

1). FreeSolv Dataset without path info:

num_layers: 3
small_hidden_dim: 142
num_heads: 9
dropout: 0.7347780293219217
weight_decay: 1.538290349900921e-18
batch_size: 2
lr: 3.7798891539041065e-05

2). FreeSolv Dataset with path info:

num_layers: 2
small_hidden_dim: 140
num_heads: 4
dropout: 0.4356401455970282
weight_decay: 0.0020369910681372685
batch_size: 9
lr: 5.4525151321520415e-05

3). ESOL Dataset without path info:

num_layers: 9
small_hidden_dim: 86
num_heads: 6
dropout: 0.15
weight_decay: 1.7486694373393174e-11
batch_size: 6
lr: 3.67247780674997e-05

3). ESOL Dataset with path info:

num_layers: 4
small_hidden_dim: 21
num_heads: 3
dropout: 0.04280483931026283
weight_decay: 0.00047149322701399004
batch_size: 3
lr: 0.00010030295499602398

5). Lipophilicity Dataset without path info:

num_layers: 1
small_hidden_dim: 167
num_heads: 10
dropout: 0.04053446947021075
weight_decay: 3.0532103567123417e-13
batch_size: 5
lr: 2.6119467092453507e-05

6). Lipophilicity Dataset with path info:

num_layers: 7
small_hidden_dim: 167
num_heads: 1
dropout: 0.0983753446086437
weight_decay: 4.086333403457301e-16
batch_size: 5
lr: 2.320541170954431e-05

7). BACE Dataset without path info:

num_layers: 6
small_hidden_dim: 47
num_heads: 3
dropout: 0.2113253945447924
weight_decay: 5.878135321726393e-12
batch_size: 3
lr: 0.0002572167798956838

8). BACE Dataset with path info:

num_layers: 5
small_hidden_dim: 141
num_heads: 2
dropout: 0.5047442534364175
weight_decay: 4.437430281721926e-11
batch_size: 7
lr: 2.8817004790329112e-05

9). BBBP Dataset without path info:

num_layers: 1
small_hidden_dim: 164
num_heads: 10
dropout: 0.10699971329382979
weight_decay: 2.8469965951126606e-14
batch_size: 2
lr: 1.7971752346298526e-05

10). BBBP Dataset with path info:

num_layers: 2
small_hidden_dim: 189
num_heads: 7
dropout: 0.7524706667718167
weight_decay: 9.298688358703593e-07
batch_size: 9
lr: 2.504908345987365e-05

11). ClinTox Dataset without path info:

num_layers: 4
small_hidden_dim: 123
num_heads: 2
dropout: 0.28912089505267613
weight_decay: 8.715810725319943e-16
batch_size: 6
lr: 6.123782868507217e-05

12). ClinTox Dataset with path info:

num_layers: 6
small_hidden_dim: 83
num_heads: 8
dropout: 0.7504659636545525
weight_decay: 1.2957637942443332e-08
batch_size: 9
lr: 2.167848298279678e-05

13) Example Usage:

```
python train_graphormer.py --use_gpu 1 --dataset ClinTox /  
--repetition 1 --epochs 200 /  
--use_path_info 1 --add_noise 1 --noise_factor 0.1 /  
--num_layers 6 --small_hidden_dim 83 --num_heads 8 /  
--dropout 0.75 --weight_decay 1.2957637942443332e-08 --batch-size 9  
/  
--lr 2.1678482982796e-05 --dir_to_save_model  
/path/to/graphormer_models
```