Efficient screening of P450 BM3 mutants for their metabolic activity and diversity towards a wide set of drug-like molecules in chemical space

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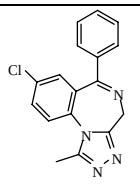
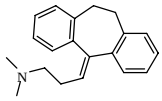
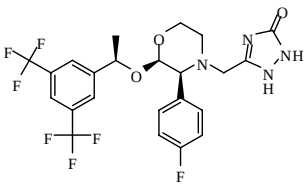
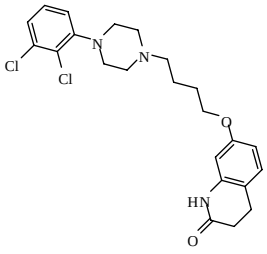
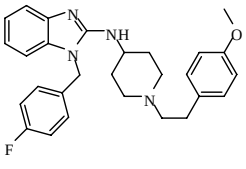
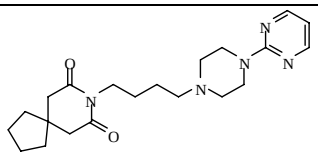
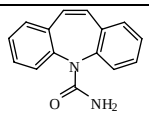
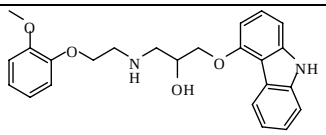
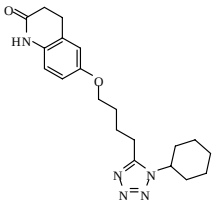
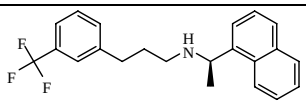
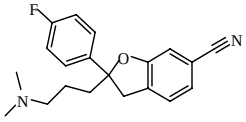
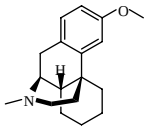
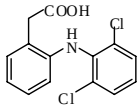
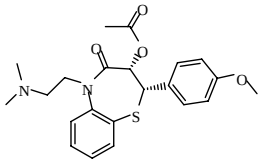
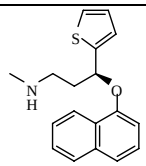
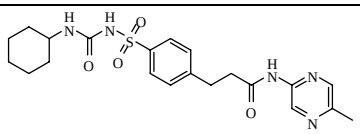
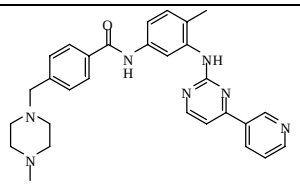
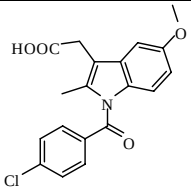
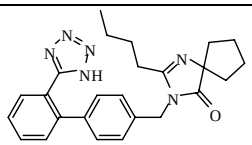
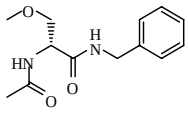
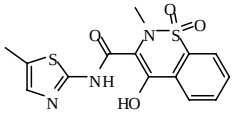
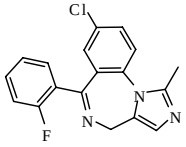
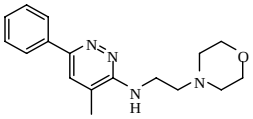
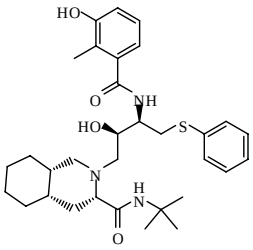
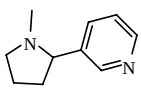
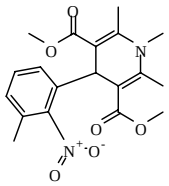
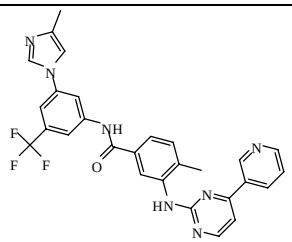
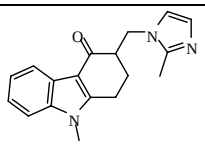
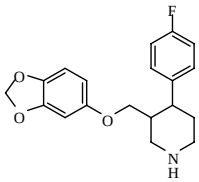
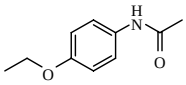
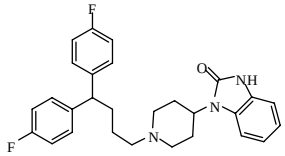
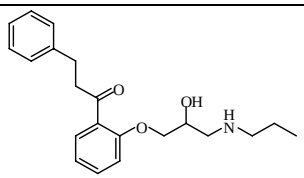
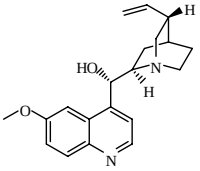
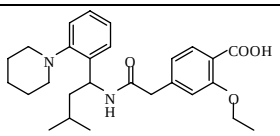
Drug Metabolism and Disposition

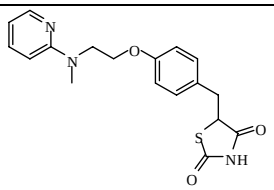
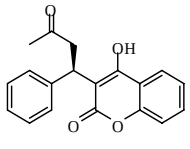
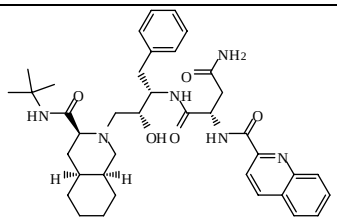
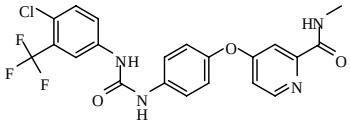
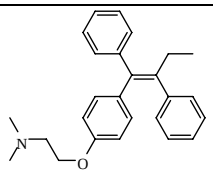
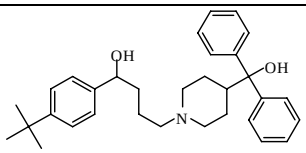
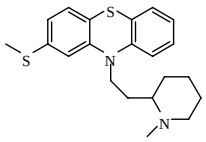
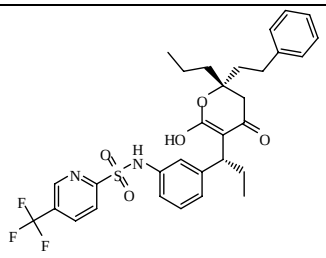
Supplemental Table 2 Detailed information of the 43 drugs used in this study.

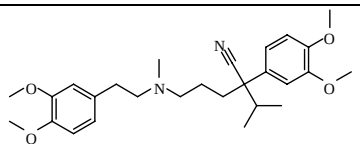
Drug name	Structure	MW	cLogP [a]	cLogD [a]	Charge [a]	PSA [a]	CYP [b]
Alprazolam		308.77	2.56	2.17	0	43.07	3A4
Amitriptyline		277.18	4.85	2.20	+	3.24	2D6 2C9 2C19 1A2
Aprepitant		534.43	4.83	6.24	0	83.24	3A4 2C19 1A2 *
Aripiprazole		448.39	5.31	4.46	+	32.7	3A4 2D6
Astemizole		458.58	6.09	4.46	+	44.81	3A4

Buspirone		385.51	2.19	1.18	+	69.64	3A4
Carbamazepine		236.27	2.38	3.22	0	46.33	3A4 2C8 *
Carvedilol		406.47	4.04	1.94	+	75.74	2D6
Cilostazol		369.46	3.53	2.97	0	81.93	3A4
Cinacalcet		357.41	6.35	3.47	+	12.03	3A4 2D6 1A2 *
Citalopram		324.39	3.13	1.19	+	36.26	2C19
Dextromethorphan		271.4	3.95	1.89	+	12.47	3A4 2D6
Diclofenac		296.15	4.73	0.74	-	49.33	2C9
Diltiazem		414.16	3.65	1.83	+	59.08	3A4
Duloxetine		297.42	4.26	1.85	+	21.26	2D6

Glipizide		445.54	2.57	-0.03	-	130.15	2C9
Imatinib		493.6	4.53	2.90	+	86.28	3A4
Indomethacin		357.79	4.18	-0.02	-	68.53	2C19
Irbesartan		428.53	6.04	3.04	-	87.13	2C9
Lacosamide		250.29	0.39	-0.06	0	67.43	2C19 **
Meloxicam		351.4	2.29	-0.07	-	99.6	2C9
Midazolam		325.77	3.42	3.08	0	30.18	3A4
Minaprine		298.38	3.19	1.83	0	50.28	2D6
Nelfinavir		567.79	5.84	4.28	0	101.9	3A4 2C19
Nicotine		162.23	0.88	0.10	+	16.13	3A4 2C19 2D6

							1A2 *
Nifedipine		346.33	3.13	1.64	0	107.77	3A4
Nilotinib		529.52	5.84	4.18	0	97.62	3A4 *
Ondansetron		293.36	2.72	1.76	+	39.82	3A4 2D6 1A2
Paroxetine		329.37	4.24	0.90	+	39.72	2D6
Phenacetine		179.22	1.77	1.46	0	38.33	2D6 1A2
Pimozide		461.55	6.40	5.37	+	41.03	3A4
Propafenone		341.44	3.64	0.88	+	58.56	2D6
Quinidine		324.42	2.79	1.46	+	45.59	3A4
Repaglinide		452.59	5.30	1.65	-	78.87	2C8

Rosiglitazone		357.43	3.02	2.12	-	71.53	2C8 2C9 *
R-warfarin		308.33	2.90	0.60	-	67.51	2C19 1A2
Saquinavir		670.85	4.73	2.33	0	166.75	3A4
Sorafenib		464.84	5.45	4.32	0	92.35	3A4 *
Tamoxifen		371.51	6.82	4.97	+	12.47	3A4 2D6 2C9
Terfenadine		471.67	6.07	4.82	+	43.7	3A4
Thioridazine		370.57	6.0	3.95	+	6.48	2D6
Tipranavir		602.66	7.55	4.62	-	105.59	3A4 *

Drug name	Structure	MW	cLogP [a]	cLogD [a]	Charge [a]	PSA [a]	CYP [b]
Verapamil		454.61	4.47	2.29	+	63.95	3A4 1A2

[a] Compound properties (cLogP, cLogD, charge and polar surface area (PSA)) were calculated using an in-house database program. Charges were defined as either positive (+), negative (-) or neutral (0).

[b] Human P450 phenotyping information was obtained from either the University of Indiana Cytochrome P450 Drug Interaction Table, the McGraw-Hill's Access Medicine database(*), or the University of Washington metabolism and transport drug interaction database(**) .