

# SUPPLEMENTARY INFORMATION

## Recurrent Neural Network Model for Constructive Peptide Design

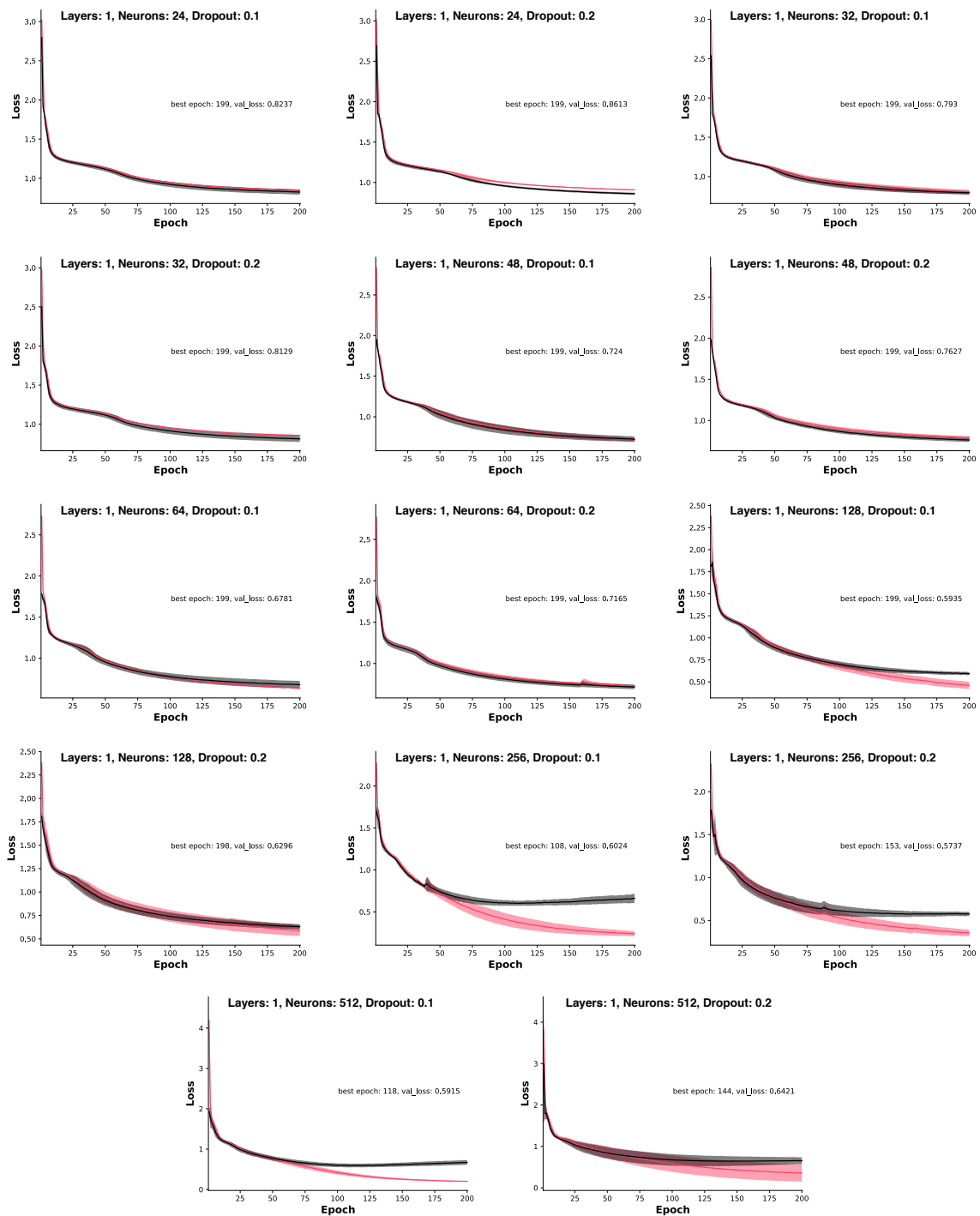
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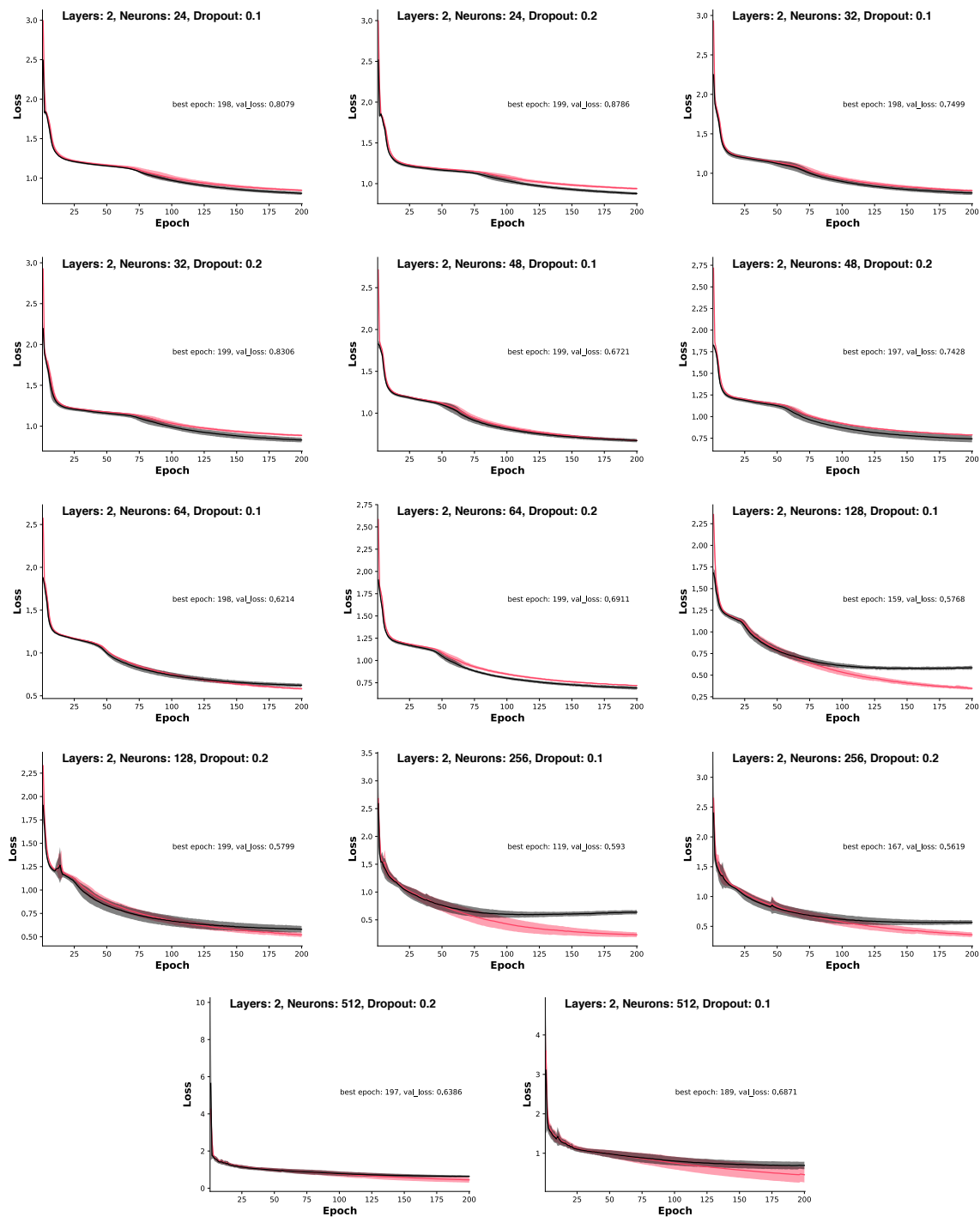
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**Table S1.** Five-fold cross-validation loss (CV loss) obtained for all tested architectures trained for 200 epochs. In each fold, weights were initialized with a different random seed.

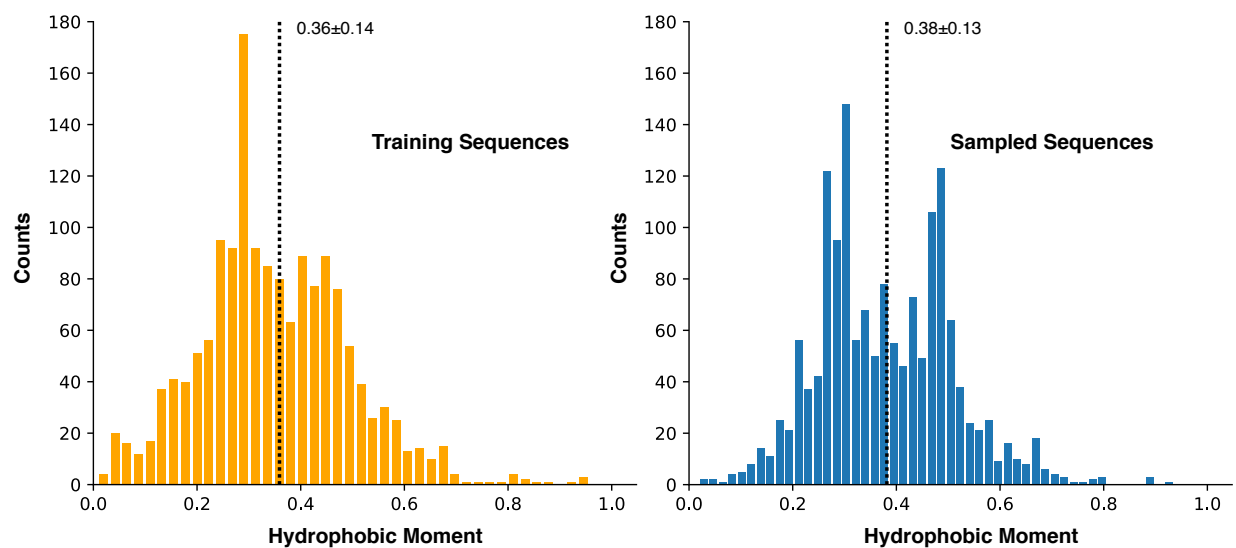
Layers	Neurons	Dropout	Best epoch	CV loss
2	256	0.2	167	0.562
1	256	0.2	153	0.574
2	128	0.1	159	0.577
2	128	0.2	199	0.580
1	512	0.1	118	0.592
2	256	0.1	119	0.593
1	128	0.1	199	0.594
1	256	0.1	108	0.602
2	64	0.1	198	0.621
1	128	0.2	198	0.630
2	512	0.2	197	0.639
1	512	0.2	144	0.642
2	48	0.1	199	0.672
1	64	0.1	199	0.678
2	512	0.1	189	0.687
2	64	0.2	199	0.691
1	64	0.2	199	0.717
1	48	0.1	199	0.724
2	48	0.2	197	0.743
2	32	0.1	198	0.750
1	48	0.2	199	0.763
1	32	0.1	199	0.793
2	24	0.1	198	0.808
1	32	0.2	199	0.813
1	24	0.1	199	0.824
2	32	0.2	199	0.831
1	24	0.2	199	0.861
2	24	0.2	199	0.879



**Figure S1.** Five-fold cross-validation loss curves for all tested architectures with one layer.



**Figure S2.** Five-fold cross-validation loss curves for all tested architectures with two layers.



**Figure S3.** Histograms of the hydrophobic moment distribution of both training (left, orange) and sampled (right, blue) sequences. Dashed lines depict the average value.