**Supplemental Information**

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

**Wang Jina, Xiaowen Liangb, Anastasia Brooksb, Kathryn Futregac, Xin Liub, Michael R. Doranc,d,e, Matthew J. Simpsona, Michael S. Robertsb,f, Haolu Wangb**

a School ofMathematical Sciences, Queensland University of Technology, Brisbane, Australia

bTherapeutics Research Centre, The University of Queensland Diamantina Institute, The University of Queensland, Translational Research Institute, Brisbane, Australia

cInstitute of Health and Biomedical Innovation, Queensland University of Technology, Translational Research Institute, Brisbane, Australia

dMater Research Institute, The University of Queensland, Translational Research Institute, Brisbane, Australia

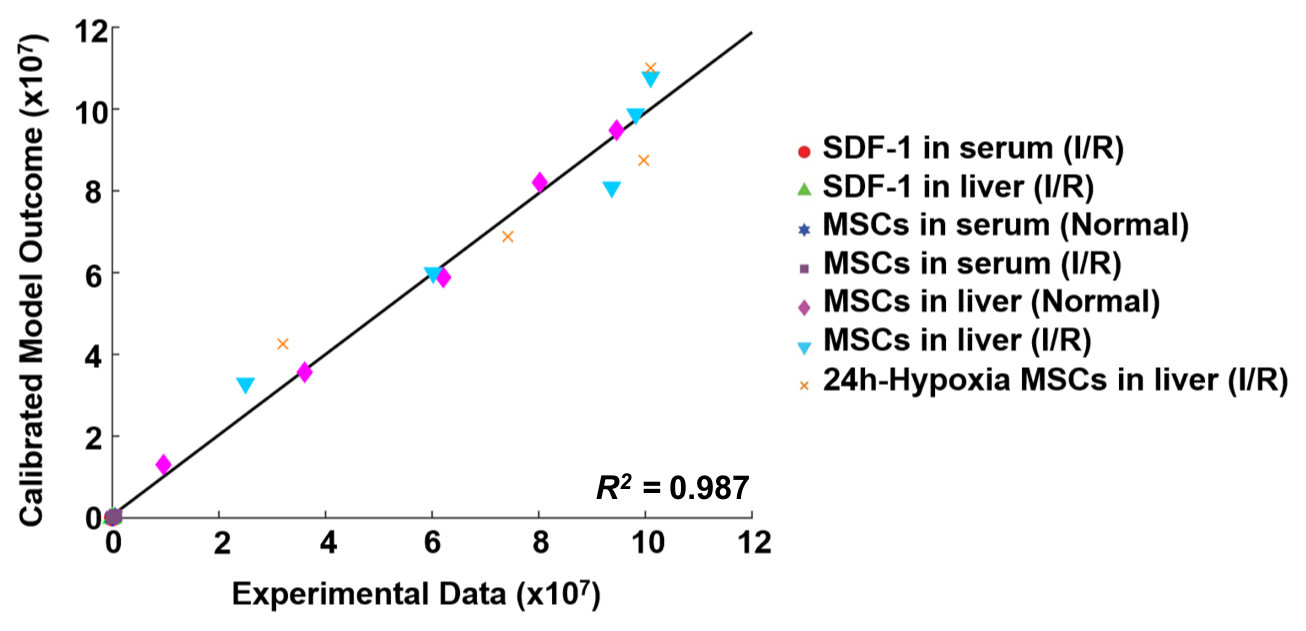
eAustralian National Centre for the Public Awareness of Science, Australian National University, Canberra, Australia

fSchool of Pharmacy and Medical Science, University of South Australia, Adelaide, Australia

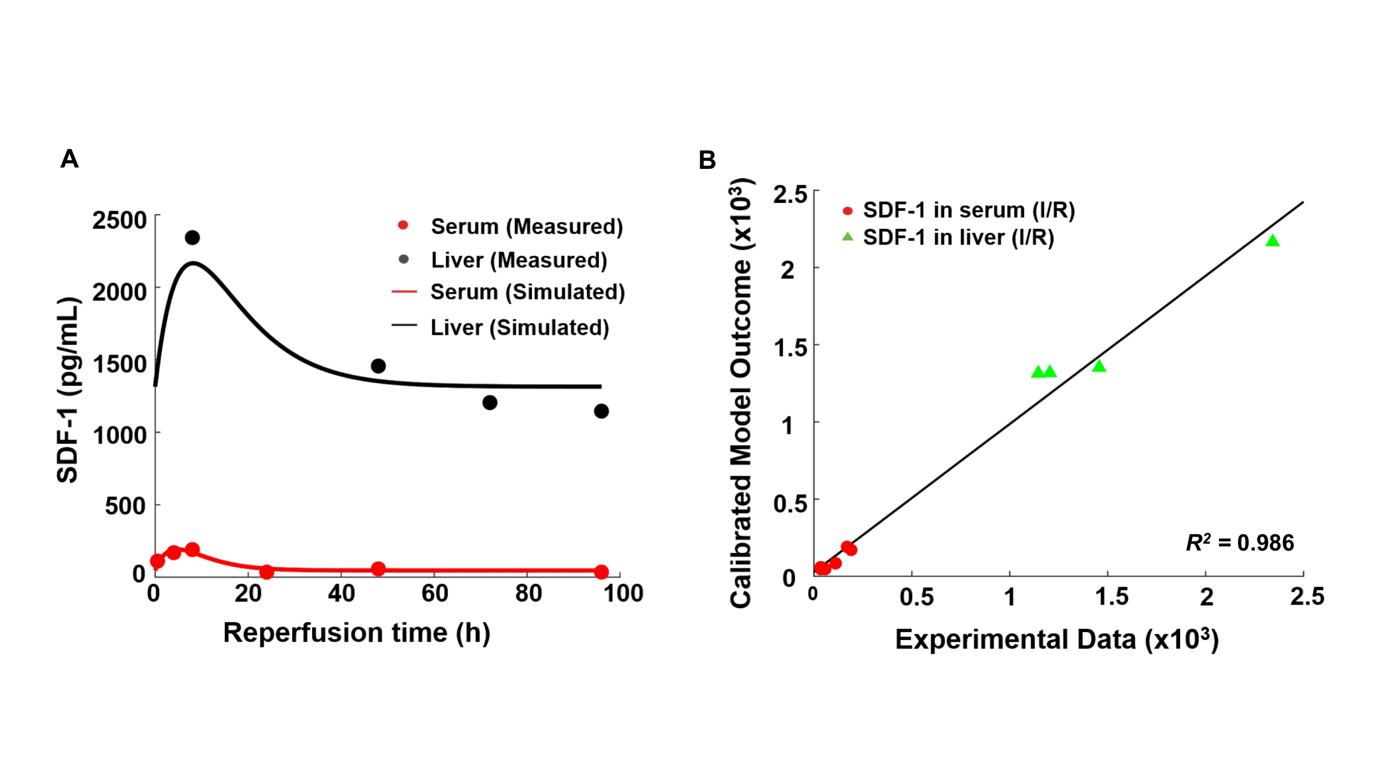
Correspondence:Michael S. Roberts, Ph.D., The University of Queensland Diamantina Institute, The University of Queensland, Translational Research Institute, QLD 4103, Australia. Telephone: 61-07-3443-8033; Email: m.roberts@uq.edu.au and Haolu Wang, MBBS., Ph.D., The University of Queensland Diamantina Institute, The University of Queensland, Translational Research Institute, QLD 4103, Australia. Telephone: 61-07-3443-7488; Email:[h.wang21@uq.edu.au](mailto:h.wang21@uq.edu.au)

**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 , , and 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).