

Pubchem CID	EC <sub>50</sub> (nM) Ave ± SD	Pubchem AID/Active Flags/Confirmed	Predictive <i>in silico</i> ADMET			
			Test (RI)	[CYP] IC <sub>50</sub> < 50 uM , IC <sub>50</sub> < 10 uM (RI)	Mouse LD <sub>50</sub> (mg/kg) (RI)	Tanimoto Score (SSG/AB)
2007	Lm: 177 ± 3 A549: >5000	171/2/0	AMES= 0.709 (0.18) hERG= 0 (0.51) SI= 0.13 OB: Good	CYP3A4= 0 (0.79) , 0 (0.87) CYP2D6= 0.02 (0.29) , 0 (0.59)	IP = 500 (0.46) OR = 800 (0.15) IV = 210 (0.32) SC = 720 (0.43)	0.2/0.2
2812	Lm: 147 ± 30 A549: >5000	345/25/13	AMES= 0.207 (0.42) hERG= 0.94 (0.46) SI= 0.49 OB: Moderate	CYP3A4= 0.94 (0.63) , 0.85 (0.54) CYP2D6= 0.61 (0.53) , 0.07 (0.6)	IP = 260 (0.47) OR = 1000 (0.33) IV = 27.74 (0.42) SC = 220 (0.36)	0.03/0.02
3117	Lm: 263 ± 20 A549: 2163 ± 1222	160/12/3	AMES= 0.436 (0.48) hERG= 0.15 (0.23) SI= 0.3 OB: Poor	CYP3A4= 0.3 (0.56) , 0.02 (0.81) CYP2D6= 0.07 (0.79) , 0.06 (0.75)	IP = 310 (0.34) OR = 1700 (0.8) IV = 46.74 (0.23) SC = 890 (0.7)	0.04/0.02
5455	Lm: 98 ± 12 A549: 750 ± 2	369/89/79	AMES= 0.651 (0.47) hERG= 0.04 (0.34) SI= 0.32 OB: Moderate	CYP3A4= 0.16 (0.51) , 0.02 (0.81) CYP2D6= 0.05 (0.76) , 0.04 (0.63)	IP = 150 (0.56) OR = 1400 (0.81) IV = 51.06 (0.42) SC = 1000 (0.71)	0.04/0.02
11352	Lm: 635 ± 26 A549: 4699 ± 311	213/20/5	AMES= 0.968 (1) hERG= 0.49 (0.23) SI= 0.37 OB: Good	CYP3A4= 0.23 (0.33) , 0.08 (0.47) CYP2D6= 0.17 (0.34) , 0.06 (0.52)	IP = 350 (0.43) OR = 240 (0.33) IV = 22.87 (0.58) SC = 350 (0.84)	0.06/0.08
89966	Lm: 392 ± 40 A549: >5000	299/15/6	AMES= 0.459 (0.33) hERG= 0.06 (0.28) SI= 0.35 OB: Good	CYP3A4= 0.05 (0.77) , 0.01 (0.7) CYP2D6= 0.11 (0.56) , 0.07 (0.45)	IP = 280 (0.55) OR = 960 (0.49) IV = 47.04 (0.41) SC = 260 (0.52)	0.02/0.03
298107	Lm: 502 ± 87 A549: >5000	282/9/0	AMES= 0.081 (0.8) hERG= 0.73 (0.48) SI= 0.37 OB: Moderate	CYP3A4= 0.49 (0.2) , 0.06 (0.38) CYP2D6= 0.84 (0.36) , 0.5 (0.08)	IP = 97.64 (0.74) OR = 310 (0.56) IV = 42.46 (0.88) SC = 230 (0.53)	0.3/0.17
359323	Lm: 46 ± 12 A549: >5000	217/10/2	AMES= 0.032 (0.74) hERG= 0.33 (0.47) SI= 0.39 OB: Poor	CYP3A4= 0.48 (0.72) , 0.11 (0.84) CYP2D6= 0.19 (0.59) , 0.11 (0.65)	IP = 68.71 (0.79) OR = 680 (0.42) IV = 28.35 (0.83) SC = 92.87 (0.79)	0.2/0.1
380438	Lm: 117 ± 22 A549: >5000	249/3/0	AMES= 0.675 (0.23) hERG= 0.21 (0.1) SI= 0.99 OB: Moderate	CYP3A4= 0.31 (0.1) , 0.03 (0.41) CYP2D6= 0.08 (0.26) , 0.01 (0.16)	IP = 360 (0.41) OR = 1100 (0.48) IV = 57.17 (0.33) SC = 430 (0.33)	0.03/0.03
422270	Lm: 289 ± 44 A549: 2919 ± 320	146/10/3	AMES= 0.321 (0.11) hERG= 0.45 (0.12) SI= 0.74 OB: Good	CYP3A4= 0.35 (0.15) , 0.09 (0.18) CYP2D6= 0.07 (0.33) , 0.03 (0.26)	IP = 110 (0.33) OR = 720 (0.44) IV = 28.74 (0.43) SC = 220 (0.43)	0.06/0.05
457964	Lm: 121 ± 20 A549: >5000	274/18/8	AMES= 0.07 (0.43) hERG= 0.02 (0.28) SI= 0.28 OB: Good	CYP3A4= 0.04 (0.53) , 0.01 (0.71) CYP2D6= 0.02 (0.58) , 0.01 (0.67)	IP = 35.64 (0.32) OR = 81.07 (0.35) IV = 30.33 (0.25) SC = 96.64 (0.24)	0.27/0.19
460747	Lm: 202 ± 11 A549: 158 ± 18	224/56/19	AMES= 0.555 (0.25) hERG= 0.04 (0.28) SI= 0.34 OB: Good	CYP3A4= 0.02 (0.56) , 0 (0.61) CYP2D6= 0.02 (0.55) , 0.01 (0.6)	IP = 72.05 (0.26) OR = 170 (0.67) IV = 20.09 (0.83) SC = 46.91 (0.52)	0.08/0.07

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625053	Lm: 403 ± 31 A549: >5000	149/2/0	AMES= 0.986 (0.77) hERG= 0.26 (0.09) SI= 0.99 OB: Good	CYP3A4= 0.76 (0.27) , 0.05 (0.3) CYP2D6= 0.27 (0.53) , 0.08 (0.22)	IP = 360 (0.51) OR = 710 (0.51) IV = 100 (0.65) SC = 300 (0.49)	0.08/0.07
629413	Lm: 379 ± 77 A549: >5000	165/6/0	AMES= 0.246 (0.55) hERG= 0.83 (0.57) SI= 0.73 OB: Poor	CYP3A4= 0.67 (0.78) , 0.38 (0.67) CYP2D6= 0.87 (0.57) , 0.34 (0.53)	IP = 59.78 (0.72) OR = 230 (0.54) IV = 12.79 (0.83) SC = 20.46 (0.82)	0.03/0.08
644992	Lm: 255 ± 21 A549: >5000	178/23/8	AMES= 0.726 (0.15) hERG= 0.35 (0.1) SI= 0.33 OB: Good	CYP3A4= 0.47 (0.15) , 0.05 (0.23) CYP2D6= 0.3 (0.22) , 0.17 (0.17)	IP = 350 (0.34) OR = 350 (0.48) IV = 49.11 (0.56) SC = 73.17 (0.63)	0.06/0.07
645317	Lm: 723 ± 24 A549: >5000	290/3/0	AMES= 0.246 (0.16) hERG= 0.24 (0.12) SI= 0.32 OB: Moderate	CYP3A4= 0.6 (0.15) , 0.08 (0.43) CYP2D6= 0.13 (0.27) , 0.05 (0.4)	IP = 320 (0.36) OR = 580 (0.42) IV = 71.55 (0.55) SC = 180 (0.37)	0.05/0.05
657546	Lm: 845 ± 136 A549: >5000	321/35/15	AMES= 0.3 (0.13) hERG= 0.68 (0.21) SI= 0.35 OB: Moderate	CYP3A4= 0.49 (0.09) , 0.05 (0.3) CYP2D6= 0.45 (0.29) , 0.25 (0.09)	IP = 91.92 (0.18) OR = 390 (0.22) IV = 22.69 (0.28) SC = 140 (0.28)	0.08/0.13
728862	Lm: 392 ± 50 A549: >5000	274/3/0	AMES= 0.337 (0.18) hERG= 0.36 (0.09) SI= 0.63 OB: Good	CYP3A4= 0.27 (0.14) , 0.02 (0.36) CYP2D6= 0.88 (0.14) , 0.34 (0.21)	IP = 390 (0.61) OR = 340 (0.4) IV = 79.06 (0.53) SC = 270 (0.29)	0.05/0.01
742546	Lm: 827 ± 116 A549: >5000	162/2/0	AMES= 0.097 (0.22) hERG= 0.79 (0.11) SI= 0.71 OB: Moderate	CYP3A4= 0.17 (0.12) , 0.01 (0.44) CYP2D6= 0.88 (0.17) , 0.67 (0.24)	IP = 56.8 (0.49) OR = 190 (0.45) IV = 79.46 (0.68) SC = 340 (0.65)	0/0.02
757789	Lm: 353 ± 25 A549: >5000	316/20/8	AMES= 0.895 (0.35) hERG= 0.27 (0.2) SI= 0.32 OB: Good	CYP3A4= 0.2 (0.35) , 0.02 (0.38) CYP2D6= 0.11 (0.22) , 0.05 (0.41)	IP = 89.1 (0.65) OR = 390 (0.42) IV = 16.38 (0.44) SC = 58.83 (0.48)	0.08/0.05
759209	Lm: 545 ± 118 A549: 2576 ± 185	152/13/4	AMES= 0.738 (0.41) hERG= 0.64 (0.19) SI= 0.32 OB: Good	CYP3A4= 0.09 (0.26) , 0.02 (0.42) CYP2D6= 0.08 (0.31) , 0.08 (0.33)	IP = 780 (0.36) OR = 760 (0.41) IV = 63.39 (0.33) SC = 860 (0.48)	0.03/0.03
760847	Lm: 108 ± 23 A549: >5000	300/8/1	AMES= 0.432 (0.28) hERG= 0.42 (0.15) SI= 0.31 OB: Moderate	CYP3A4= 0.51 (0.17) , 0.08 (0.39) CYP2D6= 0.65 (0.18) , 0.22 (0.28)	IP = 270 (0.32) OR = 610 (0.27) IV = 52.69 (0.28) SC = 370 (0.41)	0.1/0.1
786799	Lm: 180 ± 35 A549: >5000	193/4/0	AMES= 0.143 (0.33) hERG= 0.58 (0.22) SI= 0.98 OB: Moderate	CYP3A4= 0.62 (0.13) , 0.21 (0.14) CYP2D6= 0.08 (0.13) , 0.02 (0.28)	IP = 380 (0.45) OR = 2200 (0.19) IV = 82.36 (0.51) SC = 250 (0.51)	0.01/0.02
871185	Lm: 287 ± 145 A549: >5000	314/23/7	AMES= 0.261 (0.22) hERG= 0.52 (0.21) SI= 0.91 OB: Good	CYP3A4= 0.74 (0.1) , 0.25 (0.29) CYP2D6= 0.13 (0.53) , 0.02 (0.38)	IP = 800 (0.38) OR = 4400 (0.35) IV = 200 (0.52) SC = 1800 (0.43)	0.1/0.01

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952234	Lm: 205 ± 21 A549: 4082 ± 352	152/6/1	AMES= 0.891 (0.54) hERG= 0.14 (0.23) SI= 0.87 OB: Good	CYP3A4= 0.32 (0.18) , 0.1 (0.24) CYP2D6= 0.05 (0.33) , 0.02 (0.53)	IP = 420 (0.44) OR = 1700 (0.17) IV = 130 (0.48) SC = 510 (0.4)	0.1/0.1
1471937	Lm: 513 ± 52 A549: 4313 ± 540	195/13/3	AMES= 0.236 (0.06) hERG= 0.9 (0.35) SI= 0.29 OB: Moderate	CYP3A4= 0.27 (0.37) , 0.1 (0.21) CYP2D6= 0.12 (0.51) , 0.16 (0.09)	IP = 690 (0.35) OR = 940 (0.4) IV = 87.15 (0.24) SC = 210 (0.31)	0.06/0.07
1475345	Lm: 242 ± 29 A549: 955 ± 25	150/23/4	AMES= 0.717 (0.33) hERG= 0.96 (0.16) SI= 0.53 OB: Good	CYP3A4= 0.86 (0.27) , 0.37 (0.4) CYP2D6= 0.2 (0.32) , 0.08 (0.38)	IP = 50.13 (0.42) OR = 820 (0.43) IV = 32.94 (0.34) SC = 6600 (0.15)	0.09/0.1
1537038	Lm: 784 ± 36 A549: >5000	143/5/1	AMES= 0.658 (0.18) hERG= 0.33 (0.11) SI= 0.32 OB: Moderate	CYP3A4= 0.38 (0.24) , 0.09 (0.22) CYP2D6= 0.35 (0.35) , 0.08 (0.31)	IP = 110 (0.6) OR = 440 (0.65) IV = 47.45 (0.69) SC = 380 (0.5)	0.06/0.03
1736381	Lm: 87 ± 21 A549: 613 ± 109	99/18/6	AMES= 0.705 (0.29) hERG= 0.14 (0.06) SI= 0.5 OB: Poor	CYP3A4= 0.28 (0.29) , 0.03 (0.28) CYP2D6= 0.09 (0.35) , 0.08 (0.41)	IP = 480 (0.5) OR = 350 (0.08) IV = 260 (0.24) SC = 240 (0.36)	0.08/0.08
1811924	Lm: 166 ± 9 A549: >5000	170/12/2	AMES= 0.363 (0.15) hERG= 0.05 (0.37) SI= 0.58 OB: Poor	CYP3A4= 0.56 (0.38) , 0.03 (0.46) CYP2D6= 0.16 (0.31) , 0.05 (0.34)	IP = 500 (0.39) OR = 1100 (0.56) IV = 130 (0.36) SC = 340 (0.24)	0.07/0.1
1987332	Lm: 85 ± 5 A549: >5000	174/7/3	AMES= 0.697 (0.14) hERG= 0.85 (0.23) SI= 0.26 OB: Moderate	CYP3A4= 0.8 (0.19) , 0.08 (0.35) CYP2D6= 0.04 (0.38) , 0.01 (0.39)	IP = 690 (0.63) OR = 610 (0.31) IV = 37.71 (0.44) SC = 87.85 (0.3)	0.06/0.1
2137463	Lm: 499 ± 135 A549: >5000	155/7/0	AMES= 0.744 (0.13) hERG= 0.19 (0.17) SI= 0.31 OB: Good	CYP3A4= 0.26 (0.25) , 0.03 (0.36) CYP2D6= 0.16 (0.33) , 0.06 (0.32)	IP = 340 (0.39) OR = 470 (0.58) IV = 130 (0.3) SC = 410 (0.31)	0.04/0.04
2194030	Lm: 718 ± 86 A549: >5000	214/16/0	AMES= 0.678 (0.33) hERG= 0.37 (0.08) SI= 0.29 OB: Moderate	CYP3A4= 0.31 (0.63) , 0.1 (0.67) CYP2D6= 0.1 (0.39) , 0.04 (0.5)	IP = 300 (0.59) OR = 610 (0.29) IV = 120 (0.61) SC = 100 (0.23)	0.05/0.04
2766929	Lm: 767 ± 160 A549: 3546 ± 582	157/15/2	AMES= 0.165 (0.25) hERG= 0.55 (0.11) SI= 0.86 OB: Moderate	CYP3A4= 0.59 (0.24) , 0.08 (0.44) CYP2D6= 0.04 (0.32) , 0.02 (0.35)	IP = 460 (0.35) OR = 430 (0.21) IV = 59.18 (0.24) SC = 89.97 (0.23)	0.07/0.06
2846928	Lm: 35 ± 1 A549: 1635 ± 59	158/19/3	AMES= 0.103 (0.34) hERG= 0.99 (0.51) SI= 0.7 OB: Poor	CYP3A4= 0.09 (0.63) , 0.04 (0.75) CYP2D6= 0.57 (0.47) , 0.22 (0.4)	IP = 29.59 (0.66) OR = 560 (0.58) IV = 27.68 (0.66) SC = 440 (0.56)	0.02/0.03
2851545	Lm: 133 ± 35 A549: >5000	301/5/0	AMES= 0.103 (0.18) hERG= 0.7 (0.34) SI= 0.57 OB: Moderate	CYP3A4= 0.52 (0.2) , 0.45 (0.39) CYP2D6= 0.67 (0.36) , 0.36 (0.19)	IP = 240 (0.44) OR = 1600 (0.56) IV = 61.19 (0.56) SC = 440 (0.38)	0.05/0.06

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2855568	Lm: 122 ± 12 A549: >5000	257/5/0	AMES= 0.071 (0.35) hERG= 0.19 (0.27) SI= 0.85 OB: Poor	CYP3A4= 0.7 (0.14) , 0.11 (0.46) CYP2D6= 0.1 (0.38) , 0.07 (0.34)	IP = 920 (0.64) OR = 710 (0.33) IV = 94.14 (0.38) SC = 73.61 (0.3)	0.09/0.1
2856077	Lm: 751 ± 110 A549: >5000	194/9/1	AMES= 0.907 (0.58) hERG= 0.45 (0.19) SI= 0.91 OB: Moderate	CYP3A4= 0.7 (0.21) , 0.04 (0.52) CYP2D6= 0.35 (0.17) , 0.17 (0.26)	IP = 630 (0.66) OR = 1300 (0.54) IV = 85.49 (0.74) SC = 380 (0.42)	0.05/0.03
2923184	Lm: 60 ± 0.1 A549: >5000	163/3/0	AMES= 0.084 (0.41) hERG= 0.77 (0.13) SI= 0.42 OB: Moderate	CYP3A4= 0.25 (0.24) , 0.06 (0.41) CYP2D6= 0.4 (0.27) , 0.25 (0.27)	IP = 260 (0.46) OR = 440 (0.63) IV = 45.62 (0.45) SC = 460 (0.57)	0.1/0.1
2937831	Lm: 255 ± 48 A549: >5000	150/2/0	AMES= 0.331 (0.16) hERG= 0.41 (0.11) SI= 0.3 OB: Moderate	CYP3A4= 0.6 (0.21) , 0.06 (0.31) CYP2D6= 0.16 (0.17) , 0.04 (0.35)	IP = 250 (0.23) OR = 890 (0.31) IV = 41.35 (0.43) SC = 350 (0.31)	0.04/0.04
2946668	Lm: 515 ± 66 A549: >5000	269/5/0	AMES= 0.316 (0.36) hERG= 0.1 (0.18) SI= 0.27 OB: Moderate	CYP3A4= 0.81 (0.31) , 0.44 (0.25) CYP2D6= 0.05 (0.23) , 0.01 (0.42)	IP = 470 (0.45) OR = 360 (0.26) IV = 71.23 (0.28) SC = 260 (0.3)	0.07/0.07
2964134	Lm: 164 ± 42 A549: >5000	189/3/0	AMES= 0.164 (0.22) hERG= 0.48 (0.15) SI= 0.3 OB: Moderate	CYP3A4= 0.85 (0.3) , 0.38 (0.24) CYP2D6= 0.83 (0.22) , 0.55 (0.21)	IP = 240 (0.57) OR = 850 (0.52) IV = 49.3 (0.57) SC = 270 (0.27)	0.07/0.09
2999476	Lm: 187 ± 26 A549: >5000	304/4/0	AMES= 0.482 (0.1) hERG= 0.7 (0.19) SI= 0.27 OB: Moderate	CYP3A4= 0.94 (0.19) , 0.55 (0.23) CYP2D6= 0.79 (0.32) , 0.34 (0.2)	IP = 680 (0.23) OR = 570 (0.2) IV = 88.86 (0.23) SC = 94.7 (0.2)	0.02/0.04
3127155	Lm: 452 ± 74 A549: >5000	194/4/1	AMES= 0.914 (0.43) hERG= 0.14 (0.29) SI= 0.91 OB: Good	CYP3A4= 0.65 (0.16) , 0.07 (0.36) CYP2D6= 0.22 (0.25) , 0.05 (0.4)	IP = 560 (0.3) OR = 380 (0.47) IV = 120 (0.36) SC = 620 (0.41)	0.07/0.05
3164059	Lm: 218 ± 54 A549: 1059 ± 156	162/34/11	AMES= 0.525 (0.26) hERG= 0.09 (0.23) SI= 0.33 OB: Good	CYP3A4= 0.03 (0.46) , 0 (0.59) CYP2D6= 0.02 (0.53) , 0.01 (0.59)	IP = 69.95 (0.23) OR = 180 (0.66) IV = 18.97 (0.8) SC = 43.55 (0.52)	0.08/0.07
3236501	Lm: 105 ± 10 A549: >5000	332/5/0	AMES= 0.327 (0.1) hERG= 0.35 (0.07) SI= 0.44 OB: Moderate	CYP3A4= 0.71 (0.19) , 0.65 (0.19) CYP2D6= 0.29 (0.13) , 0.04 (0.37)	IP = 460 (0.46) OR = 1100 (0.29) IV = 70.96 (0.54) SC = 450 (0.38)	0.04/0.07
3237155	Lm: 743 ± 62 A549: >5000	246/3/0	AMES= 0.512 (0.27) hERG= 0.25 (0.12) SI= 0.3 OB: Poor	CYP3A4= 0.9 (0.39) , 0.36 (0.19) CYP2D6= 0.87 (0.37) , 0.17 (0.41)	IP = 580 (0.3) OR = 420 (0.16) IV = 99.8 (0.38) SC = 580 (0.31)	0.1/0.2
3242548	Lm: 111 ± 10 A549: >5000	270/2/0	AMES= 0.317 (0.1) hERG= 0.82 (0.15) SI= 0.87 OB: Moderate	CYP3A4= 0.85 (0.15) , 0.27 (0.27) CYP2D6= 0.72 (0.15) , 0.37 (0.18)	IP = 110 (0.68) OR = 460 (0.35) IV = 76.69 (0.5) SC = 200 (0.54)	0.05/0.09

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3521510	Lm: 326 ± 40 A549: >5000	163/2/0	AMES= 0.802 (0.68) hERG= 0.09 (0.19) SI= 0.39 OB: Moderate	CYP3A4= 0.71 (0.25) , 0.14 (0.33) CYP2D6= 0.14 (0.25) , 0.04 (0.33)	IP = 400 (0.26) OR = 150 (0.28) IV = 100 (0.57) SC = 170 (0.36)	0.01/0
3536067	Lm: 636 ± 60 A549: >5000	163/8/2	AMES= 0.977 (0.86) hERG= 0.01 (0.32) SI= 0.99 OB: Moderate	CYP3A4= 0.22 (0.28) , 0.01 (0.47) CYP2D6= 0.12 (0.28) , 0.05 (0.23)	IP = 450 (0.6) OR = 640 (0.45) IV = 190 (0.62) SC = 520 (0.51)	0.1/0.1
3564202	Lm: 565 ± 35 A549: 2106 ± 77	220/27/5	AMES= 0.064 (0.55) hERG= 0.94 (0.68) SI= 0.29 OB: Moderate	CYP3A4= 0.94 (0.22) , 0.75 (0.32) CYP2D6= 0.09 (0.33) , 0.02 (0.29)	IP = 270 (0.32) OR = 330 (0.42) IV = 56.14 (0.48) SC = 72.69 (0.24)	0.03/0.03
3609942	Lm: 73 ± 13 A549: 2748 ± 73	205/35/12	AMES= 0.86 (0.13) hERG= 0.71 (0.12) SI= 0.27 OB: Poor	CYP3A4= 0.94 (0.09) , 0.34 (0.19) CYP2D6= 0.07 (0.2) , 0.02 (0.33)	IP = 600 (0.49) OR = 880 (0.55) IV = 24.53 (0.52) SC = 16.53 (0.17)	0.04/0.07
3769434	Lm: 504 ± 66 A549: >5000	152/5/2	AMES= 0.34 (0.44) hERG= 0.54 (0.09) SI= 0.54 OB: Good	CYP3A4= 0.37 (0.22) , 0.06 (0.51) CYP2D6= 0.25 (0.37) , 0.08 (0.63)	IP = 310 (0.44) OR = 680 (0.35) IV = 91.91 (0.29) SC = 190 (0.36)	0.09/0.1
3932660	Lm: 61 ± 4 A549: >5000	211/6/2	AMES= 0.982 (0.8) hERG= 0.28 (0.08) SI= 0.99 OB: Good	CYP3A4= 0.64 (0.17) , 0.1 (0.56) CYP2D6= 0.32 (0.49) , 0.14 (0.49)	IP = 400 (0.43) OR = 500 (0.69) IV = 77.78 (0.3) SC = 460 (0.49)	0.03/0.03
3980962	Lm: 192 ± 2 A549: >5000	168/5/2	AMES= 0.536 (0.22) hERG= 0.49 (0.08) SI= 0.9 OB: Moderate	CYP3A4= 0.94 (0.29) , 0.24 (0.22) CYP2D6= 0.02 (0.33) , 0.01 (0.27)	IP = 980 (0.51) OR = 1100 (0.45) IV = 270 (0.49) SC = 730 (0.38)	0.04/0.04
4202676	Lm: 767 ± 76 A549: >5000	152/6/2	AMES= 0.635 (0.11) hERG= 0.06 (0.46) SI= 0.33 OB: Good	CYP3A4= 0.31 (0.3) , 0.03 (0.47) CYP2D6= 0.13 (0.24) , 0.05 (0.42)	IP = 430 (0.64) OR = 450 (0.69) IV = 210 (0.4) SC = 340 (0.37)	0.06/0.04
4271960	Lm: 545 ± 193 A549: >5000	163/4/0	AMES= 0.525 (0.08) hERG= 0.75 (0.18) SI= 0.47 OB: Moderate	CYP3A4= 0.75 (0.13) , 0.11 (0.34) CYP2D6= 0.16 (0.22) , 0.07 (0.28)	IP = 840 (0.35) OR = 690 (0.31) IV = 86.7 (0.49) SC = 100 (0.29)	0.06/0.07
5032706	Lm: 856 ± 33 A549: >5000	167/2/0	AMES= 0.692 (0.24) hERG= 0.17 (0.24) SI= 0.31 OB: Good	CYP3A4= 0.27 (0.13) , 0.05 (0.36) CYP2D6= 0.13 (0.13) , 0.02 (0.29)	IP = 340 (0.34) OR = 250 (0.18) IV = 110 (0.48) SC = 390 (0.32)	0.04/0.03
5309827	Lm: 382 ± 56 A549: >5000	286/7/1	AMES= 0.031 (0.14) hERG= 0.54 (0.09) SI= 0.45 OB: Moderate	CYP3A4= 0.66 (0.17) , 0.03 (0.25) CYP2D6= 0.08 (0.16) , 0.06 (0.24)	IP = 710 (0.39) OR = 2500 (0.33) IV = 83.63 (0.4) SC = 550 (0.35)	0.1/0.1
5833488	Lm: 788 ± 114 A549: 151 ± 10	150/16/2	AMES= 0.934 (0.17) hERG= 0.18 (0.07) SI= 0.31 OB: Poor	CYP3A4= 0.7 (0.29) , 0.06 (0.36) CYP2D6= 0.06 (0.28) , 0.01 (0.39)	IP = 430 (0.49) OR = 720 (0.35) IV = 250 (0.27) SC = 80.56 (0.26)	0.1/0.1

Pubchem CID	EC <sub>50</sub> (nM) Ave ± SD	Pubchem AID/Active Flags/Confirmed	Predictive <i>in silico</i> ADMET			
			Test (RI)	[CYP] IC <sub>50</sub> < 50 uM , IC <sub>50</sub> < 10 uM (RI)	Mouse LD <sub>50</sub> (mg/kg) (RI)	Tanimoto Score (SSG/AB)
6261459	Lm: 306 ± 31 A549: >5000	170/9/1	AMES= 0.28 (0.22) hERG= 0.61 (0.09) SI= 0.73 OB: Moderate	CYP3A4= 0.44 (0.28) , 0.03 (0.52) CYP2D6= 0.33 (0.14) , 0.08 (0.22)	IP = 320 (0.38) OR = 380 (0.42) IV = 60.82 (0.28) SC = 64.07 (0.21)	0.07/0.1
6602747	Lm: 104 ± 27 A549: >5000	311/5/1	AMES= 0.139 (0.31) hERG= 0.48 (0.12) SI= 0.14 OB: Moderate	CYP3A4= 0.53 (0.17) , 0.06 (0.46) CYP2D6= 0.7 (0.19) , 0.33 (0.1)	IP = 200 (0.4) OR = 1700 (0.23) IV = 43.75 (0.4) SC = 840 (0.41)	0.1/0.1
6602880	Lm: 10 ± 3 A549: >5000	286/7/1	AMES= 0.046 (0.2) hERG= 0.62 (0.5) SI= 0.94 OB: Moderate	CYP3A4= 0.49 (0.15) , 0.1 (0.15) CYP2D6= 0.44 (0.18) , 0.33 (0.18)	IP = 350 (0.65) OR = 650 (0.58) IV = 37.36 (0.56) SC = 200 (0.43)	0.01/0.03
6603247	Lm: 83 ± 5 A549: >5000	305/10/2	AMES= 0.301 (0.33) hERG= 0.92 (0.16) SI= 0.44 OB: Moderate	CYP3A4= 0.69 (0.3) , 0.1 (0.12) CYP2D6= 0.4 (0.24) , 0.56 (0.11)	IP = 170 (0.48) OR = 660 (0.39) IV = 46.76 (0.43) SC = 41.63 (0.3)	0.02/0.06
6603672	Lm: 274 ± 51 A549: >5000	305/3/0	AMES= 0.086 (0.16) hERG= 0.64 (0.25) SI= 0.21 OB: Poor	CYP3A4= 0.88 (0.36) , 0.34 (0.26) CYP2D6= 0.71 (0.28) , 0.23 (0.13)	IP = 250 (0.18) OR = 970 (0.28) IV = 110 (0.79) SC = 330 (0.52)	0.03/0.08
6604199	Lm: 5 ± 0.1 A549: 1903 ± 1400	210/20/5	AMES= 0.048 (0.6) hERG= 0.01 (0.31) SI= 0.3 OB: Good	CYP3A4= 0.1 (0.49) , 0.03 (0.66) CYP2D6= 0.01 (0.74) , 0.01 (0.66)	IP = 36.15 (0.62) OR = 96.4 (0.4) IV = 81.54 (0.78) SC = 220 (0.63)	0.2/0.1
9549148	Lm: 137 ± 40 A549: >5000	200/7/0	AMES= 0.115 (0.27) hERG= 0.88 (0.21) SI= 0.39 OB: Moderate	CYP3A4= 0.54 (0.24) , 0.03 (0.48) CYP2D6= 0.87 (0.09) , 0.63 (0.14)	IP = 150 (0.51) OR = 500 (0.5) IV = 27.55 (0.57) SC = 270 (0.44)	0.06/0.1
9549170	Lm: 164 ± 11 A549: 72 ± 5	176/25/2	AMES= 0.42 (0.31) hERG= 0 (0.26) SI= 0.3 OB: Poor	CYP3A4= 0.04 (0.56) , 0.01 (0.61) CYP2D6= 0.01 (0.74) , 0.01 (0.66)	IP = 220 (0.21) OR = 91.34 (0.35) IV = 120 (0.38) SC = 720 (0.29)	0.2/0.3
9550329	Lm: 50 ± 0.1 A549: >5000	216/23/9	AMES= 0.112 (0.39) hERG= 0.23 (0.37) SI= 0.69 OB: Poor	CYP3A4= 0.82 (0.37) , 0.17 (0.4) CYP2D6= 0.08 (0.32) , 0.02 (0.29)	IP = 120 (0.47) OR = 570 (0.51) IV = 32.35 (0.3) SC = 220 (0.37)	0.05/0.1
11293258	Lm: 10 ± 2 A549: 1296 ± 76	167/23/8	AMES= 0.897 (0.58) hERG= 0.96 (0.32) SI= 0.39 OB: Moderate	CYP3A4= 0.36 (0.28) , 0.05 (0.52) CYP2D6= 0.27 (0.15) , 0.08 (0.4)	IP = 160 (0.27) OR = 450 (0.47) IV = 37 (0.38) SC = 530 (0.46)	0.03/0.04
11834429	Lm: 142 ± 32 A549: >5000	188/3/0	AMES= 0.095 (0.29) hERG= 0.4 (0.09) SI= 0.39 OB: Moderate	CYP3A4= 0.51 (0.16) , 0.15 (0.19) CYP2D6= 0.69 (0.1) , 0.69 (0.15)	IP = 360 (0.56) OR = 600 (0.54) IV = 68.39 (0.53) SC = 1100 (0.51)	0.06/0.07
11834470	Lm: 211 ± 47 A549: >5000	200/24/3	AMES= 0.641 (0.22) hERG= 0.26 (0.09) SI= 0.84 OB: Moderate	CYP3A4= 0.76 (0.12) , 0.18 (0.34) CYP2D6= 0.24 (0.37) , 0.07 (0.24)	IP = 280 (0.49) OR = 1100 (0.48) IV = 68.33 (0.3) SC = 130 (0.26)	0.1/0.09

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			Test (RI)	[CYP] IC <sub>50</sub> < 50 uM , IC <sub>50</sub> < 10 uM (RI)	Mouse LD <sub>50</sub> (mg/kg) (RI)	Tanimoto Score (SSG/AB)
11948854	Lm: 607 ± 166 A549: >5000	180/4/0	AMES= 0.081 (0.2) hERG= 0.92 (0.31) SI= 0.81 OB: Moderate	CYP3A4= 0.39 (0.09) , 0.04 (0.21) CYP2D6= 0.55 (0.3) , 0.15 (0.3)	IP = 780 (0.73) OR = 270 (0.9) IV = 230 (0.75) SC = 210 (0.4)	0.04/0.01
11957314	Lm: 205 ± 21 A549: 1143 ± 53	200/26/3	AMES= 0.345 (0.1) hERG= 0.98 (0.25) SI= 0.71 OB: Poor	CYP3A4= 0.19 (0.48) , 0.06 (0.55) CYP2D6= 0.75 (0.37) , 0.24 (0.14)	IP = 77.01 (0.58) OR = 970 (0.51) IV = 14.72 (0.68) SC = 320 (0.5)	0/0.01
11958710	Lm: 174 ± 32 A549: >5000	193/10/1	AMES= 0.616 (0.2) hERG= 0.84 (0.12) SI= 0.72 OB: Poor	CYP3A4= 0.53 (0.14) , 0.04 (0.38) CYP2D6= 0.39 (0.24) , 0.17 (0.28)	IP = 24.37 (0.38) OR = 65.56 (0.69) IV = 12.2 (0.22) SC = 35.08 (0.3)	0.02/0.03
12004512	Lm: 746 ± 211 A549: >5000	162/6/2	AMES= 0.37 (0.42) hERG= 0.03 (0.27) SI= 0.48 OB: Poor	CYP3A4= 0.96 (0.86) , 0.48 (0.3) CYP2D6= 0.05 (0.39) , 0 (0.41)	IP = 47.19 (0.13) OR = 450 (0.42) IV = 6.34 (0.23) SC = 38.47 (0.33)	0.08/0.2
12004742	Lm: 491 ± 92 A549: >5000	181/25/10	AMES= 0.477 (0.21) hERG= 0.94 (0.12) SI= 0.68 OB: Poor	CYP3A4= 0.66 (0.17) , 0.09 (0.26) CYP2D6= 0.31 (0.2) , 0.34 (0.18)	IP = 11.02 (0.06) OR = 140 (0.12) IV = 8.4 (0.36) SC = 110 (0.25)	0.07/0.1
12005597	Lm: 629 ± 107 A549: 4067 ± 721	172/19/6	AMES= 0.049 (0.54) hERG= 0.99 (0.56) SI= 0.67 OB: Poor	CYP3A4= 0.09 (0.53) , 0.06 (0.66) CYP2D6= 0.32 (0.38) , 0.11 (0.45)	IP = 46.51 (0.51) OR = 700 (0.46) IV = 23.31 (0.69) SC = 350 (0.55)	0.03/0.05
13481921	Lm: 229 ± 34 A549: >5000	166/11/0	AMES= 0.646 (0.16) hERG= 0.96 (0.19) SI= 0.72 OB: Poor	CYP3A4= 0.4 (0.26) , 0.1 (0.58) CYP2D6= 0.78 (0.5) , 0.48 (0.35)	IP = 41.73 (0.46) OR = 130 (0.44) IV = 18.84 (0.44) SC = 29.98 (0.37)	0/0.01
15944965	Lm: 849 ± 99 A549: >5000	168/14/3	AMES= 0.254 (0.26) hERG= 0.87 (0.13) SI= 0.73 OB: Moderate	CYP3A4= 0.67 (0.12) , 0.11 (0.51) CYP2D6= 0.69 (0.2) , 0.42 (0.17)	IP = 580 (0.39) OR = 480 (0.27) IV = 60.54 (0.41) SC = 130 (0.32)	0.04/0.07
15944971	Lm: 505 ± 54 A549: >5000	166/23/5	AMES= 0.841 (0.25) hERG= 0.97 (0.23) SI= 0.7 OB: Poor	CYP3A4= 0.68 (0.12) , 0.08 (0.48) CYP2D6= 0.56 (0.1) , 0.35 (0.13)	IP = 76.17 (0.15) OR = 290 (0.22) IV = 12.69 (0.31) SC = 48.86 (0.16)	0.02/0.04
15945170	Lm: 178 ± 36 A549: >5000	164/2/0	AMES= 0.454 (0.19) hERG= 0.22 (0.21) SI= 0.16 OB: Poor	CYP3A4= 0.37 (0.12) , 0.01 (0.43) CYP2D6= 0.28 (0.27) , 0.07 (0.28)	IP = 680 (0.48) OR = 1700 (0.19) IV = 13.24 (0.43) SC = 1000 (0.31)	0.1/0.2
15945780	Lm: 184 ± 12 A549: >5000	168/10/1	AMES= 0.425 (0.14) hERG= 0.8 (0.14) SI= 0.3 OB: Moderate	CYP3A4= 0.28 (0.19) , 0.04 (0.45) CYP2D6= 0.58 (0.38) , 0.26 (0.35)	IP = 24.19 (0.54) OR = 550 (0.41) IV = 29.82 (0.61) SC = 110 (0.4)	0.03/0.03
16187569	Lm: 165 ± 25 A549: >5000	151/2/0	AMES= 0.188 (0.13) hERG= 0.9 (0.17) SI= 0.62 OB: Moderate	CYP3A4= 0.34 (0.16) , 0.03 (0.3) CYP2D6= 0.48 (0.08) , 0.24 (0.27)	IP = 320 (0.4) OR = 520 (0.58) IV = 47.74 (0.41) SC = 260 (0.43)	0.1/0.1

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			Test (RI)	[CYP] IC <sub>50</sub> < 50 uM , IC <sub>50</sub> < 10 uM (RI)	Mouse LD <sub>50</sub> (mg/kg) (RI)	Tanimoto Score (SSG/AB)
16187595	Lm: 14 ± 13 A549: >5000	145/2/0	AMES= 0.066 (0.29) hERG= 0.34 (0.04) SI= 0.7 OB: Moderate	CYP3A4= 0.39 (0.23) , 0.02 (0.3) CYP2D6= 0.45 (0.19) , 0.24 (0.46)	IP = 180 (0.32) OR = 1500 (0.57) IV = 36.81 (0.45) SC = 150 (0.37)	0.02/0.06
16187738	Lm: 511 ± 44 A549: >5000	149/2/0	AMES= 0.157 (0.2) hERG= 0.68 (0.1) SI= 0.48 OB: Moderate	CYP3A4= 0.2 (0.09) , 0.01 (0.26) CYP2D6= 0.45 (0.25) , 0.33 (0.25)	IP = 300 (0.26) OR = 760 (0.41) IV = 36.53 (0.6) SC = 340 (0.52)	0.09/0.1
16189740	Lm: 571 ± 113 A549: >5000	146/2/0	AMES= 0.013 (0.14) hERG= 0.48 (0.07) SI= 0.84 OB: Moderate	CYP3A4= 0.5 (0.26) , 0.1 (0.34) CYP2D6= 0.29 (0.2) , 0.2 (0.27)	IP = 110 (0.7) OR = 550 (0.59) IV = 27.54 (0.2) SC = 86.87 (0.41)	0.04/0.06
16192568	Lm: 301 ± 50 A549: >5000	148/2/0	AMES= 0.624 (0.5) hERG= 0.14 (0.19) SI= 0.3 OB: Moderate	CYP3A4= 0.31 (0.24) , 0.1 (0.38) CYP2D6= 0.1 (0.44) , 0.01 (0.54)	IP = 1100 (0.39) OR = 520 (0.59) IV = 130 (0.66) SC = 270 (0.69)	0.12/0.07
16192591	Lm: 357 ± 56 A549: 3754 ± 623	153/5/0	AMES= 0.073 (0.5) hERG= 0.68 (0.14) SI= 0.44 OB: Moderate	CYP3A4= 0.29 (0.19) , 0.04 (0.47) CYP2D6= 0.34 (0.22) , 0.09 (0.26)	IP = 220 (0.6) OR = 490 (0.72) IV = 41.19 (0.67) SC = 160 (0.37)	0.01/0.04
16196001	Lm: 50 ± 9 A549: >5000	146/2/0	AMES= 0.403 (0.15) hERG= 0.72 (0.37) SI= 0.72 OB: Poor	CYP3A4= 0.45 (0.39) , 0.12 (0.34) CYP2D6= 0.39 (0.19) , 0.18 (0.22)	IP = 57.67 (0.55) OR = 330 (0.55) IV = 12.85 (0.56) SC = 200 (0.33)	0.04/0.06
16196006	Lm: 703 ± 44 A549: >5000	145/5/1	AMES= 0.21 (0.11) hERG= 1 (0.43) SI= 0.64 OB: Poor	CYP3A4= 0.72 (0.47) , 0.32 (0.35) CYP2D6= 0.79 (0.33) , 0.29 (0.34)	IP = 14.24 (0.61) OR = 470 (0.33) IV = 1.66 (0.41) SC = 20.73 (0.36)	0.03/0.03
16196223	Lm: 18 ± 2 A549: 2325 ± 205	156/18/2	AMES= 0.469 (0.13) hERG= 0.96 (0.4) SI= 0.7 OB: Poor	CYP3A4= 0.78 (0.15) , 0.12 (0.2) CYP2D6= 0.63 (0.33) , 0.34 (0.22)	IP = 51.41 (0.54) OR = 350 (0.27) IV = 11.38 (0.55) SC = 74.17 (0.36)	0.01/0.05
16196319	Lm: 15 ± 1 A549: >5000	150/11/1	AMES= 0.304 (0.12) hERG= 0.92 (0.33) SI= 0.71 OB: Poor	CYP3A4= 0.69 (0.2) , 0.05 (0.32) CYP2D6= 0.42 (0.32) , 0.29 (0.21)	IP = 23.87 (0.48) OR = 400 (0.31) IV = 13.55 (0.59) SC = 70.87 (0.37)	0.01/0.08