

1). FreeSolv Dataset without path info:

num\_layers: 1  
small\_hidden\_dim: 161  
dropout: 0.4168274325534108  
weight\_decay: 1.635806233409211e-10  
batch\_size: 4  
lr: 0.05900224481337009

2). FreeSolv Dataset with path info:

num\_layers: 1  
small\_hidden\_dim: 12  
max\_pow: 2  
dropout: 0.14449349878813347  
weight\_decay: 1.386048955624208e-11  
batch\_size: 3  
lr: 0.06246465272211292

3). ESOL Dataset without path info:

num\_layers: 1  
small\_hidden\_dim: 138  
dropout: 0.10740849252745631  
weight\_decay: 5.829522761945421e-07  
batch\_size: 5  
lr: 0.00899803546663418

4). ESOL Dataset with path info:

num\_layers: 2  
small\_hidden\_dim: 59  
max\_pow: 5  
dropout: 0.4428927705250062  
weight\_decay: 6.117308833591867e-17  
batch\_size: 6  
lr: 0.003446531385382952

5). Lipophilicity Dataset without path info:

num\_layers: 2  
small\_hidden\_dim: 93  
dropout: 0.477217941047075  
weight\_decay: 6.236350503288137e-05  
batch\_size: 8  
lr: 0.0006731898598905812

6). Lipophilicity Dataset with path info:

num\_layers: 2  
small\_hidden\_dim: 148  
max\_pow: 4  
dropout: 0.7090744972020606  
weight\_decay: 7.552208510172316e-16  
batch\_size: 9  
lr: 4.4670389174200005e-05

7). BACE Dataset without path info:

num\_layers: 8  
small\_hidden\_dim: 163  
dropout: 0.030429863104662863  
weight\_decay: 4.963667106698153e-19  
batch\_size: 10  
lr: 0.00014261807046744095

8). BACE Dataset with path info:

num\_layers: 7  
small\_hidden\_dim: 137  
max\_pow: 3  
dropout: 0.14579599577455854  
weight\_decay: 1.8976159247030544e-11  
batch\_size: 10  
lr: 2.256250669202958e-05

9). BBBP Dataset without path info:

```
num_layers: 2
small_hidden_dim: 122
dropout: 0.05535406119748653
weight_decay: 1.1527288629473404e-14
batch_size: 6
lr: 0.00041876458799519465
```

10). BBBP Dataset with path info:

```
num_layers: 1
small_hidden_dim: 70
max_pow: 3
dropout: 0.19975030896092166
weight_decay: 2.037326704901844e-15
batch_size: 9
lr: 0.0014197707178220946
```

11). ClinTox Dataset without path info:

```
num_layers: 10
small_hidden_dim: 95
dropout: 0.45924929530332814
weight_decay: 3.9844666148289284e-20
batch_size: 6
lr: 0.04057762972479995
```

12). ClinTox Dataset with path info:

```
num_layers: 9
small_hidden_dim: 164
max_pow: 4
dropout: 0.4778545342903914
weight_decay: 0.003608476532411314
batch_size: 6
lr: 4.199957904366677e-05
```

13). Example Usage:

```
python train_mix_hop.py --use_gpu 1 --dataset ClinTox /
--repetition 3 --epochs 200 /
--use_path_info 1 --add_noise 1 --noise_factor 0.1 /
```

```
--num-layers 9      --small_hidden_dim 164      --max_pow 4 /  
--dropout 0.48 --weight_decay 0.003608476532411314 --batch-size 6 /  
--lr 4.199957904366677e-05 --dir_to_save_model /path/to/mix_hop_models
```