## 2W1_compiled Kd_supplemental
| chemical name | Kd | Kd 95% CI | ∆Amax | ∆Amax 95% CI | ∆Amax/Kd | MW | CAS | CLOGP | ROTATABLE\_BONDS | TPSA (Å²) | IUPAC name | SMILES |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ciproxifan hydrochloride | 0.382 | 0.281 to 0.514 | 0.0798 | 0.0744 to 0.0855 | 0.209 | 306.800 | 1049741-81-2 | 2.50 | 7.0 | 55.0 | cyclopropyl-[4-[3-(1H-imidazol-5-yl)propoxy]phenyl]methanone;hydrochloride | C1CC1C(=O)C2=CC=C(C=C2)OCCCC3=CN=CN3 |
| SKF96365 | 0.39 | 0.271 to 0.555 | 0.0714 | 0.0649 to 0.0783 | 0.183 | 402.910 | 130495-35-1 | NaN | 10.0 | 45.5 | 1-[2-(4-methoxyphenyl)-2-[3-(4-methoxyphenyl)propoxy]ethyl]imidazole;hydrochloride | COC1=CC=C(C=C1)CCCOC(CN2C=CN=C2)C3=CC=C(C=C3)OC |
| Miconazole impurity H | 0.403 | 0.315 to 0.512 | 0.0775 | 0.0728 to 0.0826 | 0.192 | 347.240 | 181931-30-6 | 4.70 | 6.0 | 27.0 | 1-[2-(2,4-dichlorophenyl)-2-phenylmethoxyethyl]imidazole | C1=CC=C(C=C1)COC(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl |
| Miconazole impurity B | 0.419 | 0.302 to 0.577 | 0.0731 | 0.0676 to 0.0789 | 0.174 | 381.680 | 913837-72-6 | 4.70 | 6.0 | 27.0 | 1-[2-[(3-chlorophenyl)methoxy]-2-(2,4-dichlorophenyl)ethyl]imidazole | C1=CC(=CC(=C1)Cl)COC(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl |
| 4-chlorobenzyl 2-(1H-imidazol-1-yl)-1-phenylethyl ether nitrate salt | 0.435 | 0.348 to 0.542 | 0.073 | 0.0689 to 0.0773 | 0.168 | 375.815 | NaN | 3.50 | 6.0 | 27.0 | 1-[(2S)-2-[(4-chlorophenyl)methoxy]-2-phenylethyl]imidazole | ClC1=CC=C(CO[C@@H](C2=CC=CC=C2)CN3C=CN=C3)C=C1 |
| Econazole | 0.453 | 0.347 to 0.589 | 0.0737 | 0.0684 to 0.0794 | 0.163 | 381.700 | 27220-47-9 | 5.50 | 6.0 | 27.0 | 1-[2-[(4-chlorophenyl)methoxy]-2-(2,4-dichlorophenyl)ethyl]imidazole | C1=CC(=CC=C1COC(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl)Cl |
| Neticonazole Hydrochloride | 0.456 | 0.359 to 0.577 | 0.0649 | 0.0615 to 0.0685 | 0.142 | 338.900 | 130773-02-3 | 4.10 | 8.0 | 52.4 | 1-[(E)-2-methylsulfanyl-1-(2-pentoxyphenyl)ethenyl]imidazole;hydrochloride | CCCCCOC1=CC=CC=C1C(=CSC)N2C=CN=C2 |
| Bifonazole | 0.457 | 0.317 to 0.644 | 0.076 | 0.0693 to 0.0831 | 0.166 | 310.390 | 60628-96-8 | 4.80 | 4.0 | 17.8 | 1-[phenyl-(4-phenylphenyl)methyl]imidazole | C1=CC=C(C=C1)C2=CC=C(C=C2)C(C3=CC=CC=C3)N4C=CN=C4 |
| Clotrimazole | 0.46 | 0.310 to 0.639 | 0.0673 | 0.0644 to 0.0702 | 0.146 | 344.830 | 23593-75-1 | 5.00 | 4.0 | 17.8 | 1-[(2-chlorophenyl)-diphenylmethyl]imidazole | C1=CC=C(C=C1)C(C2=CC=CC=C2)(C3=CC=CC=C3Cl)N4C=CN=C4 |
| Sulconazole Nitrate | 0.463 | 0.337 to 0.633 | 0.0778 | 0.0712 to 0.0850 | 0.168 | 460.800 | 61318-91-0 | 6.10 | 6.0 | 109.0 | 1-[2-[(4-chlorophenyl)methylsulfanyl]-2-(2,4-dichlorophenyl)ethyl]imidazole;nitric acid | C1=CC(=CC=C1CSC(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl)Cl |
| Prochloraz | 0.474 | 0.325 to 0.685 | 0.0641 | 0.0584 to 0.0702 | 0.135 | 376.670 | 67747-09-5 | 4.60 | 6.0 | 47.4 | N-propyl-N-[2-(2,4,6-trichlorophenoxy)ethyl]imidazole-1-carboxamide | CCCN(CCOC1=C(C=C(C=C1Cl)Cl)Cl)C(=O)N2C=CN=C2 |
| Miconazole impurity I | 0.477 | 0.274 to 0.809 | 0.0771 | 0.0666 to 0.0889 | 0.162 | 444.700 | 24169-00-4 | 4.70 | 6.0 | 27.0 | 1-[2-[(2-chlorophenyl)methoxy]-2-(2,4-dichlorophenyl)ethyl]imidazole | C1=CC=C(C(=C1)COC(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl)Cl |
| Enilconazole | 0.488 | 0.377 to 0.629 | 0.0706 | 0.0657 to 0.0759 | 0.145 | 297.200 | 35554-44-0 | 3.80 | 6.0 | 27.0 | 1-[2-(2,4-dichlorophenyl)-2-prop-2-enoxyethyl]imidazole | C=CCOC(CN1C=CN=C1)C2=C(C=C(C=C2)Cl)Cl |
| Butoconazole Nitrate | 0.496 | 0.363 to 0.669 | 0.0772 | 0.0712 to 0.0836 | 0.156 | 474.800 | 64872-77-1 | 6.40 | 7.0 | 109.0 | 1-[4-(4-chlorophenyl)-2-(2,6-dichlorophenyl)sulfanylbutyl]imidazole;nitric acid | C1=CC(=C(C(=C1)Cl)SC(CCC2=CC=C(C=C2)Cl)CN3C=CN=C3)Cl |
| Tioconazole | 0.498 | 0.385 to 0.638 | 0.0793 | 0.0742 to 0.0847 | 0.159 | 387.700 | 65899-73-2 | 5.30 | 6.0 | 55.3 | 1-[2-[(2-chlorothiophen-3-yl)methoxy]-2-(2,4-dichlorophenyl)ethyl]imidazole | C1=CC(=C(C=C1Cl)Cl)C(CN2C=CN=C2)OCC3=C(SC=C3)Cl |
| 1-(2,4-dichlorophenyl)-2-imidazol-1-ylethanol | 0.507 | 0.425 to 0.603 | 0.0679 | 0.0652 to 0.0707 | 0.134 | 257.120 | 24155-42-8 | 2.60 | 3.0 | 38.0 | 1-(2,4-dichlorophenyl)-2-imidazol-1-ylethanol | C1=CC(=C(C=C1Cl)Cl)C(CN2C=CN=C2)O |
| Isoconazole nitrate | 0.507 | 0.404 to 0.633 | 0.0723 | 0.0686 to 0.0762 | 0.143 | 479.100 | 24168-96-5 | 5.30 | 6.0 | 93.1 | 1-[2-(2,4-dichlorophenyl)-2-[(2,6-dichlorophenyl)methoxy]ethyl]imidazole;nitric acid | C1=CC(=C(C(=C1)Cl)COC(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl)Cl |
| Fenticonazole Nitrate | 0.541 | 0.423 to 0.689 | 0.0698 | 0.0658 to 0.0739 | 0.129 | 518.410 | 73151-29-8 | 6.70 | 8.0 | 118.0 | 1-[2-(2,4-dichlorophenyl)-2-[(4-phenylsulfanylphenyl)methoxy]ethyl]imidazole;nitric acid | C1=CC=C(C=C1)SC2=CC=C(C=C2)COC(CN3C=CN=C3)C4=C(C=C(C=C4)Cl)Cl |
| Flutrimazole | 0.566 | 0.479 to 0.661 | 0.063 | 0.0617 to 0.0643 | 0.111 | 346.400 | 119006-77-8 | 4.60 | 4.0 | 17.8 | 1-[(2-fluorophenyl)-(4-fluorophenyl)-phenylmethyl]imidazole | C1=CC=C(C=C1)C(C2=CC=C(C=C2)F)(C3=CC=CC=C3F)N4C=CN=C4 |
| NITRIC ACID COMPOUND WITH [2-(2,4-DICHLOROPHENYL)-2-(1H-IMIDAZOL-1-YLMETHYL)-1,3-DIOXOLAN-4-YL]METHYL BENZOATE | 0.572 | 0.464 to 0.702 | 0.0644 | 0.0613 to 0.0677 | 0.113 | 496.307 | 1263966-18-2 | 4.80 | 7.0 | 123.0 | [2-(2,4-dichlorophenyl)-2-(imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methyl benzoate;dihydroxy(oxo)azanium | O=C(OCC1OC(CN2C=CN=C2)(C3=CC=C(Cl)C=C3Cl)OC1)C4=CC=CC=C4 |
| 1-[5-(2,4-Dichlorophenoxy)pentyl]-1h-Imidazole | 0.59 | 0.420 to 0.820 | 0.0763 | 0.0696 to 0.0836 | 0.129 | 299.200 | NaN | 4.31 | 7.0 | 27.0 | 1-[5-(2,4-dichlorophenoxy)pentyl]-1H-imidazole | ClC1=CC=C(OCCCCCN2C=CN=C2)C(Cl)=C1 |
| Miconazole | 0.62 | 0.440 to 0.870 | 0.0766 | 0.0695 to 0.0844 | 0.124 | 416.130 | 22916-47-8 | 5.30 | 6.0 | 27.0 | 1-[2-(2,4-dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]imidazole | C1=CC(=C(C=C1Cl)Cl)COC(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl |
| Liarozole dihydrochloride | 0.634 | 0.531 to 0.755 | 0.0612 | 0.0585 to 0.0639 | 0.097 | 345.227 | 1883548-96-6 | 3.50 | 3.0 | 46.5 | 6-[(3-chlorophenyl)-imidazol-1-ylmethyl]-1H-benzimidazole;hydrochloride | C1=CC(=CC(=C1)Cl)C(C2=CC3=C(C=C2)N=CN3)N4C=CN=C4 |
| 1-[4-(2,4-dichlorophenoxy)butyl]-1H-imidazole | 0.639 | 0.438 to 0.921 | 0.078 | 0.0703 to 0.0865 | 0.122 | 285.000 | NaN | 3.79 | 6.0 | 27.0 | 1-[4-(2,4-dichlorophenoxy)butyl]-1H-imidazole | ClC1=CC=C(OCCCCN2C=CN=C2)C(Cl)=C1 |
| A112994; (cis-2-((1H-Imidazol-1-yl)methyl)-2-(2,4-dichlorophenyl)-1,3-dioxolan-4-yl)methyl 4-methylbenzenesulfonate | 0.657 | 0.541 to 0.795 | 0.0552 | 0.0527 to 0.0578 | 0.084 | 483.370 | 134071-44-6 | 4.60 | 7.0 | 88.0 | [(2R,4R)-2-(2,4-dichlorophenyl)-2-(imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methyl 4-methylbenzenesulfonate | O=S(C1=CC=C(C)C=C1)(OC[C@@H]2O[C@@](CN3C=CN=C3)(C4=CC=C(Cl)C=C4Cl)OC2)=O |
| ISCK03; Tert-Butylphenyl imidazolylphenyl sulfonamide | 0.723 | 0.576 to 0.891 | 0.0627 | 0.0608 to 0.0646 | 0.0867 | 355.500 | 945526-43-2 | 3.90 | 5.0 | 72.4 | 4-tert-butyl-N-(4-imidazol-1-ylphenyl)benzenesulfonamide | CC(C)(C)C1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(C=C2)N3C=CN=C3 |
| [2-(2,4-DICHLOROPHENYL)-2-(IMIDAZOL-1-YLMETHYL)-1,3-DIOXOLAN-4-YL]METHYL BENZOATE | 0.737 | 0.583 to 0.929 | 0.0711 | 0.0670 to 0.0755 | 0.0965 | 433.300 | 138866-89-4 | 4.80 | 7.0 | 62.6 | [2-(2,4-dichlorophenyl)-2-(imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methyl benzoate | C1C(OC(O1)(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl)COC(=O)C4=CC=CC=C4 |
| Triflumizole | 0.742 | 0.596 to 0.910 | 0.0596 | 0.0578 to 0.0614 | 0.0803 | 345.750 | 68694-11-1 | 4.00 | 6.0 | 39.4 | N-[4-chloro-2-(trifluoromethyl)phenyl]-1-imidazol-1-yl-2-propoxyethanimine | CCCOCC(=NC1=C(C=C(C=C1)Cl)C(F)(F)F)N2C=CN=C2 |
| 1-[2-(2-tert-butyl-4-chlorophenoxy)ethyl]imidazole oxalate | 0.747 | 0.634 to 0.879 | 0.0681 | 0.0653 to 0.0710 | 0.0912 | 368.810 | NaN | NaN | 6.0 | 102.0 | 1-[2-(2-tert-butyl-4-chlorophenoxy)ethyl]imidazole;oxalic acid | CC(C)(C)C1=C(C=CC(=C1)Cl)OCCN2C=CN=C2 |
| 1-[2-(2,4-Dichlorophenoxy)ethyl]-1H-imidazole | 0.874 | 0.801 to 0.951 | 0.0676 | 0.0668 to 0.0685 | 0.0773 | 257.110 | 112736-85-3 | 2.90 | 4.0 | 27.0 | 1-[2-(2,4-dichlorophenoxy)ethyl]imidazole | C1=CC(=C(C=C1Cl)Cl)OCCN2C=CN=C2 |
| Oxiconazole Nitrate | 0.875 | 0.736 to 1.03 | 0.0652 | 0.0635 to 0.0670 | 0.0745 | 492.100 | 64211-46-7 | 6.10 | 6.0 | 106.0 | (Z)-1-(2,4-dichlorophenyl)-N-[(2,4-dichlorophenyl)methoxy]-2-imidazol-1-ylethanimine;nitric acid | C1=CC(=C(C=C1Cl)Cl)CON=C(CN2C=CN=C2)C3=C(C=C(C=C3)Cl)Cl |
| 1-(2,4-dichlorophenyl)-2-(1H-imidazol-1-yl)ethan-1-one | 0.937 | 0.768 to 1.12 | 0.0624 | 0.0609 to 0.0639 | 0.0666 | 255.100 | 46503-52-0 | 2.80 | 3.0 | 34.9 | 1-(2,4-dichlorophenyl)-2-imidazol-1-ylethanone | C1=CC(=C(C=C1Cl)Cl)C(=O)CN2C=CN=C2 |
| Elubiol | 1.04 | 0.793 to 1.36 | 0.0576 | 0.0537 to 0.0618 | 0.0554 | 561.460 | 67914-69-6 | 5.10 | 9.0 | 78.3 | ethyl 4-[4-[[(2R,4S)-2-(2,4-dichlorophenyl)-2-(imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]piperazine-1-carboxylate | CCOC(=O)N1CCN(CC1)c1ccc(OC[C@H]2CO[C@@](Cn3ccnc3)(O2)c2ccc(Cl)cc2Cl)cc1 |
| 1-4-(4-Chlorophenyl)-2-hydroxylbutyl]imidazole | 1.07 | 0.913 to 1.25 | 0.0681 | 0.0666 to 0.0696 | 0.0636 | 250.730 | 67085-11-4 | 2.30 | 5.0 | 38.0 | 4-(4-chlorophenyl)-1-imidazol-1-ylbutan-2-ol | C1=CC(=CC=C1CCC(CN2C=CN=C2)O)Cl |
| Climbazole | 1.15 | 0.887 to 1.48 | 0.0625 | 0.0603 to 0.0648 | 0.0543 | 292.760 | 38083-17-9 | 3.70 | 5.0 | 44.1 | 1-(4-chlorophenoxy)-1-imidazol-1-yl-3,3-dimethylbutan-2-one | CC(C)(C)C(=O)C(N1C=CN=C1)OC2=CC=C(C=C2)Cl |
| 1-(2,4-Dichlorophenyl)-2-imidazol-1-yl-ethanone o-allyloxime | 1.27 | 0.944 to 1.70 | 0.0586 | 0.0556 to 0.0617 | 0.0461 | 310.200 | 928209-03-4 | 4.00 | 6.0 | 39.4 | (Z)-1-(2,4-dichlorophenyl)-2-imidazol-1-yl-N-prop-2-enoxyethanimine | C=CCON=C(CN1C=CN=C1)C2=C(C=C(C=C2)Cl)Cl |
| Chk2 Inhibitor II | 1.51 | 0.655 to 3.00 | 0.0164 | 0.0140 to 0.0192 | 0.0109 | 363.800 | 516480-79-8 | 4.30 | 4.0 | 81.0 | 2-[4-(4-chlorophenoxy)phenyl]-3H-benzimidazole-5-carboxamide | C1=CC(=CC=C1C2=NC3=C(N2)C=C(C=C3)C(=O)N)OC4=CC=C(C=C4)Cl |
| Medetomidine HCl | 1.57 | 1.10 to 2.20 | 0.0691 | 0.0656 to 0.0727 | 0.044 | 236.700 | 86347-15-1 | 3.10 | 2.0 | 28.7 | 5-[1-(2,3-dimethylphenyl)ethyl]-1H-imidazole;hydrochloride | CC1=C(C(=CC=C1)C(C)C2=CN=CN2)C |
| Efinaconazole | 1.68 | 1.10 to 2.43 | 0.0566 | 0.0532 to 0.0601 | 0.0337 | 348.400 | 164650-44-6 | 2.00 | 5.0 | 54.2 | (2R,3R)-2-(2,4-difluorophenyl)-3-(4-methylidenepiperidin-1-yl)-1-(1,2,4-triazol-1-yl)butan-2-ol | C[C@@H](N1CCC(CC1)=C)[C@@](CN2N=CN=C2)(O)C3=CC=C(F)C=C3F |
| Dexmedetomidine HCl (Precedex) | 1.75 | 1.19 to 2.47 | 0.0671 | 0.0638 to 0.0705 | 0.0383 | 236.740 | 145108-58-3 | 3.10 | 2.0 | 28.7 | 5-[(1S)-1-(2,3-dimethylphenyl)ethyl]-1H-imidazole;hydrochloride | C[C@H](C1=CN=CN1)C2=CC=CC(C)=C2C |
| Detomidine HCl | 2.14 | 1.83 to 2.48 | 0.0719 | 0.0703 to 0.0736 | 0.0336 | 222.714 | 90038-01-0 | 2.70 | 2.0 | 28.7 | 5-[(2,3-dimethylphenyl)methyl]-1H-imidazole;hydrochloride | CC1=C(C(=CC=C1)CC2=CN=CN2)C |
| Ketoconazole | 2.97 | 2.46 to 3.57 | 0.0584 | 0.0564 to 0.0605 | 0.0197 | 531.400 | 65277-42-1 | 4.30 | 7.0 | 69.1 | 1-[4-[4-[[(2R,4S)-2-(2,4-dichlorophenyl)-2-(imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]piperazin-1-yl]ethanone | CC(N1CCN(C2=CC=C(OC[C@@H]3O[C@@](CN4C=CN=C4)(C5=CC=C(Cl)C=C5Cl)OC3)C=C2)CC1)=O |
| Etaconazol | 3.48 | 2.07 to 5.75 | 0.049 | 0.0449 to 0.0532 | 0.0141 | 328.190 | 71245-23-3 | 3.30 | 3.0 | 49.2 | 1-[2-(2,4-dichlorophenyl)-4-ethyl-1,3-dioxolan-2-yl]-1,2,4-triazole | CCC1COC(O1)(C2=C(C=C(C=C2)Cl)Cl)N3C=NC=N3 |
| (4-fluorophenyl)(1-methyl-1H-imidazol-2-yl)methanol | 3.55 | 0.101 to 14.5 | 0.0076 | 0.00567 to 0.00980 | 0.00214 | 206.220 | 122155-26-4 | 1.00 | 2.0 | 38.0 | (4-fluorophenyl)-(1-methylimidazol-2-yl)methanol | CN1C=CN=C1C(C2=CC=C(C=C2)F)O |
| Posaconazole | 3.84 | 2.59 to 5.64 | 0.0206 | 0.0183 to 0.0233 | 0.00536 | 700.800 | 171228-49-2 | 4.60 | 12.0 | 112.0 | 4-[4-[4-[4-[[(3R,5R)-5-(2,4-difluorophenyl)-5-(1,2,4-triazol-1-ylmethyl)oxolan-3-yl]methoxy]phenyl]piperazin-1-yl]phenyl]-2-[(2S,3S)-2-hydroxypentan-3-yl]-1,2,4-triazol-3-one | O=C1N([C@@H](CC)[C@@H](O)C)N=CN1C2=CC=C(N3CCN(C4=CC=C(OC[C@@H]5CO[C@@](CN6N=CN=C6)(C7=CC=C(F)C=C7F)C5)C=C4)CC3)C=C2 |
| Propiconazole | 4.28 | 3.43 to 5.32 | 0.0553 | 0.0528 to 0.0579 | 0.01292 | 342.220 | 60207-90-1 | 3.50 | 5.0 | 49.2 | 1-[[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-yl]methyl]-1,2,4-triazole | CCCC1COC(O1)(CN2C=NC=N2)C3=C(C=C(C=C3)Cl)Cl |
| 1-[2-([1,1’-biphenyl]-4-yloxy)ethyl]-1H-imidazole | 5.99 | 4.37 to 8.14 | 0.0628 | 0.0592 to 0.0666 | 0.01048 | 264.320 | 107352-52-3 | 3.50 | 5.0 | 27.0 | 1-[2-(4-phenylphenoxy)ethyl]imidazole | C1=CC=C(C=C1)C2=CC=C(C=C2)OCCN3C=CN=C3 |
| Candesartan cilexetil | 6.04 | 0.362 to 630 | 0.025 | 0.0116 to 0.786 | 0.00414 | 610.660 | 145040-37-5 | 7.00 | 13.0 | 143.0 | 1-cyclohexyloxycarbonyloxyethyl 2-ethoxy-3-[[4-[2-(2H-tetrazol-5-yl)phenyl]phenyl]methyl]benzimidazole-4-carboxylate | CCOC1=NC2=CC=CC(=C2N1CC3=CC=C(C=C3)C4=CC=CC=C4C5=NNN=N5)C(=O)OC(C)OC(=O)OC6CCCCC6 |
| Tipifarnib (Zarnestra) | 6.56 | 4.27 to 10.0 | 0.0434 | 0.0381 to 0.0498 | 0.00662 | 489.400 | 192185-72-1 | 4.10 | 4.0 | 64.2 | 6-[(R)-amino-(4-chlorophenyl)-(3-methylimidazol-4-yl)methyl]-4-(3-chlorophenyl)-1-methylquinolin-2-one | Cn1cncc1[C@@](N)(c1ccc(Cl)cc1)c1ccc2n(C)c(=O)cc(-c3cccc(Cl)c3)c2c1 |
| Atipamezole | 7.63 | 6.32 to 9.18 | 0.0622 | 0.0598 to 0.0646 | 0.00815 | 212.290 | 104054-27-5 | 3.00 | 2.0 | 28.7 | 5-(2-ethyl-1,3-dihydroinden-2-yl)-1H-imidazole | CCC1(CC2=CC=CC=C2C1)C3=CN=CN3 |
| Isavuconazole | 7.67 | 2.30 to 22.5 | 0.0346 | 0.0270 to 0.0452 | 0.00451 | 437.500 | 241479-67-4 | 3.50 | 6.0 | 116.0 | 4-[2-[(2R,3R)-3-(2,5-difluorophenyl)-3-hydroxy-4-(1,2,4-triazol-1-yl)butan-2-yl]-1,3-thiazol-4-yl]benzonitrile | N#CC1=CC=C(C2=CSC([C@@H]([C@@](O)(C3=CC(F)=CC=C3F)CN4N=CN=C4)C)=N2)C=C1 |
| trans-2-​(2,​4-​Dichlorophenyl)​-​2-​(1H-​imidazol-​1-​ylmethyl)​-​1,​3-​dioxolane-​4-​methanol | 10.2 | 9.33 to 11.1 | 0.0637 | 0.0625 to 0.0649 | 0.00625 | 329.200 | 61441-65-4 | 2.60 | 4.0 | 56.5 | [(2R,4R)-2-(2,4-dichlorophenyl)-2-(imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methanol | OC[C@H]1O[C@@](CN2C=CN=C2)(C3=CC=C(Cl)C=C3Cl)OC1 |
| IB-MECA | 10.9 | 9.29 to 12.9 | 0.0332 | 0.0320 to 0.0344 | 0.00305 | 510.290 | 152918-18-8 | 0.90 | 5.0 | 134.0 | (2S,3S,4R,5R)-3,4-dihydroxy-5-[6-[(3-iodophenyl)methylamino]purin-9-yl]-N-methyloxolane-2-carboxamide | O=C([C@H]1O[C@@H](N2C=NC3=C(N(C4=CC=CC(I)=C4)C)N=CN=C23)[C@H](O)[C@@H]1O)NC |
| 1-(4-Chlorophenyl)imidazole | 13.6 | 10.9 to 16.7 | 0.0584 | 0.0556 to 0.0613 | 0.00429 | 178.620 | 51581-54-5 | 2.30 | 1.0 | 17.8 | 1-(4-chlorophenyl)imidazole | C1=CC(=CC=C1N2C=CN=C2)Cl |
| Lomeguatrib | 16.2 | 11.8 to 22.0 | 0.0287 | 0.0266 to 0.0309 | 0.00177 | 326.170 | 192441-08-0 | 2.00 | 3.0 | 118.0 | 6-[(4-bromothiophen-2-yl)methoxy]-7H-purin-2-amine | C1=C(SC=C1Br)COC2=NC(=NC3=C2NC=N3)N |
| Glasdegib (PF\_04449913) maleate salt | 16.8 | 12.6 to 22.2 | 0.047 | 0.0442 to 0.0501 | 0.0028 | 490.510 | 1095173-27-5 | 2.40 | 3.0 | 96.8 | 1-[(2R,4R)-2-(1H-benzimidazol-2-yl)-1-methylpiperidin-4-yl]-3-(4-cyanophenyl)urea | O=C(NC1=CC=C(C#N)C=C1)N[C@H]2C[C@H](C3=NC4=CC=CC=C4N3)N(C)CC2 |
| Imidazole | 17.8 | 16.2 to 19.6 | 0.0701 | 0.0691 to 0.0711 | 0.00394 | 68.080 | 288-32-4 | -0.10 | 0.0 | 28.7 | 1H-imidazole | C1=CN=CN1 |
| IR415; 1-[3-(1-Imidazolyl)propyl]-3-(2,4-difluorophenyl)thiourea | 21.1 | 18.0 to 24.6 | 0.063 | 0.0608 to 0.0653 | 0.00299 | 296.340 | 452967-14-5 | 1.80 | 5.0 | 74.0 | 1-(2,4-difluorophenyl)-3-(3-imidazol-1-ylpropyl)thiourea | C1=CC(=C(C=C1F)F)NC(=S)NCCCN2C=CN=C2 |
| 1-Benzylimidazole | 23.7 | 14.34 to 38.3 | 0.0617 | 0.0548 to 0.0693 | 0.0026 | 158.200 | 4238-71-5 | 1.60 | 2.0 | 17.8 | 1-benzylimidazole | C1=CC=C(C=C1)CN2C=CN=C2 |
| HC-030031 | 34.6 | 19.5 to 61.0 | 0.0263 | 0.0220 to 0.0321 | 0.00076 | 355.400 | 349085-38-7 | 1.70 | 4.0 | 87.5 | 2-(1,3-dimethyl-2,6-dioxopurin-7-yl)-N-(4-propan-2-ylphenyl)acetamide | CC(C)C1=CC=C(C=C1)NC(=O)CN2C=NC3=C2C(=O)N(C(=O)N3C)C |
| Terconazole | 38.2 | 21.2 to 67.6 | 0.0487 | 0.0419 to 0.0568 | 0.00127 | 532.460 | 67915-31-5 | 4.80 | 8.0 | 64.9 | 1-[4-[[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-4-propan-2-ylpiperazine | CC(N1CCN(C2=CC=C(OC[C@@H]3O[C@@](CN4N=CN=C4)(C5=CC=C(Cl)C=C5Cl)OC3)C=C2)CC1)C |
| 1-Butylimidazole | 40.9 | 22.5 to 73.3 | 0.0512 | 0.0439 to 0.0601 | 0.00125 | 124.180 | 4316-42-1 | 1.20 | 3.0 | 17.8 | 1-butylimidazole | CCCCN1C=CN=C1 |
| Indazole | 49.3 | 42.3 to 57.5 | 0.0613 | 0.0586 to 0.0642 | 0.00124 | 118.140 | 271-44-3 | 1.80 | 0.0 | 28.7 | 1H-indazole | C1=CC=C2C(=C1)C=NN2 |
| Voriconazole | 51.7 | 22.3 to 116 | 0.0285 | 0.0228 to 0.0363 | 0.000551 | 349.310 | 188416-29-7 | 1.50 | 5.0 | 76.7 | (2R,3S)-2-(2,4-difluorophenyl)-3-(5-fluoropyrimidin-4-yl)-1-(1,2,4-triazol-1-yl)butan-2-ol | C[C@@H](C1=NC=NC=C1F)[C@@](O)(C2=CC=C(F)C=C2F)CN3N=CN=C3 |
| 1-Vinylimidazole | 104 | 79.8 to 136 | 0.0504 | 0.0460 to 0.0556 | 0.000485 | 94.110 | 1072-63-5 | 0.50 | 1.0 | 17.8 | 1-ethenylimidazole | C=CN1C=CN=C1 |
| 1-Methylimidazole | 148 | 72.9 to 311 | 0.0347 | 0.0269 to 0.0479 | 0.000234 | 82.100 | 616-47-7 | -0.10 | 0.0 | 17.8 | 1-methylimidazole | CN1C=CN=C1 |
| Benzimidazole | 175 | 97.2 to 330 | 0.0567 | 0.0451 to 0.0752 | 0.000324 | 118.140 | 51-17-2 | 1.30 | 0.0 | 28.7 | 1H-benzimidazole | C1=CC=C2C(=C1)NC=N2 |
| (1-Methyl-1H-imidazol-2-yl)(phenyl)methanol | -- | -- | -- | -- | -- | 188.230 | 30517-60-3 | 0.90 | 2.0 | 38.0 | (1-methylimidazol-2-yl)-phenylmethanol | CN1C=CN=C1C(C2=CC=CC=C2)O |
| [2-(1H-benzimidazol-2-yl)ethyl]ethylamine dihydrochloride | -- | -- | -- | -- | -- | 262.180 | NaN | NaN | 4.0 | 40.7 | 2-(1H-benzimidazol-2-yl)-N-ethylethanamine;dihydrochloride | CCNCCC1=NC2=CC=CC=C2N1 |
| {[2-Chloro-6-(1H-imidazol-1-ylmethyl)-3-pyridinyl]oxy}acetic acid | -- | -- | -- | -- | -- | 267.670 | 105277-92-7 | 1.10 | 5.0 | 77.2 | {[2-Chloro-6-(1H-imidazol-1-ylmethyl)-3-pyridinyl]oxy}acetic acid | O=C(O)COC1=CC=C(CN2C=CN=C2)N=C1Cl |
| 1-(3,6-dibromo-9H-carbazol-9-yl)-3-(4,5-diphenyl-1H-imidazol-1-yl)-2-propanol | -- | -- | -- | -- | -- | 601.300 | NaN | 7.10 | 6.0 | NaN | 1-(3,6-dibromocarbazol-9-yl)-3-(4,5-diphenylimidazol-1-yl)propan-2-ol | N(CC(O)CN1C=NC(C2=CC=CC=C2)=C1C1C=CC=CC=1)1C2=CC=C(C=C2C2=CC(Br)=CC=C21)Br |
| 1-(4-CHLOROPHENYL)-2-((5,6-DIMETHYL-1H-BENZIMIDAZOL-2-YL)THIO)ETHANONE | -- | -- | -- | -- | -- | 330.839 | 394221-21-7 | 5.10 | 4.0 | 71.0 | 1-(4-chlorophenyl)-2-[(5,6-dimethyl-1H-benzimidazol-2-yl)sulfanyl]ethanone | CC1=C(C)C=C2N=C(SCC(C3=CC=C(Cl)C=C3)=O)NC2=C1 |
| 1-(methoxymethyl)-2-phenyl-1H-imidazole | -- | -- | -- | -- | -- | 188.230 | NaN | 1.60 | 3.0 | 27.0 | 1-(methoxymethyl)-2-phenylimidazole | COCN1C=CN=C1C2=CC=CC=C2 |
| 1-Aminobenzotriazole | -- | -- | -- | -- | -- | 134.140 | 1614-12-6 | 0.90 | 0.0 | 56.7 | benzotriazol-1-amine | C1=CC=C2C(=C1)N=NN2N |
| 1H-1,2,4-Triazole | -- | -- | -- | -- | -- | 69.070 | 288-88-0 | -0.60 | 0.0 | 41.6 | 1H-1,2,4-triazole | C1=NC=NN1 |
| 2-((1-BENZOYL-1H-BENZIMIDAZOL-2-YL)THIO)-1-(4-CHLOROPHENYL)ETHANOL | -- | -- | -- | -- | -- | 408.910 | 883813-15-8 | 5.30 | 5.0 | 80.4 | [2-[2-(4-chlorophenyl)-2-hydroxyethyl]sulfanylbenzimidazol-1-yl]-phenylmethanone | ClC1=CC=C(C(O)CSC2=NC3=CC=CC=C3N2C(C4=CC=CC=C4)=O)C=C1 |
| 2-((1-ETHYL-1H-BENZIMIDAZOL-2-YL)THIO)-N'-(4-PROPOXYBENZYLIDENE)ACETOHYDRAZIDE | -- | -- | -- | -- | -- | 396.515 | 315216-01-4 | 4.40 | 9.0 | 93.8 | 2-(1-ethylbenzimidazol-2-yl)sulfanyl-N-[(E)-(4-propoxyphenyl)methylideneamino]acetamide | O=C(NN=CC1=CC=C(OCCC)C=C1)CSC2=NC3=CC=CC=C3N2CC |
| 2-(1H-benzimidazol-1-yl)propanoic acid hydrochloride | -- | -- | -- | -- | -- | 226.660 | 1095080-29-7 | NaN | 2.0 | 55.1 | 2-(1H-benzimidazol-1-yl)propanoic acid hydrochloride | CC(C(=O)O)N1C=NC2=CC=CC=C21 |
| 2-(3-iodophenyl)-4,5-bis(4-phenoxyphenyl)-1H-imidazole | -- | -- | -- | -- | -- | 606.500 | NaN | 8.80 | 7.0 | 47.1 | 2-(3-iodophenyl)-4,5-bis(4-phenoxyphenyl)-1H-imidazole | C1=CC=C(C=C1)OC2=CC=C(C=C2)C3=C(N=C(N3)C4=CC(=CC=C4)I)C5=CC=C(C=C5)OC6=CC=CC=C6 |
| 2-[(1H-benzimidazol-2-ylmethyl)thio]ethanol hydrochloride | -- | -- | -- | -- | -- | 244.740 | NaN | NaN | 4.0 | 74.2 | 2-(1H-benzimidazol-2-ylmethylsulfanyl)ethanol;hydrochloride | C1=CC=C2C(=C1)NC(=N2)CSCCO |
| 2-{1-[2-(4-bromophenoxy)ethyl]-1H-benzimidazol-2-yl}-1-(4-chlorophenyl)vinyl 4-chlorobenzoate | -- | -- | -- | -- | -- | 608.300 | NaN | 8.50 | 9.0 | 53.4 | [(E)-2-[1-[2-(4-bromophenoxy)ethyl]benzimidazol-2-yl]-1-(4-chlorophenyl)ethenyl] 4-chlorobenzoate | C1(N(CCOC2C=CC(=CC=2)Br)C2=C(C=CC=C2)N=1)/C=C(\C1C=CC(=CC=1)Cl)/OC(=O)C1C=CC(=CC=1)Cl |
| 2-{4-[(4-chlorobenzyl)oxy]-3-iodo-5-methoxyphenyl}-4,5-diphenyl-1H-imidazole acetate | -- | -- | -- | -- | -- | 592.900 | NaN | NaN | NaN | NaN | 2-{4-[(4-chlorobenzyl)oxy]-3-iodo-5-methoxyphenyl}-4,5-diphenyl-1H-imidazole acetate | N1C(C2=CC=CC=C2)=C(NC=1C1C=C(OC)C(=C(I)C=1)OCC1=CC=C(C=C1)Cl)C1=CC=CC=C1 |
| 2-Chloro-1-(4-fluorobenzyl)benzoimidazole | -- | -- | -- | -- | -- | 260.690 | 84946-20-3 | 4.10 | 2.0 | 17.8 | 2-Chloro-1-(4-fluorobenzyl)benzoimidazole | C1=CC=C2C(=C1)N=C(N2CC3=CC=C(C=C3)F)Cl |
| 2-ET-5-HO-4-(1-HYDROXY-2-(1-METHYL-1H-BENZIMIDAZOL-2-YL)VINYL)PHENYL PIVALATE | -- | -- | -- | -- | -- | 394.475 | 308295-24-1 | 5.30 | 6.0 | 84.6 | [2-ethyl-5-hydroxy-4-[(Z)-1-hydroxy-2-(1-methylbenzimidazol-2-yl)ethenyl]phenyl] 2,2-dimethylpropanoate | CN1C2=C(C=CC=C2)N=C1/C=C(C3=CC(CC)=C(OC(C(C)(C)C)=O)C=C3O)\O |
| Astemizole | -- | -- | -- | -- | -- | 458.600 | 68844-77-9 | 6.00 | 8.0 | 42.3 | 1-[(4-fluorophenyl)methyl]-N-[1-[2-(4-methoxyphenyl)ethyl]piperidin-4-yl]benzimidazol-2-amine | COC1=CC=C(C=C1)CCN2CCC(CC2)NC3=NC4=CC=CC=C4N3CC5=CC=C(C=C5)F |
| CBR00638; 2-[2-(1H-Imidazol-1-yl)ethyl]piperidine dihydrochloride | -- | -- | -- | -- | -- | 252.180 | NaN | NaN | 3.0 | 29.8 | 2-(2-imidazol-1-ylethyl)piperidine;dihydrochloride | C1CCNC(C1)CCN2C=CN=C2 |
| CDS007822; 3-imidazol-1-yl-propionic acid | -- | -- | -- | -- | -- | 140.140 | 18999-45-6 | -0.60 | 3.0 | 55.1 | 3-imidazol-1-ylpropanoic acid | C1=CN(C=N1)CCC(=O)O |
| CDS017891; 4-([3-(1H-imidazol-1-yl)propyl]amino)-4-oxobutanoic acid | -- | -- | -- | -- | -- | 225.250 | NaN | -1.00 | 7.0 | 84.2 | 4-([3-(1H-Imidazol-1-Yl)Propyl]Amino)-4- Oxobutanoic Acid | C1=CN(C=N1)CCCNC(=O)CCC(=O)O |
| Chloro-IB-MECA | -- | -- | -- | -- | -- | 544.700 | 163042-96-4 | 1.90 | 5.0 | 134.0 | (2S,3S,4R,5R)-5-[2-chloro-6-[(3-iodophenyl)methylamino]purin-9-yl]-3,4-dihydroxy-N-methyloxolane-2-carboxamide | O=C([C@H]1O[C@@H](N2C=NC3=C(N(C4=CC=CC(I)=C4)C)N=C(Cl)N=C23)[C@H](O)[C@@H]1O)NC |
| Fluconazole | -- | -- | -- | -- | -- | 306.270 | 86386-73-4 | 0.40 | 5.0 | 81.6 | 2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol | NaN |
| Fosfluconazole | -- | -- | -- | -- | -- | 386.250 | 194798-83-9 | -0.60 | 7.0 | 128.0 | [2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-yl] dihydrogen phosphate | C1=CC(=C(C=C1F)F)C(CN2C=NC=N2)(CN3C=NC=N3)OP(=O)(O)O |
| Letrozole | -- | -- | -- | -- | -- | 285.300 | 112809-51-5 | 2.70 | 3.0 | 78.3 | 4-[(4-cyanophenyl)-(1,2,4-triazol-1-yl)methyl]benzonitrile | C1=CC(=CC=C1C#N)C(C2=CC=C(C=C2)C#N)N3C=NC=N3 |
| N-(1-(1-(4-CHLOROBENZYL)-1H-BENZIMIDAZOL-2-YL)ETHYL)-4-FLUOROBENZAMIDE | -- | -- | -- | -- | -- | 407.879 | 430451-95-9 | 5.00 | 5.0 | 46.9 | N-[1-[1-[(4-chlorophenyl)methyl]benzimidazol-2-yl]ethyl]-4-fluorobenzamide | O=C(NC(C1=NC2=CC=CC=C2N1CC3=CC=C(Cl)C=C3)C)C4=CC=C(F)C=C4 |
| NGP555 | -- | -- | -- | -- | -- | 407.530 | 1304630-27-0 | 6.30 | 5.0 | 71.0 | N-(5-ethyl-2,4-dimethylphenyl)-4-[3-fluoro-4-(4-methylimidazol-1-yl)phenyl]-1,3-thiazol-2-amine | CCC1=CC(=C(C=C1C)C)NC2=NC(=CS2)C3=CC(=C(C=C3)N4C=C(N=C4)C)F |
| Oteseconazole | -- | -- | -- | -- | -- | 527.400 | 1340593-59-0 | 4.20 | 8.0 | 86.0 | (2R)-2-(2,4-difluorophenyl)-1,1-difluoro-3-(tetrazol-1-yl)-1-[5-[4-(2,2,2-trifluoroethoxy)phenyl]pyridin-2-yl]propan-2-ol | O[C@@](CN1N=NN=C1)(C2=CC=C(F)C=C2F)C(F)(F)C3=NC=C(C4=CC=C(OCC(F)(F)F)C=C4)C=C3 |
| Ozagrel hydrochloride hydrate | -- | -- | -- | -- | -- | 264.710 | 78712-43-3 | 1.60 | 4.0 | 56.1 | (E)-3-[4-(imidazol-1-ylmethyl)phenyl]prop-2-enoic acid;hydrochloride | C1=CC(=CC=C1CN2C=CN=C2)C=CC(=O)O |
| PC945 | -- | -- | -- | -- | -- | 682.700 | 1931946-73-4 | NaN | NaN | NaN | NaN | FC1=C(C=CC(F)=C1)[C@]2(C[C@H](COC(C=CC(N3CCN(C4=CC=C(C(NC5=CC=C(F)C=C5)=O)C=C4)CC3)=C6)=C6C)CO2)CN7C=NC=N7 |
| PTC-028 | -- | -- | -- | -- | -- | 405.300 | 1782970-28-8 | 4.70 | 3.0 | 55.6 | 6-(5,6-difluoro-2-methylbenzimidazol-1-yl)-N-[4-(trifluoromethyl)phenyl]pyrazin-2-amine | Cc1nc2cc(F)c(F)cc2n1-c1cncc(Nc2ccc(cc2)C(F)(F)F)n1 |
| pyrazole, 3(5)-phenyl-1H--pyrazol-5-yl (4-phenyl-1H-pyrazol-5-amine) | -- | -- | -- | -- | -- | 159.190 | 5591-70-8 | 1.50 | 1.0 | 54.7 | 4-phenyl-1H-pyrazol-5-amine | C1=CC=C(C=C1)C2=C(NN=C2)N |
| RAF265 (CHIR-265) | -- | -- | -- | -- | -- | 518.400 | 927880-90-8 | 5.40 | 5.0 | 80.6 | 1-methyl-5-[2-[5-(trifluoromethyl)-1H-imidazol-2-yl]pyridin-4-yl]oxy-N-[4-(trifluoromethyl)phenyl]benzimidazol-2-amine | Cn1c(Nc2ccc(cc2)C(F)(F)F)nc2cc(Oc3ccnc(c3)-c3ncc([nH]3)C(F)(F)F)ccc12 |
| StemRegenin 1 | -- | -- | -- | -- | -- | 428.500 | 1227633-49-9 | 5.40 | 6.0 | 104.0 | 4-[2-[[2-(1-benzothiophen-3-yl)-9-propan-2-ylpurin-6-yl]amino]ethyl]phenol | CC(C)N1C=NC2=C(N=C(N=C21)C3=CSC4=CC=CC=C43)NCCC5=CC=C(C=C5)O |
| TNP | -- | -- | -- | -- | -- | 443.400 | 519178-28-0 | 4.40 | 6.0 | 124.0 | 6-N-[(4-nitrophenyl)methyl]-2-N-[[3-(trifluoromethyl)phenyl]methyl]-7H-purine-2,6-diamine | C1=CC(=CC(=C1)C(F)(F)F)CNC2=NC3=C(C(=N2)NCC4=CC=C(C=C4)[N+](=O)[O-])NC=N3 |
| triazole, 1H-1,2,3- (1-(Rufinamide;2,6-Difluorobenzyl)-1H-1,2,3-triazole-4-carboxamide) | -- | -- | -- | -- | -- | 69.070 | 288-36-8 | -0.30 | 0.0 | 73.8 | 2H-triazole | C1=NNN=C1 |
| Triclabendazole (CPD000466357) | -- | -- | -- | -- | -- | 359.660 | 68786-66-3 | 5.70 | 3.0 | 63.2 | 6-chloro-5-(2,3-dichlorophenoxy)-2-methylsulfanyl-1H-benzimidazole | CSC1=NC2=CC(=C(C=C2N1)Cl)OC3=C(C(=CC=C3)Cl)Cl |