



Figure S1. PBPK simulations of the plasma concentrations of montelukast A (perfusion-limited distribution; $f_{m,CYP2C8}=0.55$, $f_{m,CYP3A4}=0.16$) and montelukast B (permeability-limited distribution; $f_{m,CYP2C8}=0.60$, $f_{m,CYP3A4}=0.16$) following intravenous administration. Montelukast 3, 9 and 18 mg were administered as 15 min infusions to 6 healthy male subjects. Thin lines represent individual trials, the thick line represents the mean of ten trials. Circles refer to clinical data from Cheng et al. (1996).