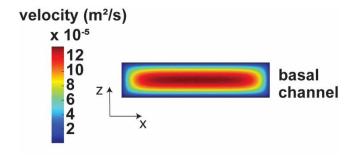
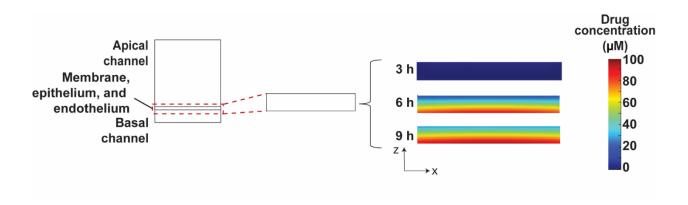
Electronic Supplementary Material (ESI) for Lab on a Chip. This journal is © The Royal Society of Chemistry 2021

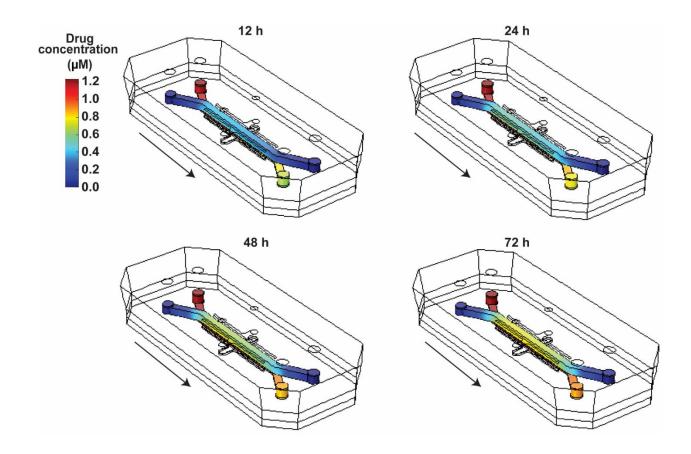
## **SUPPLEMENTARY INFORMATION**



**Figure S1.** Heat map of the velocity distribution in a vertical cross section of the basal channel along the xz axis.



**Figure S2**. 2D heat maps of the concentration profiles of the drug in vertical cross sections of the epithelium, membrane, and endothelium along the xz axis. The epithelium, membrane, and endothelium are combined into one geometry.



**Figure S3.** 3D surface heat maps showing amodiaquine concentrations in the Organ Chip over a 72 h dosing period. The heat maps were generated using P= 40 and D<sub>pdms</sub> =  $3.8 \times 10^{-13} \frac{m^2}{s}$ .

Table S1. Physiochemical properties of amodiaquine and FITC.

	Amodiaquine (from DrugBank)¹	FITC (from PubChem) <sup>2</sup>
Molecular weight (g/mol)	355.86	398.4
Log P	3.7	4.8 (XLogP2 value)
Hydrogen acceptor count	4	7
Hydrogen donor count	2	2
Number of rings	3	5

 Table S2. Model parameters.

Parameter	Description	Value	Unit	Ref
Q	Basal channel flow rate	60	$\frac{\mu L}{h}$	
T	Incubator temperature	37	°C	
P	Atmospheric pressure	1	atm	
$D_{med}$	Diffusion coefficient of the drug in medium	$1 \times 10^{-9}$	$\frac{m^2}{s}$	3–5
c <sub>o</sub>	Concentration of drug dosed into the chip	1.24	μМ	
$D_{pdms}$	Diffusion coefficient of the drug in PDMS	Unknown	$\frac{m^2}{s}$	
P	Partition coefficient of the compound	Unknown		
C <sub>pdms</sub>	Concentration of the drug in PDMS	Unknown	μΜ	
C <sub>med</sub>	Concentration of the drug in cell culture medium	Unknown	μΜ	

## References

- 1 Wishart DS, Knox C, Guo AC, Shrivastava S, Hassanali M, Stothard P, et al. Drugbank: a comprehensive resource for in silico drug discovery and exploration. Nucleic Acids Res. 2006 Jan 1;34 (Database issue):D668-72. 16381955.
- 2National Center for Biotechnology Information (2021). PubChem Compound Summary for CID 18730, Fluorescein-5-isothiocyanate. Retrieved March 25, 2021 from https://pubchem.ncbi.nlm.nih.gov/compound/Fluorescein-5-isothiocyanate.
- 3P. Buchwald, Theor. Biol. Med. Model., 2011, 8, 20.
- 4J. Wang and T. Hou, J. Comput. Chem., 2011, 32, 3505-3519.
- 5J. Järnefelt, T. Laurent and R. Rigler, *FEBS Lett.*, 1988, **242**, 129–133.