**Table S1** - Hyper-parameters of NPI-RGCNAE

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Dataseta | Dropout ratio | Initial learning rate | Weight decay | *step\_size* | *γ* | Epochs |
| RPI2241 | 0.1 | 0.0007 | 0.001 | 50 | 0.7 | 25 |
| RPI2241\_random | 0.1 | 0.0007 | 0.001 | 50 | 0.7 | 25 |
| RPI2241\_sort\_random | 0.1 | 0.0007 | 0.001 | 50 | 0.7 | 25 |
| RPI369 | 0.3 | 0.0007 | 0.001 | 50 | 0.7 | 50 |
| RPI369\_random | 0.8 | 0.0007 | 0.07 | 50 | 0.7 | 50 |
| RPI369\_sort\_random | 0.3 | 0.0007 | 0.001 | 50 | 0.7 | 50 |
| NPInter10412 | 0.1 | 0.001 | 0.001 | 10 | 0.7 | 30 |
| NPInter10412\_random | 0.1 | 0.001 | 0.001 | 10 | 0.7 | 30 |
| NPInter10412\_sort\_random | 0.1 | 0.001 | 0.001 | 10 | 0.7 | 30 |
| NPInter10412\_20% | 0.1 | 0.0007 | 0.001 | 50 | 0.7 | 25 |
| NPInter10412\_40% | 0.1 | 0.001 | 0.001 | 20 | 0.7 | 50 |
| NPInter10412\_60% | 0.1 | 0.003 | 0.001 | 30 | 0.7 | 50 |
| NPInter10412\_80% | 0.1 | 0.003 | 0.001 | 30 | 0.7 | 50 |
| RPI7317 | 0.1 | 0.003 | 0.001 | 30 | 0.7 | 50 |
| RPI7317\_random | 0.1 | 0.003 | 0.001 | 30 | 0.7 | 50 |
| RPI7317\_sort\_random | 0.1 | 0.003 | 0.001 | 30 | 0.7 | 50 |
| NPInter4158 | 0.1 | 0.001 | 0.001 | 20 | 0.7 | 50 |

aNPInter10412\_20%, NPInter10412\_40%, NPInter10412\_60%, and NPInter10412\_80% were randomly selected from the NPInter10412 with 20%, 40%, 60%, and 80% ratio. "random" means negative samples of the dataset were generated by the "random" strategy. "sort\_random" means negative samples of the dataset were generated by the "sort\_random" strategy.