**Supplemental Information**

**Modelling of the SDF-1/CXCR4 Regulated *In vivo* Homing of Therapeutic Mesenchymal Stem/stromal Cells**

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**Additional results**

Fig. S1 shows the overall goodness-of-fit of the model calibration with an initial MSC does of 5 × 105 cells/animal. Fig. S2 shows the model calibration and validation with the independent external data, as well as the corresponding goodness-of-fit plot. To validate the model for SDF-1 in the liver, we first calibrate Equation (3) in the main manuscript to the published independent external data (Wilson et al., 2016), to estimate parameters *a*B, *b*B, and *c*B. The parameter estimates are then inputted into Equation (4) with the association coefficients $η\_{1}$, $η\_{2}$, and $η\_{3}$ estimated by calibrating both Equations (3) and (4) into the data of SDF-1level presented in the main manuscript, to predict the SDF-1 level in the liver. The predicted SDF-1 level (black solid line in Fig. S2A) is then superimposed onto the independent external data.



**Figure S1.** Goodness-of-fit plot of model calibration. Model predictions and experimental data are analyzed using linear regression, with *R2*=0.987 (n = 34).



**Figure S2.** Model validation results with independent external data. **(A)** Model validation with the SDF-1 concentrations in the blood and liver of mice with hepatic ischemia/reperfusion (I/R) injury. The solid line in each panel represents the concentration-time profile of the SDF-1 simulated by the model while the circles represent measured data. Concentrations of the SDF-1 is expressed as SDF-1 amount per kilogram of tissue. **(B)** Goodness-of-fit plot of model validation. Model predictions and experimental data are analyzed using linear regression, with *R2*=0.986 (n = 10).