# PD-BertEDL: An Ensemble Deep Learning Method Using BERT and Multivariate Representation to Predict Peptide Detectability

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## Supporting Tables

**Table S1.** Amino acid properties details of 15 physicochemical information.

| category | Amino acid properties |
|---|---|
| structure | 0-alpha-CH chemical shifts |
| | 1-Helix termination parameter at posision j-2, j-1, j |
| | 2-Optimized propensity to form reverse turn |
| | 3-Normalized frequency of alpha-helix in all-alpha class All-alpha |
| | 4-Correlation coefficient in regression analysis |
| | 5-Weights for alpha-helix at the window position of -1 |
| | 6-Average relative fractional occurrence in ER(i-1) |
| | 7-Relative preference value at N1 |
| | 8-Normalized frequency of isolated helix |
| | 9-Normalized frequency of zeta R |
| Hydrophobicity | Hydrophobicity coefficient in RP-HPLC, C18 with 0.1%TFA/2-PrOH/MeCN/H2O |
| energy | 0-Activation Gibbs energy of unfolding |
| | 1-Slopes tripeptide FDPB PARSE neutral |
| charge | Positive charge |
| AAC | AA composition of EXT2 of single-spanning proteins |

**Table S2.** Amino acid properties details of 15 physicochemical information value.

| Amino acid | str0 | str1 | str2 | str3 | str4 | str5 | str6 | str7 | str8 | str9 | Hydroph-obicity | Energy0 | Energy1 | charge | AAC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | 4.349 | 1.2 | 1.34 | 1.08 | 0.687 | 0.34 | 0.99 | 1.2 | 0.946 | 0.328 | -2.34 | -0.729 | 18.56 | 0 | 5.04 |
| C | 4.686 | 1 | 1.07 | 1.22 | 0.263 | -0.18 | 2.32 | 0.8 | 0.481 | 0 | 5.03 | -0.408 | 17.84 | 0 | 2.2 |
| D | 4.765 | 0.7 | 3.32 | 0.86 | 0.632 | 0.06 | 1.18 | 0.8 | 1.311 | 3.379 | -0.48 | -0.545 | 17.94 | 0 | 5.26 |
| E | 4.295 | 0.7 | 2.2 | 1.09 | 0.669 | 0.2 | 1.36 | 2.2 | 0.698 | 0 | 1.3 | -0.532 | 17.97 | 0 | 6.07 |
| F | 4.663 | 1 | 0.8 | 0.96 | 0.577 | 0.15 | 1.25 | 0.5 | 0.963 | 1.336 | 2.57 | -0.454 | 17.95 | 0 | 3.72 |
| G | 3.972 | 0.8 | 2.07 | 0.85 | 0.67 | -0.88 | 1.4 | 0.3 | 0.36 | 0.5 | -1.06 | -0.86 | 18.57 | 0 | 7.09 |
| H | 4.63 | 1.2 | 1.27 | 1.02 | 0.594 | -0.09 | 1.06 | 0.7 | 2.168 | 1.204 | -3 | -0.519 | 18.64 | 1 | 2.99 |
| I | 4.224 | 0.8 | 0.66 | 0.98 | 0.564 | -0.03 | 0.81 | 0.9 | 1.283 | 2.078 | 7.26 | -0.361 | 19.21 | 0 | 4.32 |
| K | 4.358 | 1.7 | 0.61 | 1.01 | 0.407 | -0.11 | 0.91 | 0.6 | 1.203 | 0.835 | 1.56 | -0.508 | 18.36 | 1 | 6.31 |
| L | 4.385 | 1 | 0.54 | 1.04 | 0.541 | 0.2 | 1.26 | 0.9 | 1.192 | 0.414 | 1.09 | -0.462 | 19.01 | 0 | 9.88 |
| M | 4.513 | 1 | 0.7 | 1.11 | 0.328 | 0.43 | 1 | 0.3 | 0 | 0.982 | 0.62 | -0.518 | 18.49 | 0 | 1.85 |
| N | 4.755 | 1.2 | 2.49 | 1.05 | 0.489 | -0.33 | 1.15 | 0.7 | 0.432 | 1.498 | 2.81 | -0.597 | 18.24 | 0 | 5.94 |
| P | 4.471 | 1 | 2.12 | 0.91 | 0.6 | -0.81 | 0 | 2.6 | 2.093 | 0.415 | -0.15 | NA | 18.77 | 0 | 6.22 |
| Q | 4.373 | 1 | 1.49 | 0.95 | 0.527 | 0.01 | 1.52 | 0.7 | 1.615 | 0 | 0.16 | -0.492 | 18.51 | 0 | 4.5 |
| R | 4.396 | 1.7 | 0.95 | 0.93 | 0.59 | 0.22 | 1.19 | 0.7 | 1.128 | 2.088 | 1.6 | -0.535 | 0 | 1 | 3.73 |
| S | 4.498 | 1.5 | 0.94 | 0.95 | 0.692 | -0.35 | 1.5 | 0.7 | 0.523 | 1.089 | 1.93 | -0.278 | 18.06 | 0 | 8.05 |
| T | 4.346 | 1 | 1.09 | 1.15 | 0.713 | -0.37 | 1.18 | 0.8 | 1.961 | 1.732 | 0.19 | -0.367 | 17.71 | 0 | 5.2 |
| V | 4.184 | 0.8 | 1.32 | 1.03 | 0.529 | 0.13 | 1.01 | 1.1 | 0.409 | 0.946 | 2.06 | -0.323 | 18.98 | 0 | 6.19 |
| W | 4.702 | 1 | -4.65 | 1.17 | 0.632 | 0.07 | 1.33 | 2.1 | 1.925 | 1.781 | 3.59 | -0.455 | 16.87 | 0 | 2.1 |
| Y | 4.604 | 1 | -0.17 | 0.8 | 0.495 | -0.31 | 1.09 | 1.8 | 0.802 | 0 | -2.58 | -0.439 | 18.23 | 0 | 3.32 |

**Table S3.** Cross-validation mean results and independent test results of 21 classifiers on the Mus.culus dataset.

| | | **Cross-validation** | **Independent test** |
|---|---|---|---|
| **Descriptor** | **Classifier**[a] | **mean_Acc±std_Acc** | **Acc** |
| One-hot | kNN | 0.5202±0.0052 | 0.5368 |
| | LR | 0.5996±0.0097 | 0.6154 |
| | RF | 0.5731±0.0037 | 0.5914 |
| | GBDT | 0.6093±0.0163 | 0.6212 |
| | CNN | 0.7129±0.0112 | 0.7112 |
| | BiLSTM | 0.7407±0.0041 | 0.7430 |
| | CNN+BiLSTM | **0.7434±0.0046** | **0.7502** |
| AP3-A | kNN | 0.5377±0.0090 | 0.5500 |
| | LR | 0.5960±0.0050 | 0.6041 |
| | RF | 0.5593±0.0129 | 0.5773 |
| | GBDT | 0.6199±0.0153 | 0.6276 |
| | CNN | 0.7190±0.0106 | 0.7242 |
| | BiLSTM | 0.7162±0.0079 | 0.7142 |
| | CNN+BiLSTM | **0.7336±0.0084** | **0.7331** |
| BERT-mini | kNN | 0.5472±0.0072 | 0.5521 |
| | LR | 0.6050±0.0052 | 0.6307 |
| | RF | 0.5478±0.0081 | 0.5516 |
| | GBDT | 0.6059±0.0072 | 0.6217 |
| | CNN | 0.6214±0.0104 | 0.6195 |
| | BiLSTM | **0.7037±0.0081** | **0.7055** |
| | CNN+BiLSTM | 0.6197±0.0134 | 0.6252 |

a kNN: k-nearest neighbor, LR: logistic regression, RF: random forest, GBDT: Gradient Boosting Decision Tree. The best results for each descriptor are highlighted in bold.

**Table S4.** Cross-validation mean results and independent test results of 21 classifiers on the Homo.spaines dataset.

| | | **Cross-validation** | **Independent test** |
|---|---|---|---|
| **Descriptor** | **Classifier[a]** | **mean_Acc±std_Acc** | **Acc** |
| One-hot | kNN | 0.5694±0.0046 | 0.5717 |
| | LR | 0.6775±0.0097 | 0.6844 |
| | RF | 0.7047±0.0072 | 0.7550 |
| | GBDT | 0.6752±0.0061 | 0.6833 |
| | CNN | 0.8037±0.0020 | 0.8009 |
| | BiLSTM | 0.8141±0.0041 | 0.7920 |
| | CNN+BiLSTM | **0.8147±0.0032** | **0.8107** |
| AP3-A | kNN | 0.6209±0.0115 | 0.6206 |
| | LR | 0.6648±0.0111 | 0.6692 |
| | RF | 0.6817±0.0113 | 0.6992 |
| | GBDT | 0.6848±0.0092 | 0.6944 |
| | CNN | 0.7968±0.0039 | 0.7983 |
| | BiLSTM | 0.7908±0.0067 | 0.7799 |
| | CNN+BiLSTM | **0.8058±0.0078** | **0.8117** |
| BERT-mini | kNN | 0.5896±0.0111 | 0.6087 |
| | LR | 0.7185±0.0050 | 0.7428 |
| | RF | 0.6275±0.0149 | 0.6148 |
| | GBDT | 0.7000±0.0104 | 0.7094 |
| | CNN | 0.7001±0.0243 | 0.6909 |
| | BiLSTM | **0.7988**±0.0068 | **0.8042** |
| | CNN+BiLSTM | 0.7864±0.0098 | 0.7921 |

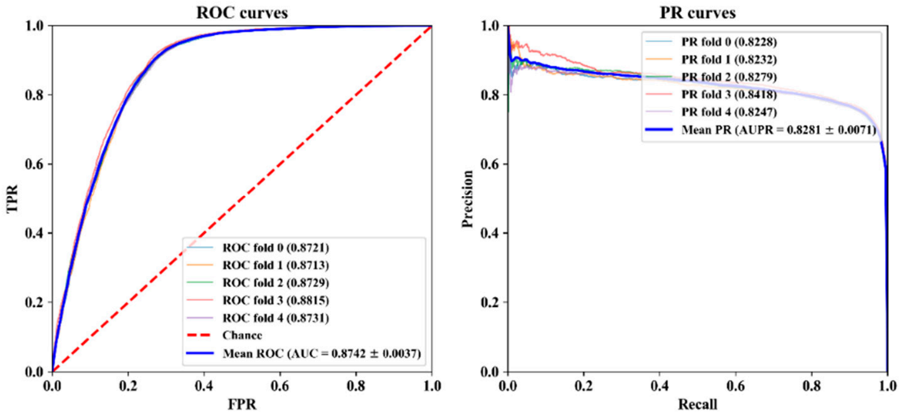
[a] kNN: k-nearest neighbor, LR: logistic regression, RF: random forest, GBDT: Gradient Boosting Decision Tree. The best results for each descriptor are highlighted in bold.

× $10^{-5}$

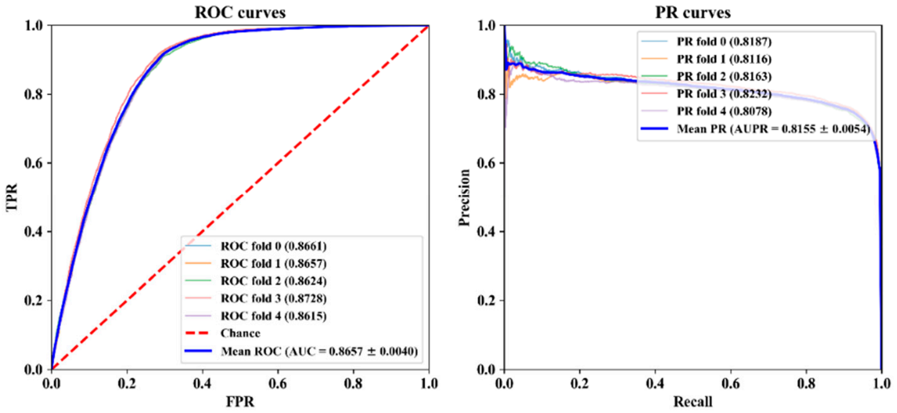
**Table S5.** The variance of indicators with different models.

| | **Sn** | **Sp** | **ACC** | **MCC** | **AUC** | **AUPR** |
|---|---|---|---|---|---|---|
| DNN | $3.65\times10^{-4}$ | $3.59\times10^{-4}$ | $2.56\times10^{-6}$ | $1.26\times10^{-5}$ | $2.25\times10^{-5}$ | $4.77\times10^{-5}$ |
| CapsNet | $6.30\times10^{-5}$ | $1.53\times10^{-4}$ | $2.93\times10^{-5}$ | $1.07\times10^{-4}$ | $1.40\times10^{-5}$ | $3.08\times10^{-5}$ |
| DeepMS | $1.33\times10^{-4}$ | $2.17\times10^{-4}$ | $1.81\times10^{-5}$ | $6.13\times10^{-5}$ | $9.47\times10^{-6}$ | $1.87\times10^{-5}$ |
| PepFormer | $5.66\times10^{-4}$ | $1.41\times10^{-3}$ | $1.29\times10^{-5}$ | $1.69\times10^{-3}$ | $3.76\times10^{-5}$ | $7.76\times10^{-5}$ |
| PD-BertEDL | $2.24\times10^{-4}$ | $1.59\times10^{-4}$ | $2.17\times10^{-5}$ | $2.32\times10^{-4}$ | $3.00\times10^{-5}$ | $3.19\times10^{-5}$ |

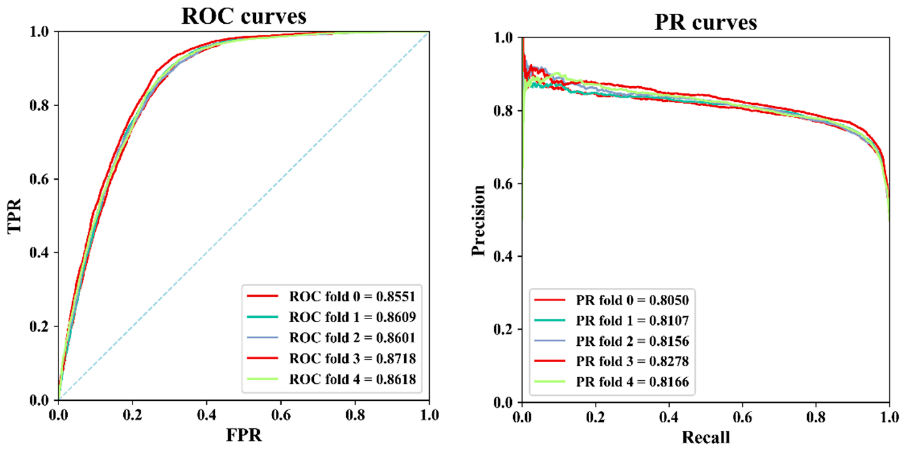
## Supporting Figures



**(a)** AUROC and AUPR curve of sequence information-CNN+BiLSTM.

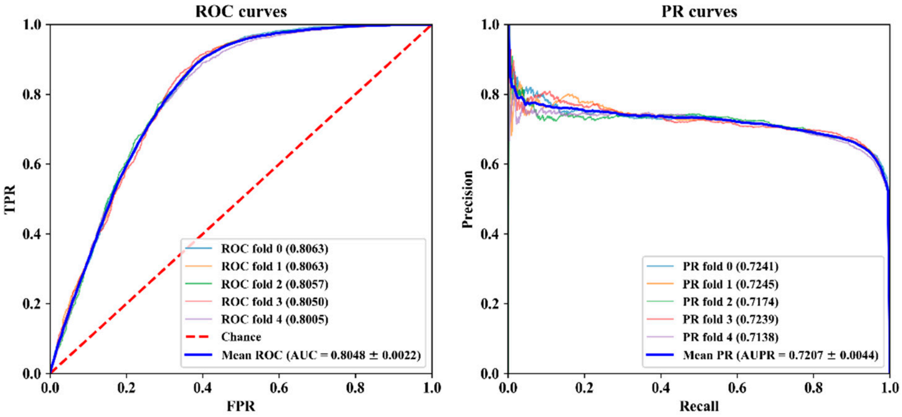


**(b)** AUROC and AUPR curve of physicochemical information-CNN+BiLSTM.

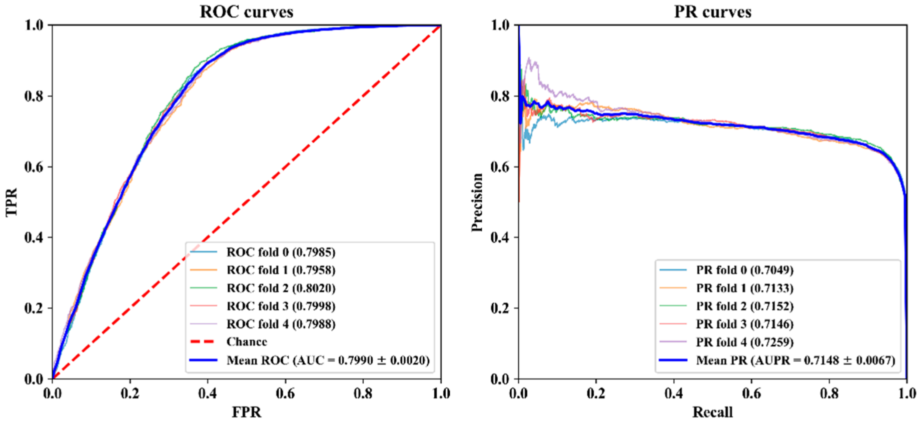


**(c)** AUROC and AUPR curve of context information-BiLSTM.

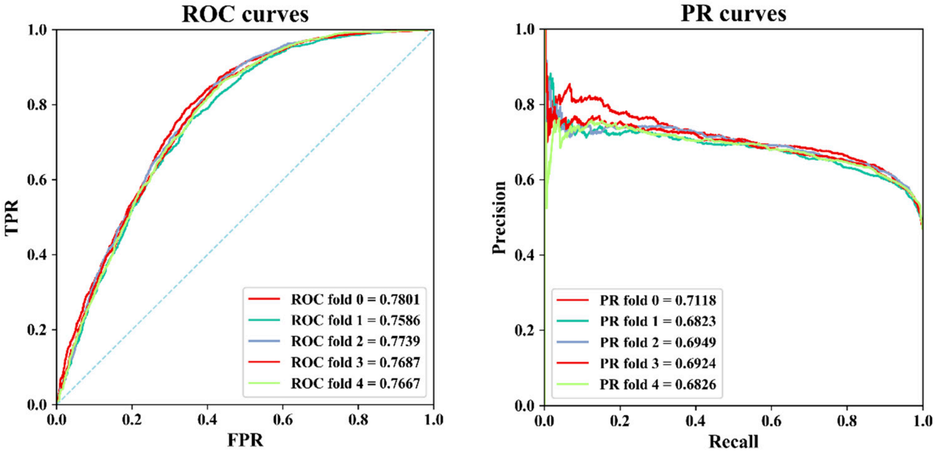
**Figure S1.** Cross-validation results of DL classifiers with three feature descriptors on the Homo.sapiens dataset.



**(a)** AUROC and AUPR curve of sequence information-CNN+BiLSTM.

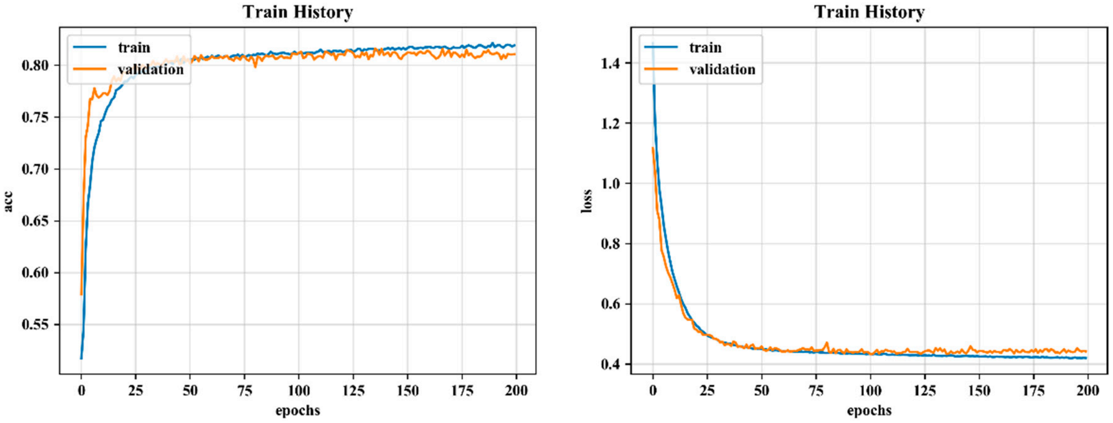


**(b)** AUROC and AUPR curve of physicochemical information-CNN+BiLSTM.

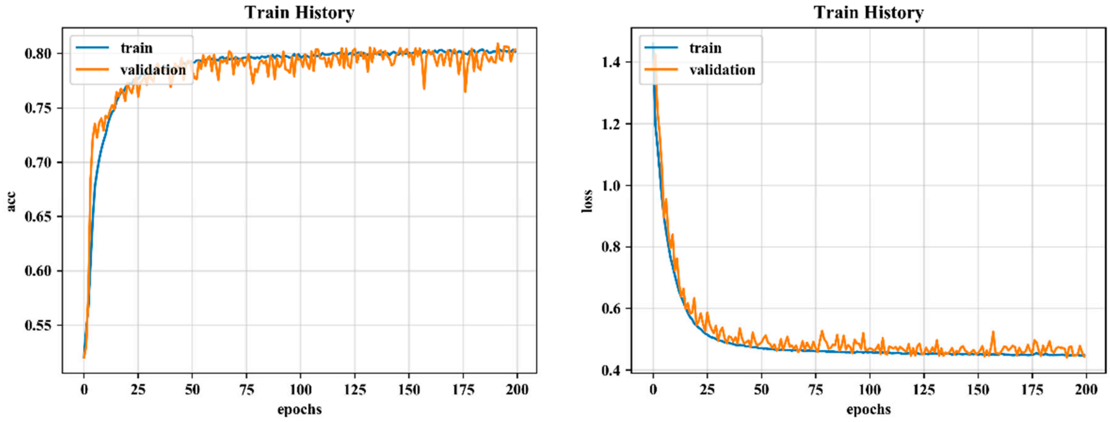


**(c)** AUROC and AUPR curve of context information-BiLSTM.

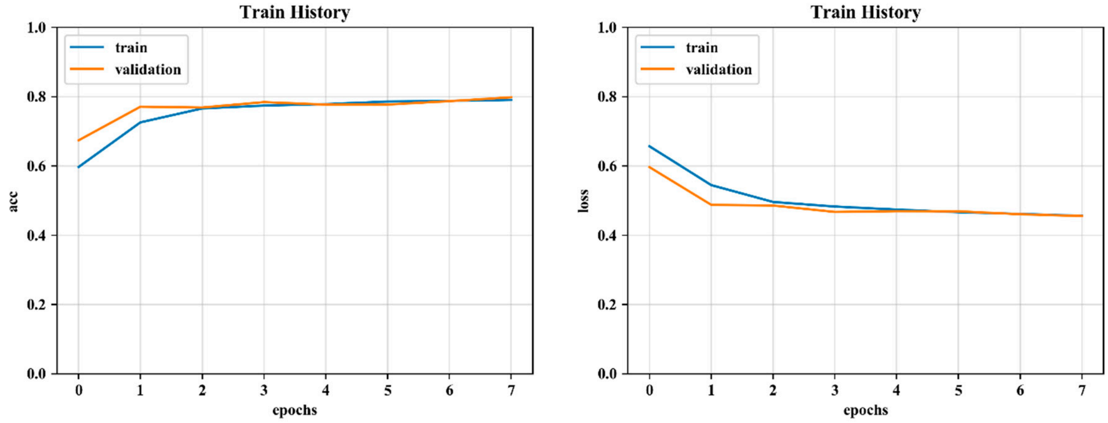
**Figure S2.** Cross-validation results of DL classifiers with three feature descriptors on the Mus.culus dataset.



**(a)** Accuracy and loss curve of sequence information-CNN+BiLSTM.

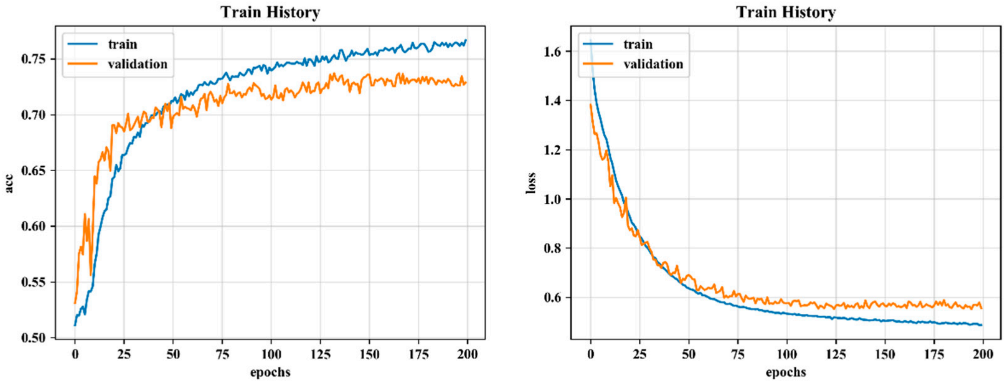


**(b)** Accuracy and loss curve of physicochemical information-CNN+BiLSTM.

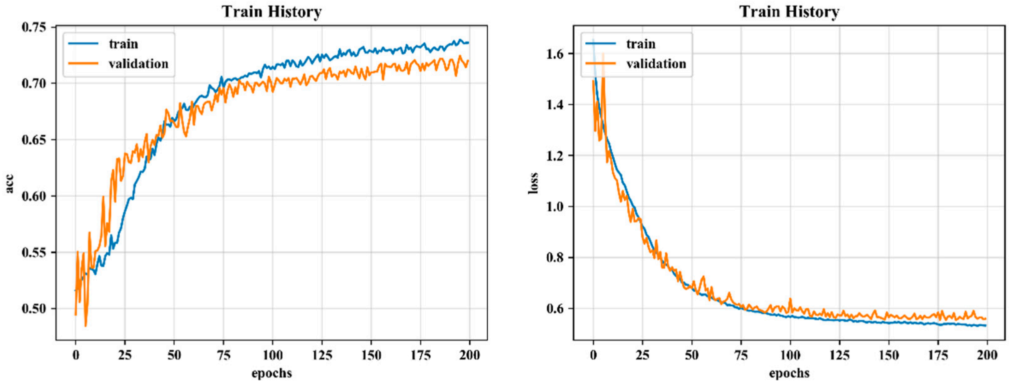


**(c)** Accuracy and loss curve of context information-BiLSTM.

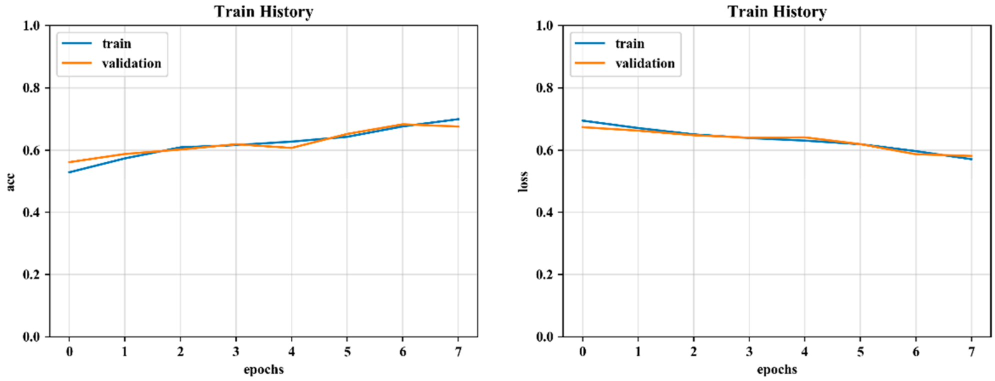
**Figure S3.** Accuracy and loss of the feature1-3 on the Homo.sapiens dataset during training.



**(a)** Accuracy and loss curve of sequence information-CNN+BiLSTM.



**(b)** Accuracy and loss curve of physicochemical information-CNN+BiLSTM.



**(c)** Accuracy and loss curve of context information-BiLSTM.

**Figure S4.** Accuracy and loss of the feature1-3 on the Mus.culus dataset during training.