In this section, we list the values of each module hyper parameter during the training and prediction process of the model. The details are shown in Table 1.

|  |  |  |
| --- | --- | --- |
| **Position Hyper parameters Values** | | |
| Train model | seed | 2024 |
| Learning Rate | 1.2e-4 |
| Batch Size | 5 |
| Epoch | 90 |
| Weight\_decay | 1e-6 |
| Optimizer | Adam W |
| T\_max | 45 |
| Eta\_min | 1e-6 |
| Dropout | 0.1 |
| Predict-CASF-2016 | Batch Size | 36 |
| Predict-CASF-2013 | Batch Size | 42 |
| MSIC | Graph node feature size | 120 |
| Activation function | ReLU，PReLU |
| Dilation rate | 1,2,4,8,16 |
| Lig Update | Graph node feature size | 120 |
| Activation function | ReLU |
| Dilated GCN | Graph node feature size | 120 |
| Graph edge feature size | 0 |
| Attention heads | 4 |
| Dilation rate | 1,2,4,8,16 |
| Activation function | PReLU,LeakyReLU, Tanh, Sigmoid |
| Hidden node size | 120 |
| Recall | 2 |
| Adaptive GCN | Graph node feature size | 120 |
| Graph edge feature size | 8 |
| Attention heads | 4 |
| Activation function | PReLU,LeakyReLU, Tanh, Sigmoid |
| Hidden node size | 120 |
| Hidden edge size | 4 |
| Recall | 2 |
| GCN | Distance cutoff | 8 Å |
| Graph node feature size | 120 |
| Graph edge feature size | 8 |
| Activation function | ReLU |
| times | 3 |
| Recall | 3 |

**Table 1** Hyper parameter settings.