

Table S1. The results for different numbers of neurons and hidden layers in one-to-one models.

Neurons \ Hidden layers	1	2	3	4	5
Model-one2one-pH					
10	0.9848476	0.971357	0.953484798	0.954261901	0.935829253
20	0.9754152	0.9555762	0.9197198	0.9002266	0.92427372
30	0.9820058	0.9617688	0.932304591	0.935559627	0.917999874
40	0.9664938	0.916116	0.8442692	0.963318652	0.913097957
50	0.9672274	0.9626812	0.891620379	0.866483005	0.949478747
Model-one2one-Ammonia					
10	0.611046938	0.80191725	0.9311222	0.951218	0.85933125
20	0.620400529	0.9637746	0.9108704	0.954741	0.915169
30	0.699313069	0.928434	0.9383212	0.9350872	0.9089766
40	0.685227953	0.8634278	0.9701732	0.9324702	0.9722256
50	0.822607278	0.8896118	0.9769406	0.7939088	0.9354836
Model-one2one-Nitrate					
10	0.8201416	0.808759723	0.8686296	0.9213178	0.921094
20	0.8389318	0.772615553	0.8064408	0.9360036	0.809162306
30	0.832612	0.73981197	0.9090174	0.9138644	0.858056418
40	0.9456164	0.789051415	0.9241816	0.9005736	0.828969966
50	0.9144294	0.787557424	0.90253675	0.8246382	0.849695
Model-one2one-Nitrite					
10	0.7943326	0.73439	0.8133944	0.7708438	0.82989125
20	0.8048794	0.8006312	0.8245906	0.7205042	0.7915685
30	0.8716404	0.6908702	0.81118	0.7394598	0.74191575
40	0.7854664	0.8031024	0.8261715	0.8328022	0.7899918
50	0.8363742	0.8390184	0.8546905	0.8128962	0.7962372

Table S2. The results for different numbers of neurons and hidden layers in three-to-three models.

Neurons \ Hidden layers	1	2	3	4	5
Model-three2three-Ammonia					
10	0.8735712	0.9443026	0.8261558	0.8652142	0.858767485
20	0.756514989	0.824957	0.876923	0.8449568	0.9375296
30	0.651539141	0.9525096	0.893859804	0.9304564	0.960905
40	0.5853024	0.9543996	0.9411882	0.8780854	0.9027912
50	0.574231774	0.9164828	0.9379708	0.9166182	0.876281732
Model-three2three-Nitrate					
10	0.929497	0.877113	0.811462333	0.80537825	0.8248664
20	0.9384	0.8430188	0.903493	0.8921334	0.8954212
30	0.9152188	0.912306	0.8893176	0.9111682	0.84579975
40	0.9332484	0.9213568	0.8835972	0.8877516	0.8950808
50	0.9403308	0.8664396	0.873103	0.9065164	0.883753
Model-three2three-Nitrite					
10	0.9366238	0.8406232	0.8649152	0.8602478	0.8447752
20	0.9053134	0.8626128	0.918536	0.8814656	0.9409446
30	0.848762467	0.8721938	0.903084	0.9130408	0.8746872
40	0.6920218	0.854776	0.9329312	0.8990174	0.9389334
50	0.607016829	0.8457166	0.9111608	0.9386606	0.81479675

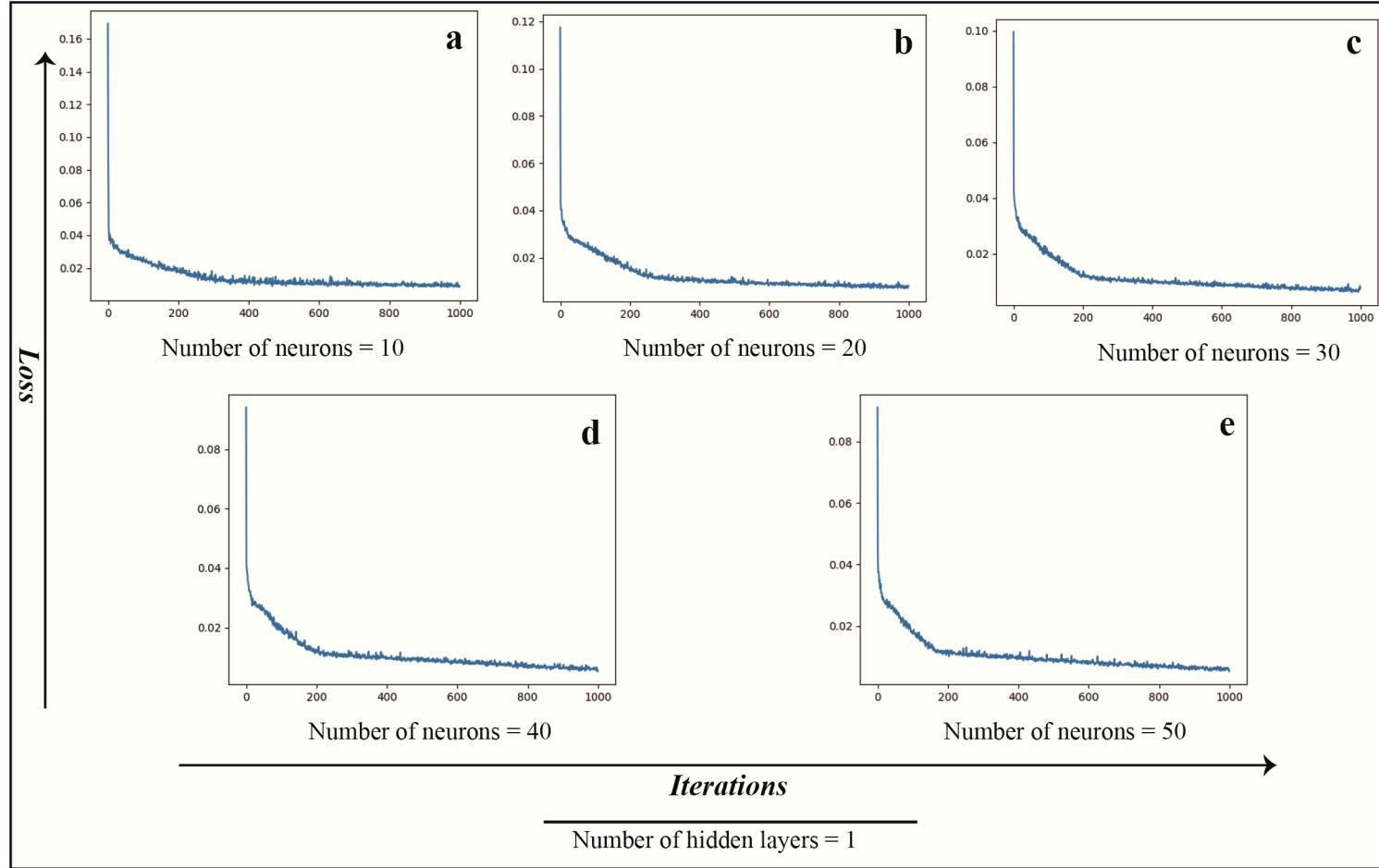


Figure S1 The loss values of different neurons and at single hidden layers for three-to-three models at 1000 iterations.

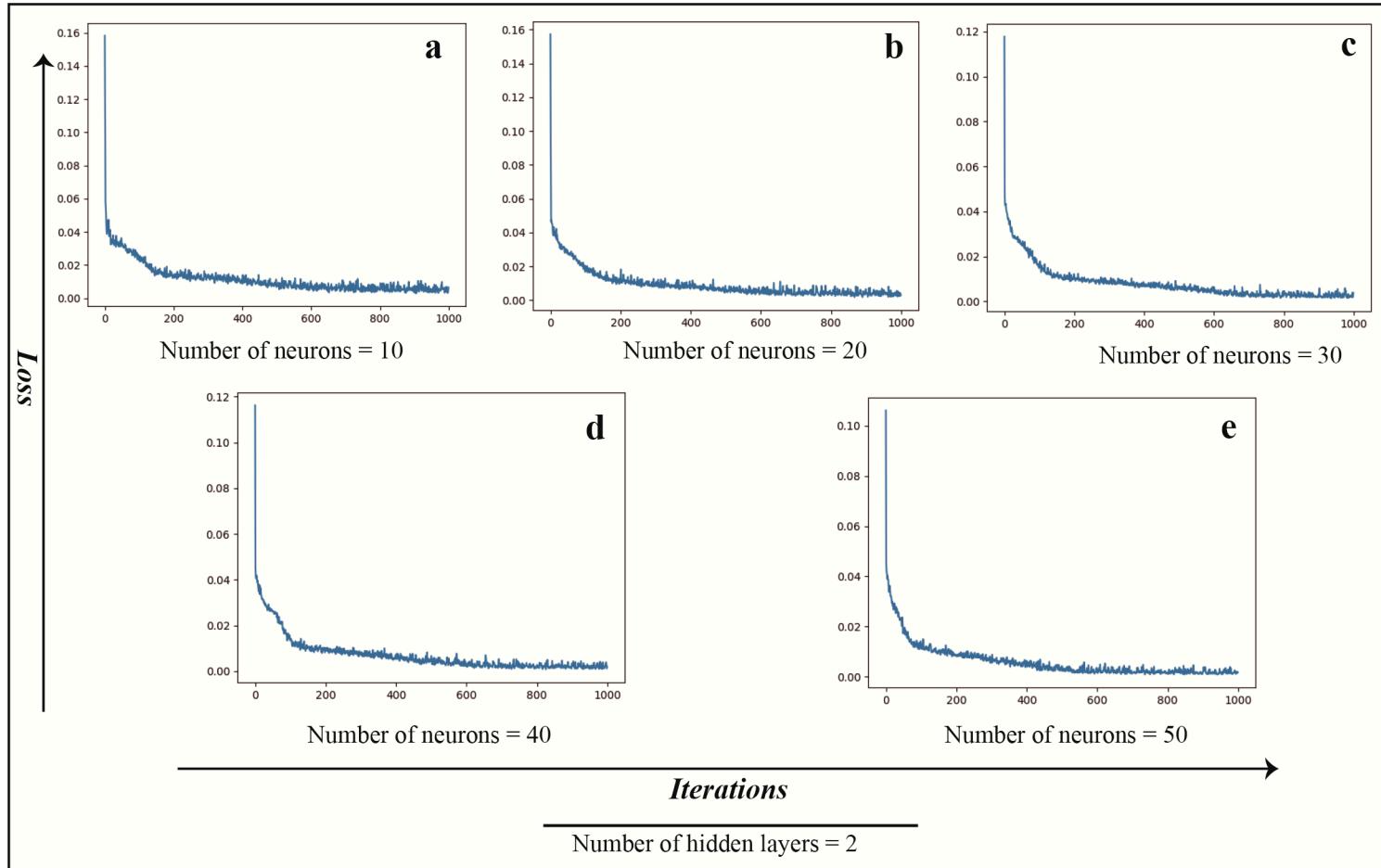


Figure S2 The loss values of different neurons and 2 hidden layers for three-to-three models at 1000 iterations.

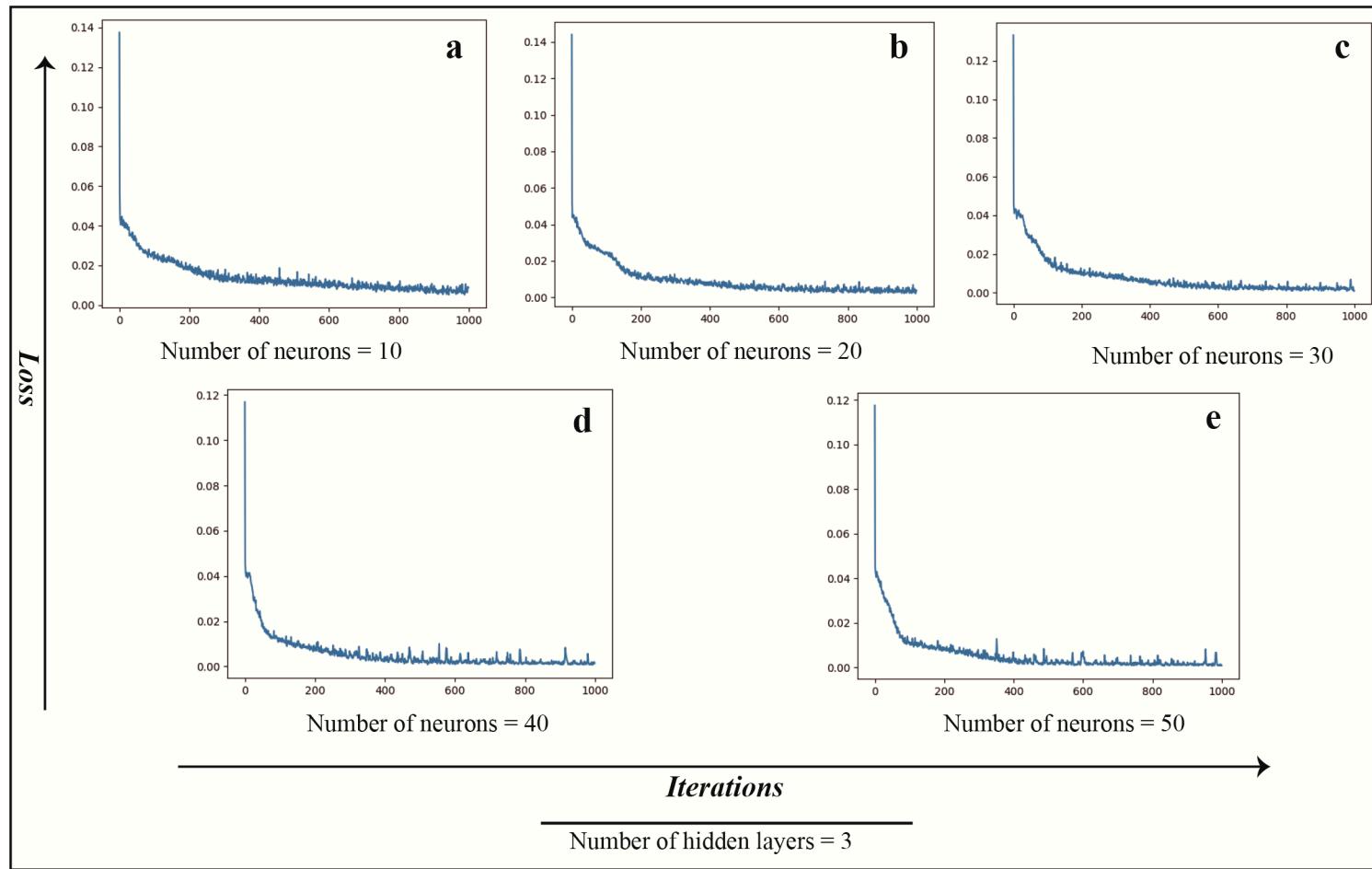


Figure S3 The loss values of different neurons and 3 hidden layers for three-to-three models at 1000 iterations.

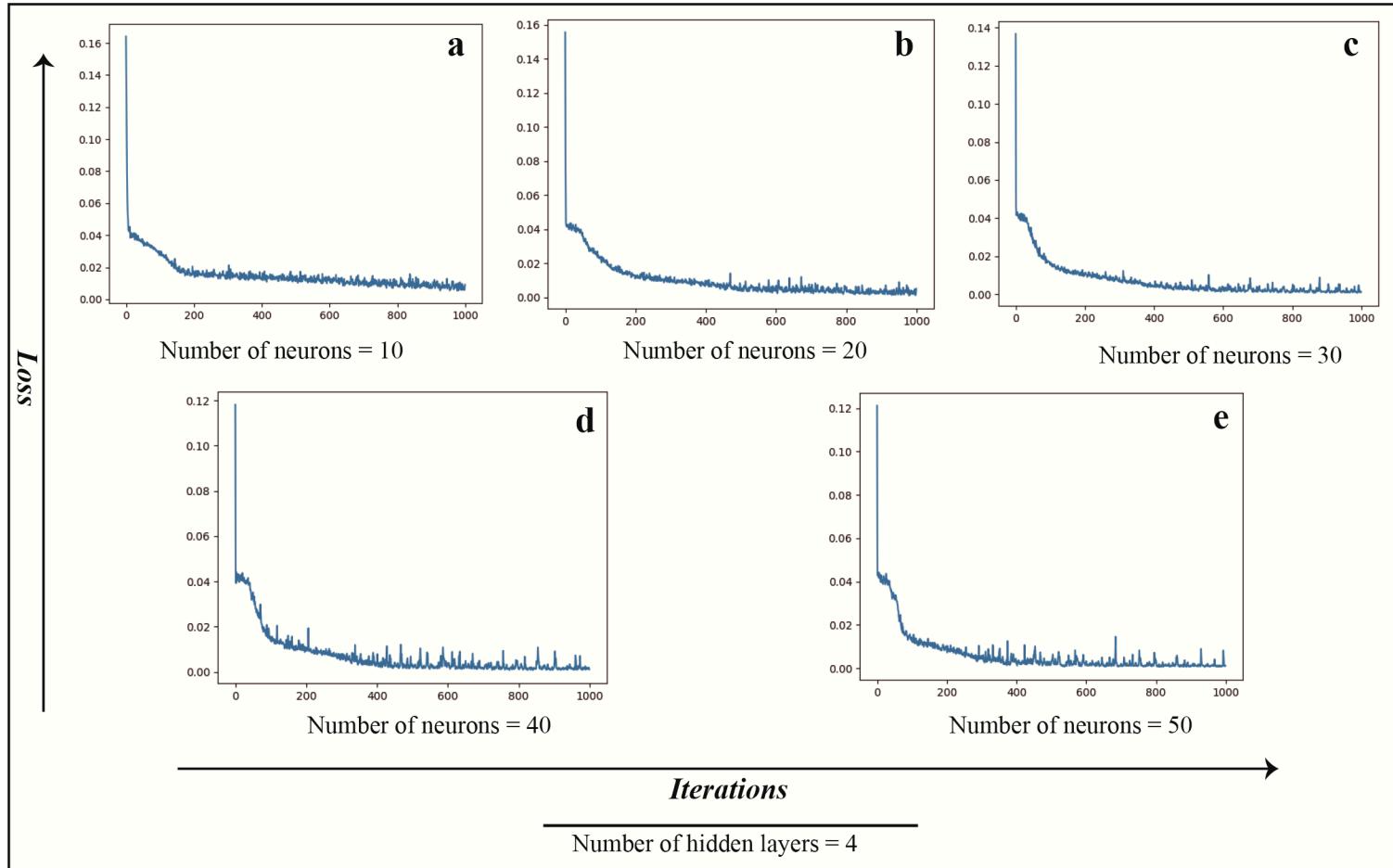


Figure S4 The loss values of different neurons and 4 hidden layers for three-to-three models at 1000 iterations.

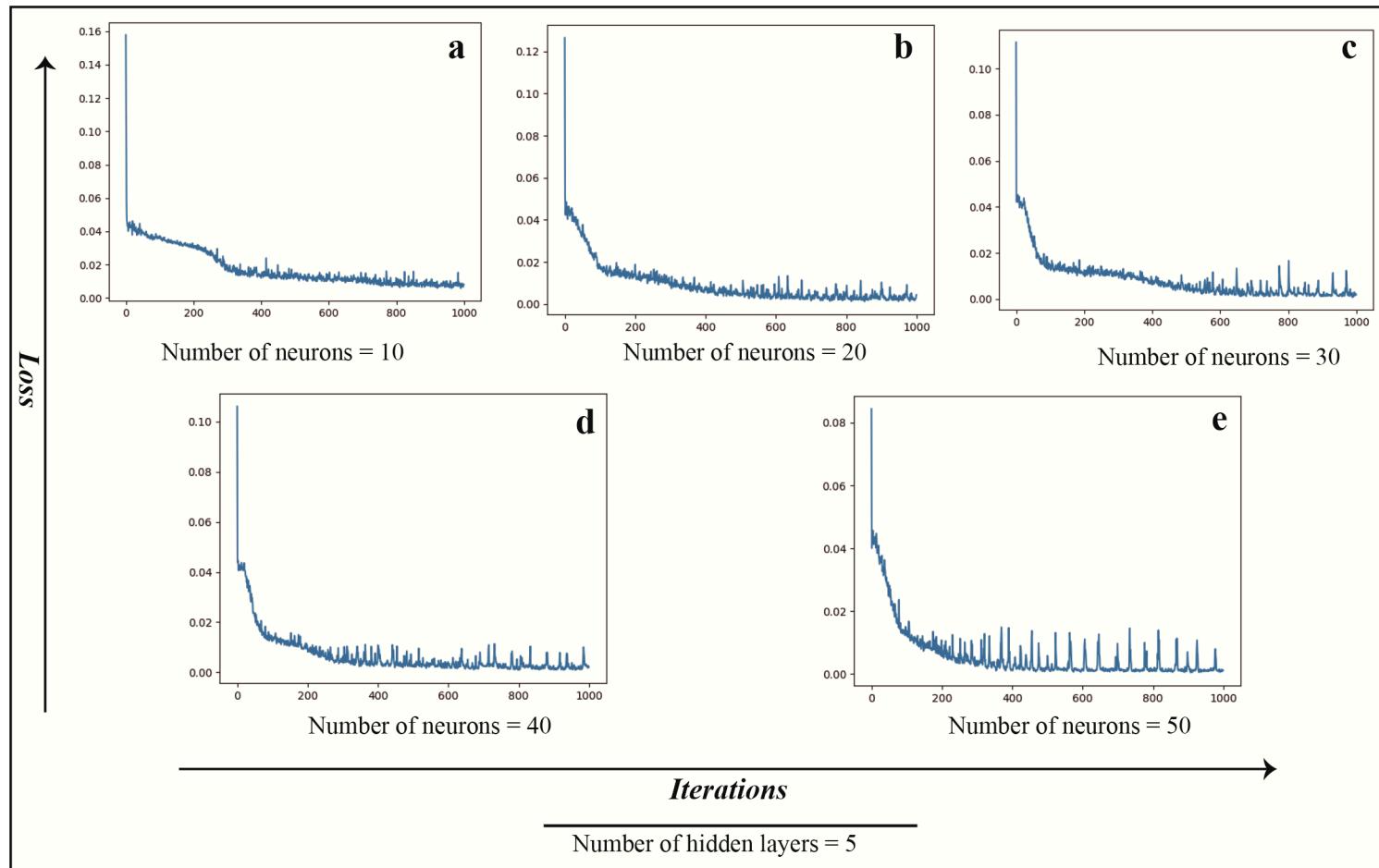


Figure S5 The loss values of different neurons and 5 hidden layers for three-to-three models at 1000 iterations.