

Supplementary file

Dose-response fit function

The dose response curves were derived from a mathematical fit function. The used function is used to describe sigmoidal dose-response curves. The fit function contains the baseline E_{\min} , the maximum response E_{\max} , the half inhibitory concentration (IC_{50}), and the hill slope p :

$$y = E_{\min} + \frac{E_{\max} - E_{\min}}{1 + 10^{(IC_{50} - c_x) \cdot p}} \quad (1)$$

Deep learning

Table S1. Dataset composition

Cisplatin concentration [μ M]	Estimated cell death Ψ (%)	Number of images
0 (untreated)	16.2	1000
0.625	17.1	415
1.0	17.6	315
1.25	18.1	215
2	19.5	410
2.5	20.7	657
3	21.9	265
5	28.3	355
10	51.9	637
50	81.8	705
Total		4974

Table S2. Hyperparameter search space and optimal configuration obtained via Bayesian Optimization

Hyperparameter	Type	Search interval	Optimum value
Neural architecture	Categorical	alexnet [1], vgg11 [2], vgg16 [2], resnet18 [3], resnet50 [3], inception [4]	vgg11
Optimizer	Categorical	Adam [5], SDG [6], RMSProp [6]	Adam [5]
Learning rate	Numerical	$1 \times 10^{-6} - 1 \times 10^{-1}$	1.69×10^{-4}
Weight decay	Numerical	$1 \times 10^{-4} - 1 \times 10^{-1}$	1.55×10^{-2}
Momentum (not for Adam)	Numerical	0 – 0.99	N/A (Adam)
Batch size	Numerical	8 – 64	20

Table S3. Transformations used for data augmentation.

Transformation	Range
Scaling (zoom)	0.5 – 2.0
Rotation (around spheroid mass center)	0° – 360°
X translation	-60 px – 60 px
X translation	-60 px – 60 px
Contrast correction – gamma	0.5 – 2.0
Contrast correction – gain	0.5 – 1.5
Vertical flip	No – Yes
Horizontal flip	No – Yes

Images are transformed differently at each epoch. The transformation parameters are randomly sampled from the indicated ranges.

References

1. Alex Krizhevsky, Ilya Sutskever, Geoffrey E. Hinton. ImageNet Classification with Deep Convolutional Neural Networks.
2. K. Simonyan, A. Zisserman, *Very Deep Convolutional Networks for Large-Scale Image Recognition 2014*.
3. Kaiming He, Xiangyu Zhang, Shaoqing Ren, et al. Deep Residual Learning for Image Recognition.
4. Christian Szegedy, Wei Liu, Yangqing Jia, et al. Going Deeper With Convolutions.
5. D. P. Kingma, J. Ba, *Adam: A Method for Stochastic Optimization 2014*.
6. S. Ruder, *An overview of gradient descent optimization algorithms 2016*.