Supplementary Information for **Quantifying and Predicting the Promiscuity and Isoform Specificity of Small-Molecule Cytochrome P450 Inhibitors**

Drug Metabolism and Disposition

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Table S1. SMILES structures for all 64 compounds included in the set S_{64}.

Albendazole	CCCSC1=CC=C2N=C(NC(=O)OC)NC2=C1
Amiodarone	CCCCC1=C(C(=O)C2=CC(I)=C(OCCN(CC)CC)C(I)=C2)C3=C(O1)C=CC=C3
Amitriptyline	CN(C)CC\C=C1/C2=CC=CC=C2CCC3=C1C=CC=C3
Artemisinin	[H][C@@]12CC[C@@H](C)[C@]3([H])CC[C@@]4(C)OO[C@@]13[C@]([H])(OC(=O)[C@@H]2C)O4
Astemizole	COC1=CC=C(CCN2CCC(CC2)NC3=NC4=C(C=CC=C4)N3CC5=CC=C(F)C=C5)C=C1
Atenolol	CC(C)NCC(O)COC1=CC=C(CC(N)=O)C=C1
Bepridil	CC(C)COCC(CN(CC1=CC=CC=C1)C2=CC=CC=C2)N3CCCC3
Budesonide	[H][C@@]12C[C@@]3([H])[C@]4([H])CCC5=CC(=O)C=C[C@]5(C)[C@@]4([H])[C@@H](O)C[C@]3(C)[C@@]1(OC(CCC)O2)C(=O)CO
Carbamazepine	NC(=O)N1C2=CC=CC=C2C=CC3=C1C=CC=C3
chloroquine	CCN(CC)CCCC(C)NC1=CC=NC2=C1C=CC(Cl)=C2
Chlorpheniramine	CN(C)CCC(C1=CC=C(Cl)C=C1)C2=CC=CC=N2
Chlorthalidone	NS(=O)(=O)C1=C(Cl)C=CC(=C1)C2(O)NC(=O)C3=CC=CC=C23
Cimetidine	CN\C(NCCSCC1=C(C)NC=N1)=N\C#N
Cisapride	CO[C@H]1CN(CCCOC2=CC=C(F)C=C2)CCC1NC(=O)C3=C(OC)C=C(N)C(Cl)=C3
Clotrimazole	ClC1=C(C=CC=C1)C(N2C=CN=C2)(C3=CC=CC=C3)C4=CC=CC=C4
Clozapine	CN1CCN(CC1)C2=NC3=CC(Cl)=CC=C3NC4=CC=CC=C24
Cyclosporin	CCCCC1N(C)C(=O)NC(=O)C(CC)NC(=O)C(C(O)C(C)C\C=C\C)N(C)C(=O)C(CCC)N(C)C(=O)C(CCCC)N(C)C(=O)C(CCCC)N(C)C(=O)C(C)NC(=O)C(C)NC(=O)C(CCCC)N(C)C(=O)C(CCC)NC1=O
Danazol	[H]C#C[C@]1(O)CC[C@@]2([H])[C@]3([H])CCC4=CC5=C(C[C@]4(C)[C@@]3([H])CC[C@]12C)C=NO5
Dexamethasone	[H][C@@]12C[C@@H](C)[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]3(F)[C@@]2([H])CCC4=CC(=O)C=C[C@]34C
Digoxin	[H][C@@]1(C[C@H](O)[C@H](O)[C@@H](C)O1)O[C@H]2[C@@H](O)C[C@]([H])(O[C@@]3([H])[C@@H](O)C[C@]([H])(O[C@H]4CC[C@@]5(C)[C@]([H])(CC[C@]6([H])[C@]5([H])C[C@@H](O)[C@]7(C)[C@H](CC[C@]67O)C8=CC(=O)OC8)C4)O[C@@H]3C)O[C@@H]2C

Diltiazem	COC1=CC=C(C=C1)[C@@H]2SC3=CC=CC=C3N(CCN(C)C)C(=O)[C@@H]2OC(C)=O
Diphenhydramine	CN(C)CCOC(C1=CC=CC=C1)C2=CC=CC=C2
Diphenylhydantoin	O=C1NC(=O)C(N1)(C2=CC=CC=C2)C3=CC=CC=C3
Disulfiram	CCN(CC)C(=S)SSC(=S)N(CC)CC
Erythromycin	CC[C@H]1OC(=O)[C@H](C)[C@H](C[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C)(O)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)O[C@H]3C[C@@](C)(OC)[C@@H](O)[C@H](C)O3
Felbamate	NC(=O)OCC(COC(N)=O)C1=CC=CC=C1
Fluconazole	OC(CN1C=NC=N1)(CN2C=NC=N2)C3=C(F)C=C(F)C=C3
Flurbiprofen	CC(C([O-])=O)C1=CC(F)=C(C=C1)C2=CC=CC=C2
Fluvoxamine	COCCCC\C(=N\OCC[NH3+])C1=CC=C(C=C1)C(F)(F)F
Haloperidol	OC1(CCN(CCCC(=O)C2=CC=C(F)C=C2)CC1)C3=CC=C(Cl)C=C3
Indomethacin	COC1=CC=C2N(C(=O)C3=CC=C(Cl)C=C3)C(C)=C(CC(O)=O)C2=C1
Isradipine	COC(=O)C1=C(C)NC(C)=C(C1C2=CC=CC3=NON=C23)C(=O)OC(C)C
Ivermectin	[H][C@@]12OC\C3=C/C=C/[C@H](C)[C@H](O[C@@H]4O[C@@H](C)[C@H](O[C@H]5C[C@H](OC)[C@@H](O)[C@H](C)O5)[C@@H](OC)O4)\C(C)=C\C[C@@H]6C[C@@H](C[C@]7(CC[C@H](C)[C@]([H])(O7)[C@@H](C)CC)O6)OC(=O)C(C=C(C)[C@H]1O)[C@@]23O
Ketoconazole	CC(=O)N1CCN(CC1)C2=CC=C(OCC3COC(CN4C=CN=C4)(O3)C5=C(Cl)C=C(Cl)C=C5)C=C2
Ketoprofen	CC(C(O)=O)C1=CC(=CC=C1)C(=O)C2=CC=CC=C2
Lansoprazole	CC1=C(CS(=O)C2=NC3=CC=CC=C3N2)N=CC=C1OCC(F)(F)F
Loratadine	CCOC(=O)N1CC\C(CC1)=C2/C3=C(CCC4=C2N=CC=C4)C=C(Cl)C=C3
Lovastatin	[H][C@]12[C@H](C[C@@H](C)C=C1C=C[C@H](C)[C@@H]2CC[C@@H]3C[C@@H](O)CC(=O)O3)OC(=O)[C@@H](C)CC
Mefloquine	OC(C1CCCCN1)C2=CC(=NC3=C2C=CC=C3C(F)(F)F)C(F)(F)F
Methoxypsoralen	COC1=CC2=CC3=C(OC(=O)C=C3)C=C2O1 |c:11,14,t:2,4,6|
Naproxen	COC1=CC2=C(C=C1)C=C(C=C2)[C@H](C)C(O)=O
Nicardipine	COC(=O)C1=C(C)NC(C)=C(C1C2=CC=CC(=C2)[N+]([O-])=O)C(=O)OCCN(C)CC3=CC=CC=C3
Nifedipine	COC(=O)C1=C(C)N=C(C)C(C(=O)OC)=C1C2=C(C=CC=C2)[N+]([O-])=O
Norfloxacin	CCN1C=C(C(O)=O)C(=O)C2=C1C=C(N3CCNCC3)C(F)=C2
Omeprazole	COC1=CC2=C(NC(=N2)S(=O)CC3=NC=C(C)C(OC)=C3C)C=C1
Orphenadrine	CN(C)CCOC(C1=CC=CC=C1)C2=CC=CC=C2C

Paclitaxel	C[C@H]([C@@H](NC(=O)C1=CC=CC=C1)C2=CC=CC=C2)C(=O)O[C@H]3C[C@@]4(O)[C@@H](OC(=O)C5=CC=CC=C5)[C@]6(C)[C@@]7(CO[C@@H]7C[C@H](O)[C@@]6(C)C(=O)[C@H](OC(C)=O)C(=C3C)C4(C)C)OC(C)=O
Paroxetine	FC1=CC=C(C=C1)[C@@H]2CCNC[C@H]2COC3=CC4=C(OCO4)C=C3
Perphenazine	OCCN1CCN(CCCN2C3=CC=CC=C3SC4=C2C=C(Cl)C=C4)CC1
Pimozide	FC1=CC=C(C=C1)C(CCCN2CCC(CC2)N3C(=O)NC4=CC=CC=C34)C5=CC=C(F)C=C5
Pravastatin	[H][C@]12[C@H](C[C@H](O)C=C1C=C[C@H](C)[C@H]2CC[C@@H](O)C[C@@H](O)CC(O)=O)OC(=O)[C@@H](C)CC
Promethazine	CC(CN1C2C=CC=CC2SC3=CC=CC=C13)N(C)C
Propranolol	CC(C)NCC(O)COC1=CC=CC2=C1C=CC=C2
Quercetin	OC1=CC2=C(C(O)=C1)C(=O)C(O)=C(O2)C3=CC=C(O)C(O)=C3
Quinapril	CCOC(=O)[C@H](CCC1=CC=CC=C1)N[C@@H](C)C(=O)C2CC3=C(C[C@H]2C(O)=O)C=CC=C3
Quinidine	COC1=CC2=C(C=CN=C2C=C1)[C@H](O)C3C[C@@H]4CC[N@]3C[C@H]4C=C
Ranolazine	COC1=CC=CC=C1OCC(O)CN2CCN(CC(=O)NC3=C(C)C=CC=C3C)CC2
Sertraline	CN[C@H]1CC[C@@H](C2=CC=C(Cl)C(Cl)=C2)C3=C1C=CC=C3
Simvastatin	[H][C@]12[C@H](C[C@@H](C)C=C1C=C[C@H](C)[C@@H]2CCC3C[C@@H](O)CC(=O)O3)OC(=O)C(C)(C)CC
Tamoxifen	CC\C(C1=CC=CC=C1)=C(/C2=CC=CC=C2)C3=CC=C(OCCN(C)C)C=C3
Terfenadine	CC(C)(C)C1=CC=C(C=C1)C(O)CCCN2CCC(CC2)C(O)(C3=CC=CC=C3)C4=CC=CC=C4
Ticlopidine	ClC1=C(CN2CCC3=C(C2)C=CS3)C=CC=C1
Verapamil	COC1=CC=C(CCN(C)CCCC(C#N)(C(C)C)C2=CC=C(OC)C(OC)=C2)C=C1OC
Warfarin	CC(=O)CC(C1=CC=CC=C1)C2=C(O)C3=CC=CC=C3OC2=O