### Table S1. Definitions of symbols

| Symbol | Definition                                                                 |
|--------|---------------------------------------------------------------------------|
| $C_{\text{aq,milk}}$ | Total drug concentration in the aqueous phase of whole milk               |
| $C_{\text{fat,milk}}$ | Total drug concentration in the lipid phase (milk fat) of whole milk      |
| $C_{\text{milk}}$ | Total drug concentration in whole milk                                    |
| $C_{\text{plasma}}$ | Total drug concentration in plasma                                         |
| $C_{\text{skim}}$ | Total drug concentration in skim milk                                     |
| $C_{\text{u,aq,milk}}$ | Unbound drug concentration in the aqueous phase of whole milk             |
| $C_{\text{u,aq,milk}}^{\text{un}}$ | Unbound, unionised drug concentration in the aqueous phase of whole milk |
| $C_{\text{u,plasma}}^{\text{un}}$ | Unbound, unionised drug concentration in plasma                           |
| $C_{\text{u,skim}}$ | Unbound drug concentration in skim milk                                   |
| $C_{\text{u,skim}}^{\text{un}}$ | Unbound, unionised drug concentration in skim milk                        |
| $D_{\text{milk}}$ | Milk lipid-to-ultrafiltrate distribution coefficient at a specified pH    |
| $f_{\text{aq,milk}}$ | Fraction of the volume of whole milk occupied by aqueous phase            |
| $f_{\text{fat,milk}}$ | Fraction of the volume of whole milk occupied by lipid phase (milk fat)   |
| $f_{\text{plasma}}^{\text{un}}$ | Unionised fraction of unbound drug in plasma                             |
| $f_{\text{skim}}^{\text{un}}$ | Unionised fraction of unbound drug in skim milk                          |
| $f_{\text{u,milk}}$ | Unbound fraction of drug in whole milk                                    |
| $f_{\text{u,plasma}}$ | Unbound fraction of drug in plasma                                        |
| $f_{\text{u,skim}}$ | Unbound fraction of drug in skim milk                                     |
| Log $D_{\text{ow}}$ | Logarithm of octanol-to-water distribution coefficient at a specified pH |
| Log $D_{\text{milk}}$ | Logarithm of milk lipid-to-ultrafiltrate distribution coefficient at a specified pH |
| Log $P_{\text{ow}}$ | Logarithm of octanol-to-water partition coefficient                       |
| $P_{\text{ow}}$ | Octanol-to-water partition coefficient                                     |
| $S/M$ | Skim-to-whole milk drug concentration ratio                               |
| $V_{\text{aq,milk}}$ | Volume of the aqueous phase of whole milk                                |
| $V_{\text{fat,milk}}$ | Volume of the lipid phase (milk fat) of whole milk                       |
| $V_{\text{milk}}$ | Volume of whole milk                                                     |