11 | 5 | 2 | 25 | 45 | 41 | 41 | 0 | 6 | 2 | 79.909 | 25.15 | 6 | 7 | 15 | 4 | 7 | 94.27 | 334.38 | 5.7 |

| | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|--------|----|----|----|----|----|---|---|----|----|----|----|---|---|---|--------|-------|---|---|----|----|----|--------|---------|-------|
| 65 | 47.246 | 0 | 45 | 25 | 20 | 11 | 4 | 2 | 24 | 44 | 40 | 40 | 0 | 4 | 4 | 78.324 | 24.14 | 5 | 6 | 15 | 3 | 6 | 85.04 | 325.59 | 5.644 |
| 66 | 51.141 | 0 | 49 | 27 | 22 | 12 | 5 | 2 | 26 | 48 | 44 | 44 | 0 | 4 | 4 | 84.526 | 26.15 | 6 | 7 | 15 | 3 | 8 | 94.27 | 351.676 | 5.755 |
| 67 | 48.048 | 0 | 46 | 26 | 20 | 11 | 5 | 2 | 25 | 45 | 41 | 41 | 0 | 4 | 3 | 79.909 | 25.15 | 6 | 7 | 15 | 2 | 7 | 94.27 | 334.38 | 5.7 |
| 68 | 50.339 | 0 | 48 | 26 | 22 | 12 | 4 | 2 | 25 | 47 | 43 | 43 | 0 | 4 | 5 | 82.941 | 25.14 | 5 | 6 | 15 | 4 | 7 | 85.04 | 342.886 | 5.7 |
| 69 | 48.048 | 0 | 46 | 26 | 20 | 11 | 5 | 2 | 25 | 45 | 41 | 41 | 0 | 4 | 3 | 79.659 | 25.15 | 6 | 7 | 15 | 0 | 7 | 94.27 | 334.38 | 5.7 |
| 70 | 48.048 | 0 | 46 | 26 | 20 | 11 | 5 | 2 | 25 | 45 | 41 | 41 | 0 | 4 | 4 | 79.736 | 25.15 | 6 | 7 | 15 | 3 | 7 | 105.27 | 334.38 | 5.7 |
| 71 | 51.141 | 0 | 49 | 27 | 22 | 12 | 5 | 2 | 26 | 48 | 44 | 44 | 0 | 6 | 3 | 84.526 | 26.15 | 6 | 7 | 15 | 2 | 8 | 94.27 | 351.676 | 5.755 |
| 72 | 44.954 | 0 | 43 | 25 | 18 | 10 | 5 | 2 | 24 | 42 | 38 | 38 | 0 | 4 | 3 | 75.119 | 24.15 | 6 | 7 | 15 | 2 | 6 | 105.27 | 317.084 | 5.644 |
| 73 | 43.252 | 0 | 40 | 25 | 15 | 10 | 4 | 2 | 24 | 39 | 34 | 34 | 0 | 3 | 3 | 75.164 | 24.15 | 6 | 7 | 15 | 2 | 5 | 108.83 | 314.018 | 5.644 |
| 74 | 33.258 | 0 | 32 | 12 | 20 | 9 | 1 | 0 | 11 | 31 | 31 | 31 | 0 | 4 | 3 | 46.262 | 11.03 | 1 | 2 | 4 | 0 | 3 | 9.23 | 195.418 | 4.585 |
| 75 | 36.351 | 0 | 35 | 13 | 22 | 10 | 1 | 0 | 12 | 34 | 34 | 34 | 0 | 4 | 4 | 51.129 | 12.03 | 1 | 2 | 5 | 3 | 4 | 9.23 | 212.714 | 4.7 |
| 76 | 33.334 | 0 | 29 | 11 | 18 | 8 | 1 | 0 | 10 | 28 | 28 | 28 | 0 | 4 | 3 | 41.722 | 10.03 | 1 | 2 | 3 | 2 | 2 | 20.23 | 188.188 | 4.459 |
| 77 | 34.642 | 6 | 31 | 13 | 18 | 11 | 0 | 0 | 12 | 30 | 30 | 24 | 3 | 2 | 4 | 54.022 | 12.02 | 0 | 1 | 6 | 6 | 5 | 3.88 | 202.411 | 4.7 |
| 78 | 36.158 | 6 | 31 | 24 | 7 | 9 | 4 | 2 | 23 | 30 | 25 | 19 | 3 | 1 | 0 | 67.165 | 23.15 | 6 | 7 | 15 | 2 | 5 | 112.71 | 277.913 | 5.585 |
| 79 | 21.368 | 6 | 17 | 10 | 7 | 7 | 0 | 0 | 9 | 16 | 15 | 9 | 3 | 1 | 0 | 33.768 | 9.03 | 1 | 2 | 3 | 2 | 1 | 27.67 | 138.951 | 4.322 |
| 80 | 36.419 | 0 | 34 | 12 | 22 | 10 | 0 | 0 | 11 | 33 | 33 | 33 | 0 | 4 | 5 | 49.544 | 11.02 | 0 | 1 | 4 | 4 | 3 | 0 | 207.997 | 4.585 |
| 81 | 47.023 | 5 | 44 | 17 | 27 | 14 | 0 | 0 | 16 | 43 | 43 | 38 | 0 | 2 | 8 | 72.502 | 16.03 | 1 | 2 | 10 | 10 | 9 | 8.81 | 267.932 | 5.087 |
| 82 | 34.649 | 5 | 32 | 13 | 19 | 10 | 0 | 0 | 12 | 31 | 31 | 26 | 0 | 2 | 4 | 54.034 | 12.03 | 1 | 2 | 6 | 6 | 5 | 8.81 | 198.748 | 4.7 |
| 83 | 22.275 | 5 | 20 | 9 | 11 | 6 | 0 | 0 | 8 | 19 | 19 | 14 | 0 | 2 | 0 | 35.566 | 8.03 | 1 | 2 | 1 | 0 | 1 | 8.81 | 129.564 | 4.17 |
| 84 | 47.008 | 5 | 45 | 20 | 25 | 13 | 0 | 0 | 19 | 44 | 44 | 39 | 0 | 2 | 7 | 78.071 | 19.07 | 1 | 2 | 9 | 9 | 8 | 8.81 | 298.21 | 5.322 |
| 85 | 34.633 | 5 | 33 | 16 | 17 | 9 | 0 | 0 | 15 | 32 | 32 | 27 | 0 | 2 | 3 | 59.603 | 15.07 | 1 | 2 | 5 | 5 | 4 | 8.81 | 229.026 | 5 |
| 86 | 34.633 | 5 | 33 | 16 | 17 | 9 | 0 | 0 | 15 | 32 | 32 | 27 | 0 | 4 | 2 | 59.679 | 15.07 | 1 | 2 | 5 | 4 | 4 | 8.81 | 229.026 | 5 |
| 87 | 35.019 | 5 | 33 | 18 | 15 | 9 | 3 | 1 | 17 | 32 | 30 | 25 | 0 | 2 | 2 | 53.692 | 17.09 | 4 | 5 | 8 | 4 | 4 | 74.39 | 229.323 | 5.17 |
| 88 | 49.439 | 5 | 46 | 27 | 19 | 12 | 4 | 2 | 26 | 45 | 41 | 36 | 0 | 2 | 4 | 87.431 | 26.15 | 6 | 7 | 15 | 6 | 9 | 93.85 | 337.71 | 5.755 |
| 89 | 34.244 | 5 | 34 | 19 | 15 | 10 | 0 | 0 | 18 | 33 | 33 | 28 | 0 | 2 | 2 | 60.269 | 18.09 | 2 | 3 | 9 | 4 | 5 | 8.81 | 230.939 | 5.248 |
| 90 | 29.963 | 5 | 28 | 14 | 14 | 7 | 4 | 1 | 13 | 27 | 25 | 20 | 0 | 2 | 0 | 45.412 | 13.07 | 5 | 6 | 6 | 0 | 2 | 83.62 | 185.319 | 4.807 |
| 91 | 43.923 | 6 | 40 | 16 | 24 | 14 | 0 | 0 | 15 | 39 | 39 | 33 | 2 | 3 | 6 | 66.896 | 15.02 | 0 | 1 | 8 | 8 | 7 | 3.88 | 254.299 | 5 |
| 92 | 22.268 | 6 | 19 | 9 | 10 | 7 | 0 | 0 | 8 | 18 | 18 | 12 | 3 | 2 | 0 | 35.554 | 8.02 | 0 | 1 | 1 | 0 | 1 | 3.88 | 133.227 | 4.17 |
| 93 | 28.462 | 0 | 26 | 11 | 15 | 8 | 0 | 0 | 10 | 25 | 24 | 24 | 0 | 3 | 3 | 41.767 | 10.03 | 1 | 2 | 3 | 2 | 1 | 23.79 | 175.056 | 4.459 |
| 94 | 59.391 | 6 | 55 | 21 | 34 | 19 | 0 | 0 | 20 | 54 | 54 | 48 | 5 | 3 | 8 | 88.975 | 20.02 | 0 | 1 | 14 | 10 | 11 | 0 | 340.779 | 5.392 |
| 95 | 46.094 | 11 | 41 | 21 | 20 | 15 | 0 | 0 | 21 | 41 | 41 | 30 | 7 | 2 | 4 | 81.714 | 21.06 | 0 | 1 | 6 | 6 | 5 | 3.88 | 290.639 | 5.392 |
| 96 | 40.96 | 0 | 38 | 25 | 13 | 9 | 5 | 2 | 24 | 37 | 32 | 32 | 0 | 5 | 0 | 72.132 | 24.16 | 7 | 8 | 15 | 2 | 5 | 118.06 | 305.512 | 5.644 |
| 97 | 44.054 | 5 | 41 | 26 | 15 | 10 | 5 | 2 | 25 | 40 | 36 | 31 | 0 | 2 | 1 | 78.741 | 25.16 | 7 | 8 | 15 | 3 | 8 | 103.08 | 311.908 | 5.7 |
| 98 | 40.158 | 0 | 37 | 24 | 13 | 9 | 4 | 2 | 23 | 36 | 31 | 31 | 0 | 3 | 2 | 70.547 | 23.15 | 6 | 7 | 15 | 2 | 5 | 108.83 | 296.722 | 5.585 |

| | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|--------|---|----|----|----|----|---|---|----|----|----|----|---|---|---|--------|-------|---|---|---|---|---|------|--------|-------|
| 99 | 38.643 | 0 | 37 | 13 | 24 | 11 | 0 | 0 | 12 | 36 | 36 | 36 | 0 | 4 | 6 | 54.161 | 12.02 | 0 | 1 | 6 | 6 | 5 | 0 | 221.22 | 4.7 |
| 100 | 31.54 | 5 | 30 | 15 | 15 | 8 | 0 | 0 | 14 | 29 | 29 | 24 | 0 | 2 | 2 | 54.986 | 14.07 | 1 | 2 | 5 | 4 | 3 | 8.81 | 211.73 | 4.907 |

Table S3. Values of Crippen and Mannhold LogP

| Sample | CrippenLogP | MannholdLogP |
|--------|-------------|--------------|
| 1 | 1.283 | 2.450 |
| 2 | -0.278 | 2.010 |
| 3 | 1.961 | 3.330 |
| 4 | 0.112 | 2.120 |
| 5 | 0.892 | 2.340 |
| 6 | 1.673 | 2.560 |
| 7 | -0.278 | 2.010 |
| 8 | 0.985 | 2.340 |
| 9 | -0.278 | 2.010 |
| 10 | 5.281 | 1.900 |
| 11 | 3.238 | 1.350 |
| 12 | 5.579 | 2.010 |
| 13 | 3.628 | 1.460 |
| 14 | -0.150 | 2.340 |
| 15 | -0.594 | 2.450 |
| 16 | 4.826 | 1.900 |
| 17 | 3.674 | 1.900 |
| 18 | -1.369 | 1.790 |
| 19 | 0.928 | 1.900 |
| 20 | 2.158 | 1.900 |
| 21 | 2.303 | 1.240 |
| 22 | 5.939 | 0.910 |
| 23 | 7.499 | 1.350 |
| 24 | 1.470 | 1.570 |
| 25 | 1.413 | 1.570 |
| 26 | 4.274 | 1.790 |
| 27 | 0.007 | 2.340 |

| | | |
|----|--------|-------|
| 28 | -0.189 | 2.450 |
| 29 | 0.591 | 2.670 |
| 30 | 6.028 | 1.350 |
| 31 | 2.381 | 1.900 |
| 32 | -0.022 | 2.230 |
| 33 | 4.303 | 1.900 |
| 34 | 3.340 | 1.680 |
| 35 | 4.120 | 1.900 |
| 36 | -0.022 | 2.230 |
| 37 | 0.787 | 2.560 |
| 38 | 0.787 | 2.560 |
| 39 | 5.083 | 2.120 |
| 40 | -3.030 | 1.900 |
| 41 | -1.112 | 2.010 |
| 42 | 4.303 | 1.900 |
| 43 | 5.863 | 2.340 |
| 44 | 4.331 | 2.010 |
| 45 | 6.585 | 1.240 |
| 46 | 5.805 | 1.020 |
| 47 | 0.369 | 2.340 |
| 48 | 0.007 | 2.340 |
| 49 | -1.972 | 2.010 |
| 50 | 4.245 | 0.910 |
| 51 | 4.232 | 1.020 |
| 52 | 4.220 | 1.020 |
| 53 | -1.343 | 2.230 |
| 54 | 4.232 | 1.020 |
| 55 | 3.629 | 3.770 |
| 56 | 5.428 | 2.230 |
| 57 | 1.132 | 2.670 |
| 58 | 1.616 | 2.340 |
| 59 | 3.678 | 0.800 |
| 60 | 3.331 | 0.800 |
| 61 | 3.721 | 0.910 |

| | | |
|----|--------|-------|
| 62 | 3.067 | 0.800 |
| 63 | 3.721 | 0.910 |
| 64 | 4.484 | 1.020 |
| 65 | 5.248 | 1.130 |
| 66 | 4.874 | 1.130 |
| 67 | 4.484 | 1.020 |
| 68 | 5.638 | 1.240 |
| 69 | 4.832 | 1.020 |
| 70 | 4.220 | 1.020 |
| 71 | 4.874 | 1.130 |
| 72 | 3.830 | 0.910 |
| 73 | 4.428 | 0.910 |
| 74 | -1.385 | 2.120 |
| 75 | -1.343 | 2.230 |
| 76 | -2.387 | 2.010 |
| 77 | 0.759 | 2.450 |
| 78 | 3.785 | 0.800 |
| 79 | -2.432 | 1.900 |
| 80 | -0.579 | 2.340 |
| 81 | 2.063 | 2.670 |
| 82 | 0.502 | 2.230 |
| 83 | -1.058 | 1.790 |
| 84 | 5.969 | 2.120 |
| 85 | 4.408 | 1.680 |
| 86 | 4.501 | 1.680 |
| 87 | 3.083 | 1.460 |
| 88 | 6.719 | 1.130 |
| 89 | 5.118 | 1.570 |
| 90 | 1.345 | 1.460 |
| 91 | 1.567 | 2.780 |
| 92 | -0.802 | 2.010 |
| 93 | -1.789 | 2.010 |
| 94 | 2.068 | 3.330 |
| 95 | 6.208 | 2.450 |

| | | |
|-----|--------|-------|
| 96 | 3.274 | 0.690 |
| 97 | 4.770 | 0.800 |
| 98 | 4.037 | 0.800 |
| 99 | -0.189 | 2.450 |
| 100 | 4.018 | 1.570 |

Table S4. Observed and predicted activities for Models 1, 2 and 3 in the external validation

| Samples | LogEC ₅₀ measured | Predicted Model | Residual Model | Predicted Model | Residual Model | Predicted Model | Residual Model |
|---------|---------------------------------|-----------------|----------------|-----------------|----------------|-----------------|----------------|
| | | 1 | 1 | 2 | 2 | 3 | 3 |
| 81 | 1.340 | 1.662 | -0.322 | 1.647 | -0.307 | 2.586 | -1.246 |
| 82 | 2.820 | 2.813 | 0.007 | 2.784 | 0.036 | 2.536 | 0.284 |
| 83 | 3.860 | 4.394 | -0.534 | 4.242 | -0.382 | 2.463 | 1.397 |
| 84 | 1.650 | 1.790 | -0.140 | 1.522 | 0.128 | 3.045 | -1.395 |
| 85 | 3.090 | 2.960 | 0.130 | 2.659 | 0.431 | 3.007 | 0.083 |
| 86 | 3.260 | 3.110 | 0.150 | 2.814 | 0.446 | 3.007 | 0.253 |
| 87 | 3.000 | 3.364 | -0.364 | 3.326 | -0.326 | 3.244 | -0.244 |
| 88 | 2.240 | 2.566 | -0.326 | 2.527 | -0.287 | 3.707 | -1.467 |
| 89 | 2.180 | 2.808 | -0.628 | 2.741 | -0.561 | 3.253 | -1.073 |
| 90 | 4.200 | 4.516 | -0.316 | 4.362 | -0.162 | 2.982 | 1.218 |
| 91 | 2.970 | 1.998 | 0.972 | 2.131 | 0.839 | 2.886 | 0.084 |
| 92 | 4.220 | 4.139 | 0.081 | 4.258 | -0.038 | 2.650 | 1.570 |
| 93 | 4.580 | 4.071 | 0.509 | 3.803 | 0.777 | 1.898 | 2.682 |
| 94 | 0.650 | 1.162 | -0.512 | 1.283 | -0.633 | 3.057 | -2.407 |
| 95 | 1.070 | 1.894 | -0.824 | 2.086 | -1.016 | 4.703 | -3.633 |
| 96 | 3.530 | 3.991 | -0.461 | 3.805 | -0.275 | 3.074 | 0.456 |
| 97 | 3.340 | 3.320 | 0.020 | 3.416 | -0.076 | 3.685 | -0.345 |
| 98 | 3.810 | 3.934 | -0.124 | 3.670 | 0.140 | 2.960 | 0.850 |
| 99 | 1.630 | 2.798 | -1.168 | 2.663 | -1.033 | 1.698 | -0.068 |
| 100 | 3.110 | 3.271 | -0.161 | 2.944 | 0.166 | 2.995 | 0.115 |

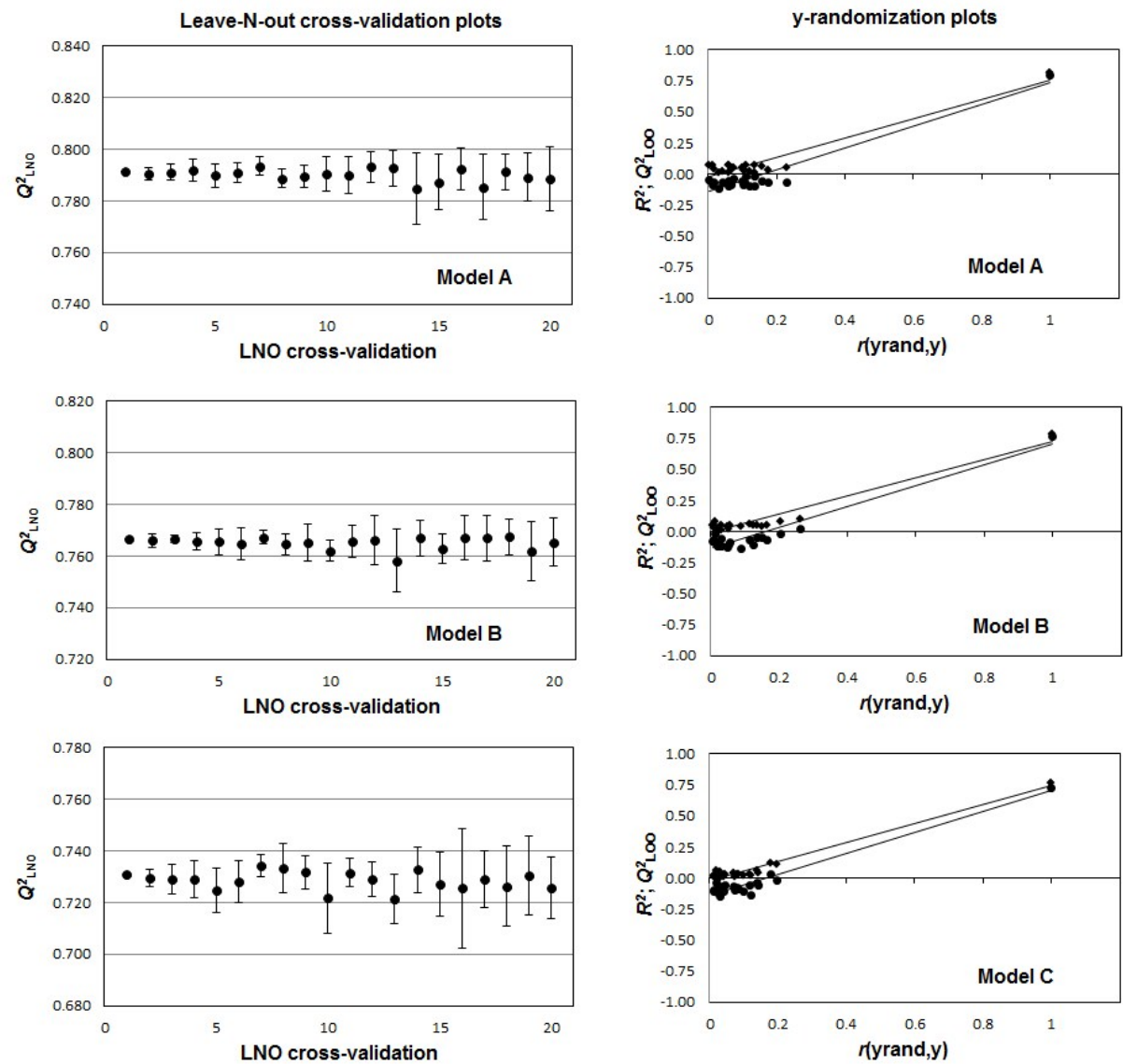


Fig. S1. Leave-N-out cross-validation and y-randomization plots for the three models. The bars represent the standard deviations.