**Table S3.** Predicted PK parameters by SimCYP Simulator of each group.

|  |  |  |  |
| --- | --- | --- | --- |
|   | **V0** | **V1** | **V2** |
| **TMax (h)** | **CMax (ng/mL)** | **AUC (ng/mL.h)** | **TMax (h)** | **CMax (ng/mL)** | **AUC (ng/mL.h)** | **TMax (h)** | **CMax (ng/mL)** | **AUC (ng/mL.h)** |
| **A-1** | 1.56 | 32.83 | 489.24 | 1.57 | 34.70 | 543.78 | 1.09 | 134.80 | 1029.77 |
| **A-2** | 2.05 | 27.26 | 301.76 | 1.92 | 23.64 | 220.52 | 1.69 | 51.44 | 368.52 |
| **B-1** | 1.81 | 11.50 | 90.49 | 1.45 | 7.78 | 41.83 | 2.16 | 8.89 | 52.77 |
| **B-2** | 1.56 | 599.76 | 4987.74 | 1.20 | 480.26 | 2894.68 | 2.04 | 111.93 | 902.70 |
| **C-1** | 1.16 | 285.58 | 1745.00 | 1.43 | 135.74 | 997.00 | 1.31 | 118.71 | 907.86 |
| **C-2** | 1.50 | 84.44 | 673.03 | 1.70 | 102.08 | 861.95 | 1.28 | 1455.19 | 9744.15 |
| **D-1** | 0.60 | 24.14 | 73.21 | 0.48 | 13.52 | 25.17 | 0.77 | 75.75 | 447.09 |
| **D-2** | 1.56 | 69.79 | 903.96 | 1.09 | 25.88 | 267.20 | 0.37 | 59.60 | 228.05 |
| **E-1** | 1.92 | 7.39 | 115.82 | 1.92 | 5.72 | 113.98 | 0.36 | 11.88 | 82.52 |
| **E-2** | 1.13 | 28.82 | 391.50 | 1.33 | 30.50 | 541.49 | 1.13 | 26.58 | 342.62 |
| **F-1** | 0.72 | 18.73 | 112.33 | 0.96 | 20.96 | 187.37 | 1.20 | 27.27 | 340.55 |
| **F-2** | 1.56 | 2.45 | 33.74 | 1.08 | 1.26 | 15.46 | 0.37 | 2.69 | 13.64 |
| **G-1** | 3.17 | 2629.04 | 57296.38 | 3.17 | 2629.02 | 57294.61 | 0.74 | 235.49 | 620.85 |
| **G-2** | 2.06 | 352.27 | 11977.41 | 2.07 | 655.13 | 29764.21 | 2.06 | 4833.39 | 847522.37 |
| **H-1** | 4.34 | 6.51 | 121.20 | 4.23 | 5.64 | 103.68 | 2.52 | 13.66 | 130.62 |
| **H-2** | 1.25 | 178.63 | 1565.18 | 0.72 | 68.62 | 234.49 | 1.72 | 10.84 | 189.81 |
| **I-1** | 0.84 | 23.50 | 69.71 | 0.48 | 22.17 | 67.13 | 1.08 | 3.51 | 7.11 |
| **I-2** | 1.33 | 4.01 | 14.42 | 1.32 | 0.88 | 2.99 | 0.88 | 49.64 | 87.57 |
| **J-1** | 0.63 | 1.35 | 4.17 | 0.50 | 0.88 | 1.81 | 0.86 | 1.89 | 17.23 |
| **J-2** | 0.72 | 74.37 | 421.55 | 0.37 | 38.06 | 272.29 | 0.37 | 34.57 | 226.19 |
| **K-1** | 0.98 | 159.28 | 1845.88 | 1.33 | 139.77 | 2466.26 | 0.89 | 32.66 | 194.88 |
| **K-2** | 0.50 | 25.10 | 73.42 | 0.50 | 13.87 | 25.13 | 0.77 | 37.94 | 354.16 |
| **L-1** | 1.24 | 3822.30 | 33567.68 | 1.23 | 2180.61 | 18538.33 | 2.16 | 1768.43 | 13202.95 |
| **L-2** | 0.75 | 2468.92 | 14595.42 | 0.64 | 2374.07 | 12320.61 | 0.56 | 1898.85 | 7753.21 |
| **M-1** | 5.62 | 13.53 | 550.05 | 6.43 | 17.61 | 896.25 | 8.03 | 57.56 | 3596.48 |
| **M-2** | 2.83 | 25.33 | 380.99 | 3.23 | 29.20 | 490.96 | 2.83 | 54.77 | 776.18 |