

Multi-Target in silico prediction of Inhibitors for Mitogen Activated Protein Kinase-Interacting Kinases

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Table S2. The architecture of Deep Neural Network (DNN) model used in the current work and in a previous report of Sosnin et al. [1].

Hidden Layer	Neurons	Batch Normalization	Dropout ratio
1	512	Yes	0.50
2	256	Yes	0.50
3	128	Yes	0.50
4	64	Yes	0.50
5	32	Yes	0.25
6	32	No	0.10

References

1. Sosnin, S.; Karlov, D.; Tetko, I.V.; Fedorov, M.V. Comparative Study of Multitask Toxicity Modeling on a Broad Chemical Space. *J. Chem. Inf. Model.* **2019**, *59*, 1062-1072.