Dataset	Baseline	MapLight	Chemprop	Minimol
Hard Tasks (Baseline < 0.70)				
Cyp2C9 Sub. Carbonmangels	0.600 (0.50 - 0.70)	0.622 (0.52 - 0.72)	**0.633** (0.53 - 0.73)	0.617 (0.51 - 0.72)
Bioavailability Ma	0.656 (0.55 - 0.77)	**0.734*** (0.64 - 0.83)	0.671 (0.57 - 0.77)	0.712 (0.61 - 0.82)
Cyp3A4 Sub. Carbonmangels	0.660 (0.57 - 0.75)	0.644 (0.55 - 0.74)	0.627 (0.53 - 0.72)	**0.671** (0.57 - 0.77)
Medium Tasks (0.70 - 0.85)				
Cyp2D6 Sub. Carbonmangels	0.760 (0.67 - 0.85)	0.805 (0.72 - 0.89)	**0.848*** (0.78 - 0.91)	0.803 (0.72 - 0.88)
Ames	0.822 (0.80 - 0.84)	**0.870*** (0.85 - 0.89)	0.850** (0.83 - 0.87)	0.853** (0.83 - 0.87)
Herg	0.827 (0.75 - 0.91)	**0.871** (0.80 - 0.94)	0.717 (0.61 - 0.82)	0.780 (0.68 - 0.88)
Dili	0.848 (0.77 - 0.92)	0.877 (0.81 - 0.95)	0.887 (0.82 - 0.96)	**0.924*** (0.87 - 0.98)
Cyp2D6 Veith	0.849 (0.83 - 0.87)	**0.889*** (0.87 - 0.91)	0.866* (0.85 - 0.89)	0.870* (0.85 - 0.89)
Easy Tasks (Baseline > 0.85)				
Bbb Martins	0.866 (0.82 - 0.91)	**0.915*** (0.88 - 0.95)	0.867 (0.82 - 0.91)	0.913** (0.88 - 0.95)
Cyp2C9 Veith	0.871 (0.86 - 0.89)	0.896*** (0.88 - 0.91)	0.891*** (0.88 - 0.90)	**0.897*** (0.88 - 0.91)
Cyp3A4 Veith	0.871 (0.86 - 0.88)	0.901*** (0.89 - 0.91)	**0.903*** (0.89 - 0.91)	0.884* (0.87 - 0.90)
Pgp Broccatelli	0.904 (0.87 - 0.94)	**0.933** (0.90 - 0.96)	0.905 (0.87 - 0.94)	0.922 (0.89 - 0.96)
Hia Hou	0.960 (0.92 - 1.00)	0.985 (0.96 - 1.00)	0.945 (0.88 - 1.02)	**0.992** (0.98 - 1.00)