**Table H1 The RNA-Ligand binding information of test sets**

|  |  |  |
| --- | --- | --- |
| **Test sets** | **PDBID** | **Ligand** |
| **Test18** | 1ddy | B12,NME |
| 1f1t | ROS |
| 1fmn | FMN |
| 1nem | BDR,BDG,NEB,IDG |
| 1q8n | MGR |
| **Test18** | 2juk | G0B |
| 2mis | MG |
| 2pwt | LHA |
| 2tob | TOA,2TB,TOC |
| 4f8u | SIS |
| 4pqv | MG |
| 4yaz | 4BW,MG |
| 5bjo | MG,747 |
| 5v3f | 74G |
| 6ez0 | U37 |
| 364d | MG |
| 379d | CO |
| 430d | MG |
| **Test3** | 1y26 | ADE,MG |
| 3d2x | D2X,MG |
| 3gx2 | SFG,MG |
| **CL1** | 4tzx | ADE,MG |
| 4xnr | ADE,MG |
| 5swe | ADE |
| **CL2** | 1j7t | PAR |
| 1mwl | GET |
| 2be0 | JS5 |
| 2et3 | LLL |
| 2et4 | NMY |
| **CL3** | 1uts | P13 |
| 1uud | P14 |
| 2l8h | R, L8H |
| 1uui | P12 |
| 1arj | ARG |

**Table H2. Performance of MultiModRLBP with differentlearning rate and dropout on Test18 and Test3 set.**

|  |  |  |  |
| --- | --- | --- | --- |
| **learning rate** | **dropout** | **Test18-AUC** | **Test3-AUC** |
| **0.001** | **0.1** | **0.781** | **0.843** |
| **0.001** | **0.2** | **0.753** | **0.831** |
| **0.03** | **0.1** | **0.72** | **0.82** |
| **0.005** | **0.1** | **0.737** | **0.935** |

**Table H3. The hyperparameter configuration of MultiModRLBP**

|  |  |  |
| --- | --- | --- |
| **Neural network component** | **Hyperparameters** | **Value of hyperparameter** |
| **RGCN Module** | **Number of RGCN layers in RGCN Module** | **3** |
| **Number of neurons for the dense layers** | **192** |
| **Activation function of the dense layers** | **ReLU** |
| **RNABert Module** | **Maximum sequence embedding length** | **440** |
| **Number of Transformer blocks** | **6** |
| **Activation function of the dense layers** | **GELU** |
| **Number of neurons for the laste dense layer** | **120** |
| **ELBFS Module** | **Convolutional kernel size of the CNN layer** | **17×71** |
| **Sliding window size** | **11** |
| **Activation function of CNN layer** | **ReLU** |
| **MFFusion Module** | **Number of dense layers** | **3** |
| **Number of neurons for the first dense layer** | **192** |
| **Activation function of the first dense layer** | **ReLU** |
| **Number of neurons for the second dense layer** | **96** |
| **Activation function of the second dense layer** | **ReLU** |
| **Number of neurons for the third dense layer** | **1** |
| **Activation function of the third dense layer** | **Sigmod** |
| **Overall architecture** | **Loss function** | **Binary Cross-Entropy Loss** |
| **Neural network component** | **Hyperparameters** | **Value of hyperparameter** |
| **Overall architecture** | **Optimizer** | **Adam** |
| **Adam learning rate** | **0.001** |
| **Adam decay** | **0** |
| **Adam bata\_1** | **0.9** |
| **Adam bata\_2** | **0.999** |
| **Dropout rate** | **0.1** |
| **Batch size** | **5** |
| **Epochs** | **80** |

**Table H4 Performance of RLBind with different local window sizes on Test18 set.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sizes of local windows (nts)** | **Precision** | **Recall** | **MCC** | **AUC** |
| **7** | **0.568** | **0.389** | **0.296** | **0.733** |
| **9** | **0.769** | **0.435** | **0.326** | **0.742** |
| **11** | **0.644** | **0.523** | **0.378** | **0.78** |
| **13** | **0.56** | **0.461** | **0.323** | **0.738** |
| **15** | **0.585** | **0.417** | **0.323** | **0.715** |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **convolution kernel sizes** | **Precision** | **Recall** | **MCC** | **AUC** |
| **13×71** | **0.678** | **0.351** | **0.315** | **0.722** |
| **17×71** | **0.644** | **0.523** | **0.378** | **0.78** |
| **21×71** | **0.648** | **0.473** | **0.356** | **0.768** |

**Table H5 Performance of MultiModRLBP with different convolution kernel sizes on Test18 set .**