

Supplemental Figure 1. Schema of sample collection

a.

Supplemental Figure 2. Visual predictive check of total MPA (a), unbound MPA (b), total MPAG (c) and IMPDH activity (d) on a linear scale. Dashed lines represent the 5th and 95th percentile of the observed data. Solid lines represent the 5th and 95th percentile of simulated data. Open circles and crosses represent 50th percentile of observed and simulated data, respectively.

c.



b.





Supplemental Figure 3.Goodness-of-fit plots: population prediction (PRED) vs. observed, individual prediction vs. observed, conditional weighted residual (CWRES) vs. PRED, and CWRES vs. time post dose. a) total MPA; b) unbound MPA; c) total MPAG; d) IMPDH activity. a.



b.



d.



Supplemental Figure 4. Effect of concomitant calcineurin inhibitor (cyclosporine or CSP, n=20 and tacrolimus or TAC, n=7), on total MPA AUC_{0-8h} in validation cohort.



Calcineurin inhibitor



Supplemental Figure 5. No effect of calcineurin inhibitor or graft source upon E_0 or IC_{50} of IMPDH activity on day +21

Supplemental Figure 6. 5th ,50th, and 95th percentiles of simulated data plotted against the observed data from the validation dataset. a) total MPA, b) unbound MPA, c) total MPAG, d) IMPDH activity.



Supplemental Figure 7. Association of IMPDH AUEC with acute GVHD (A), CMV reactivation (B), non-relapse mortality (C), and overall mortality (D) in 11 patients receiving a related donor graft. Only events on or after day +26 are shown.

