

Imperial College London

Department of Life Sciences

Final Year Project

Supplementary Information

Feature engineering and selection to improve autoencoder-based classification of wildtype and mutant c-Myc molecular dynamics trajectories

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SUPERVISED BY

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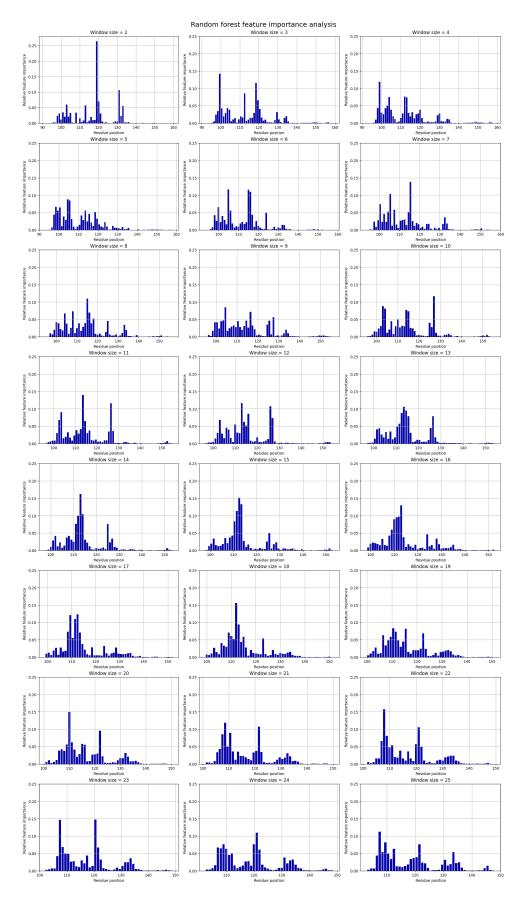
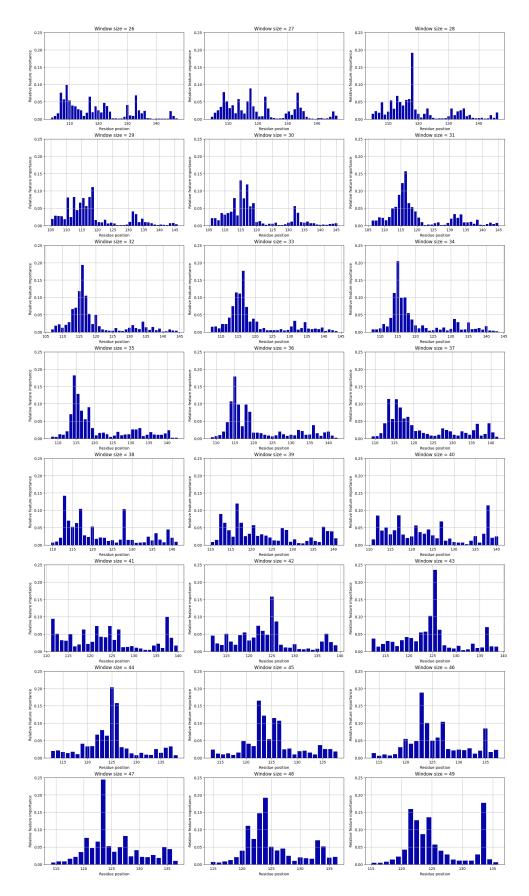


Figure S1: Random forest feature importance analysis for window size 2-25



 $\textbf{Figure S1:} \ \ \text{Random forest feature importance analysis for window size } 26\text{--}50$

Training history of Multi-Layer Perceptron classifier
Trained on wild-type and mutant local compaction data generated using window size 12.

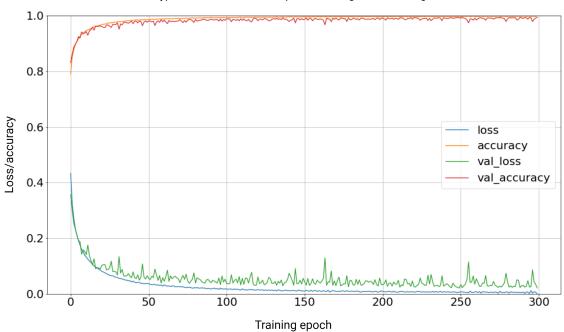
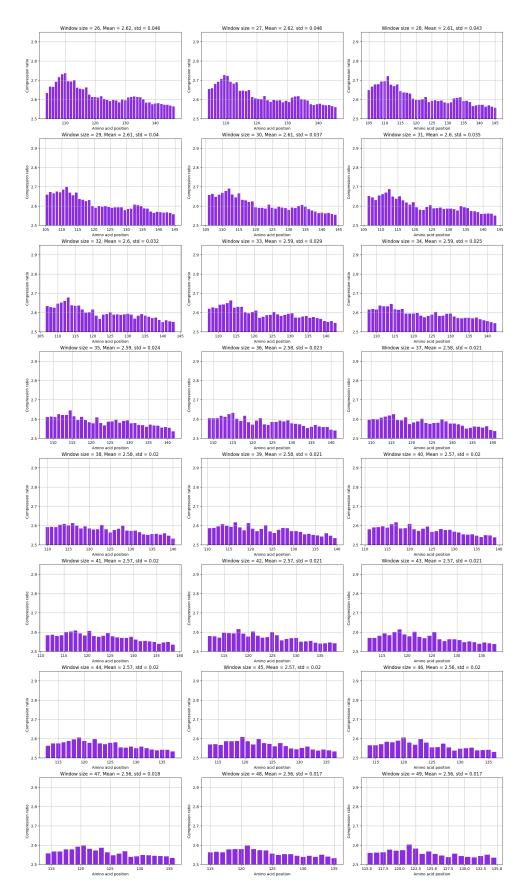


Figure S2: Traning history for multi-layer perceptron classifier, trained on wild-type and mutant local compaction data generated using window size = 12.



 $\textbf{Figure S3:} \ \ \text{gzip compression ratios for local compaction data generated using window size 2-25}$



 $\textbf{Figure S3:} \ \text{gzip compression ratios for local compaction data generated using window size } 26\text{-}50$