## Data S2

## DNA shape features improve transcription factor binding site predictions *in vivo*

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Related to Figure 2. Impact of DNA shape on predicting TFBSs. A. Comparison of the AUROC obtained for the 400 ENCODE human ChIP-seq data sets when using either the PSSM scores (x-axis) or the classifiers combining PSSM scores and DNA shape features (y-axis). The dashed line represents equal AUROC values obtained with the two methods. B. Comparison of the median AUROC over all ChIP-seq data sets associated with each TF (one data point per TF) when using either the PSSM scores (x-axis) or the PSSM + DNA shape classifiers (y-axis). The dashed line represents equal AUROC values obtained with the two methods. C. Improvement in predictive power obtained when considering DNA shape features (y-axis) as the difference between the AUROC values obtained with the PSSM + DNA shape classifiers and PSSM scores. The higher the difference, the stronger the improvement when DNA shape information is incorporated. Note that the data sets (x-axis) were ranked by increasing difference values. D. For each TF family (y-axis), an associated data set is represented at the corresponding x-coordinate where the data set appears in B. The name of the TF families are given on the y-axis along with the Mann-Whitney U test p-values of enrichment for significant improvement in parenthesis. Note that the given p-values are not corrected for multiple hypothesis testing.



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