

Supporting information Comparative Study of Multitask Toxicity Modeling on a Broad Chemical Space

Sergey Sosnin,[†] Dmitry Karlov,[†] Igor V. Tetko,[‡] and Maxim V. Fedorov^{*,†,¶}

[†]*Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow
143026, Russia*

[‡]*Helmholtz Zentrum München - Research Center for Environmental Health (GmbH),
Institute of Structural Biology, Ingolstädter Landstraße 1 b. 60w, D-85764 Neuherberg
Germany*

[¶]*University of Strathclyde, Department of Physics, John Anderson Building, 107
Rottenrow East, Glasgow, UK G40NG*

E-mail: m.fedorov@skoltech.ru

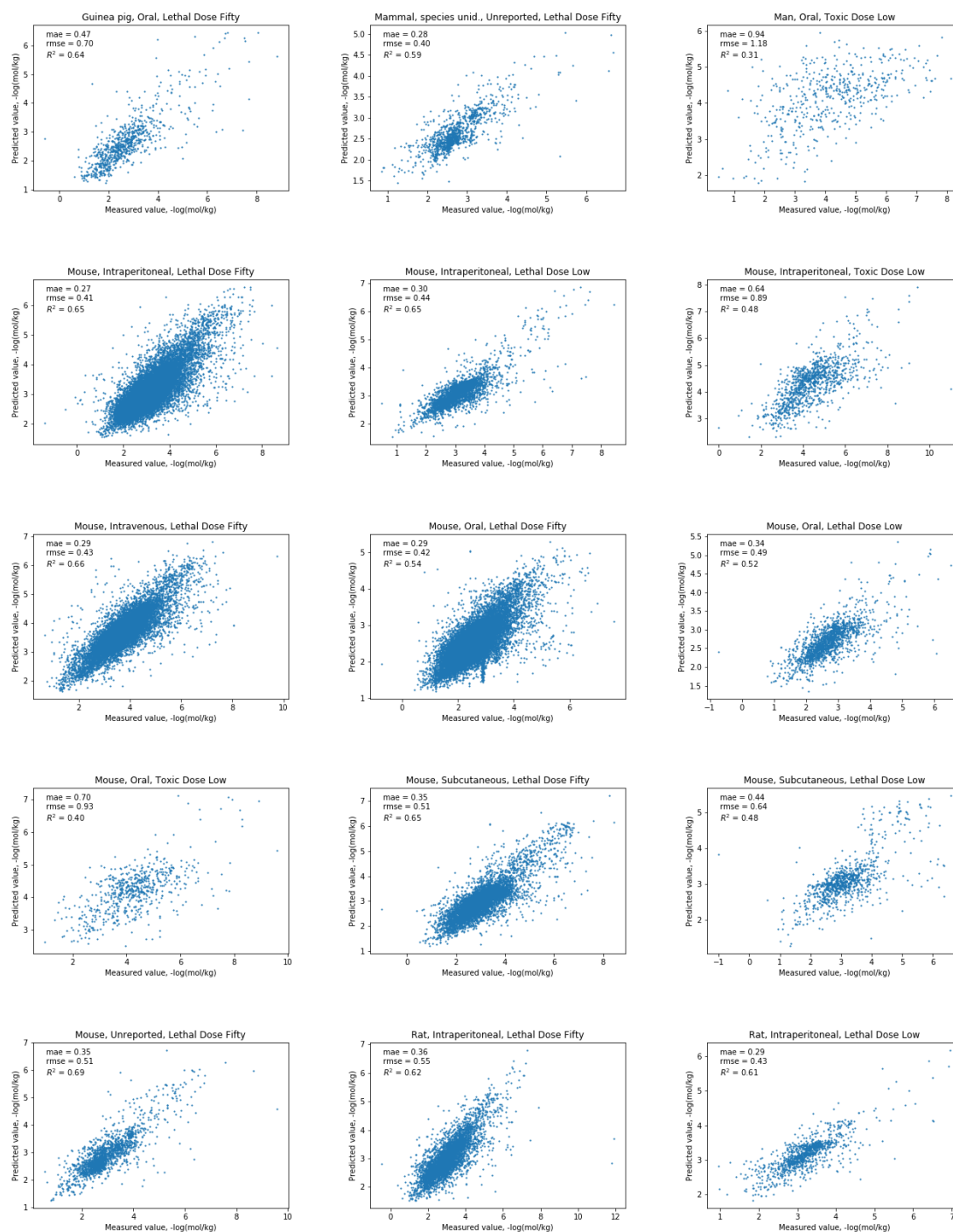
The architecture and training parameters for ANN used in the experiments

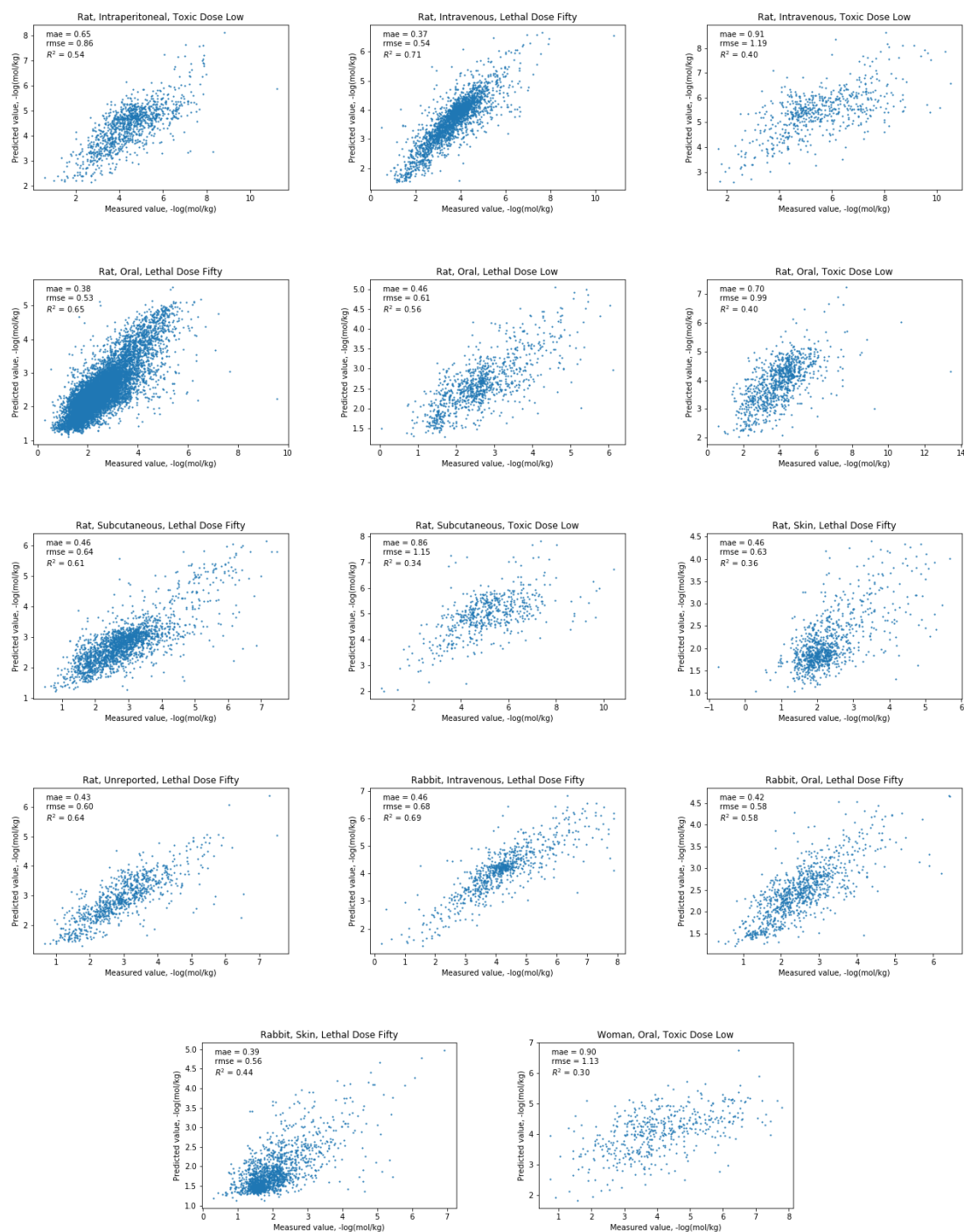
The architecture presented in the *Table S1*. In our experiments Adam¹ optimizer with default parameters was used for neural network training.

Table S1: The architecture of our neural network

Hidden Layer	Neurons	Batch Normalization	Dropout ratio
1	512	Yes	0.5
2	256	Yes	0.5
3	128	Yes	0.5
4	64	Yes	0.5
5	32	Yes	0.25
6	32	No	0.1

Endpoints prediction charts





References

- (1) Kingma D.P.; Ba J. Adam: A Method for Stochastic Optimization *Published as a conference paper at the 3rd International Conference for Learning Representations*, San Diego, USA, 2015, arXiv:1412.6980 .