

Discrimination of blood species using Raman spectroscopy combined with a recurrent neural network: supplement

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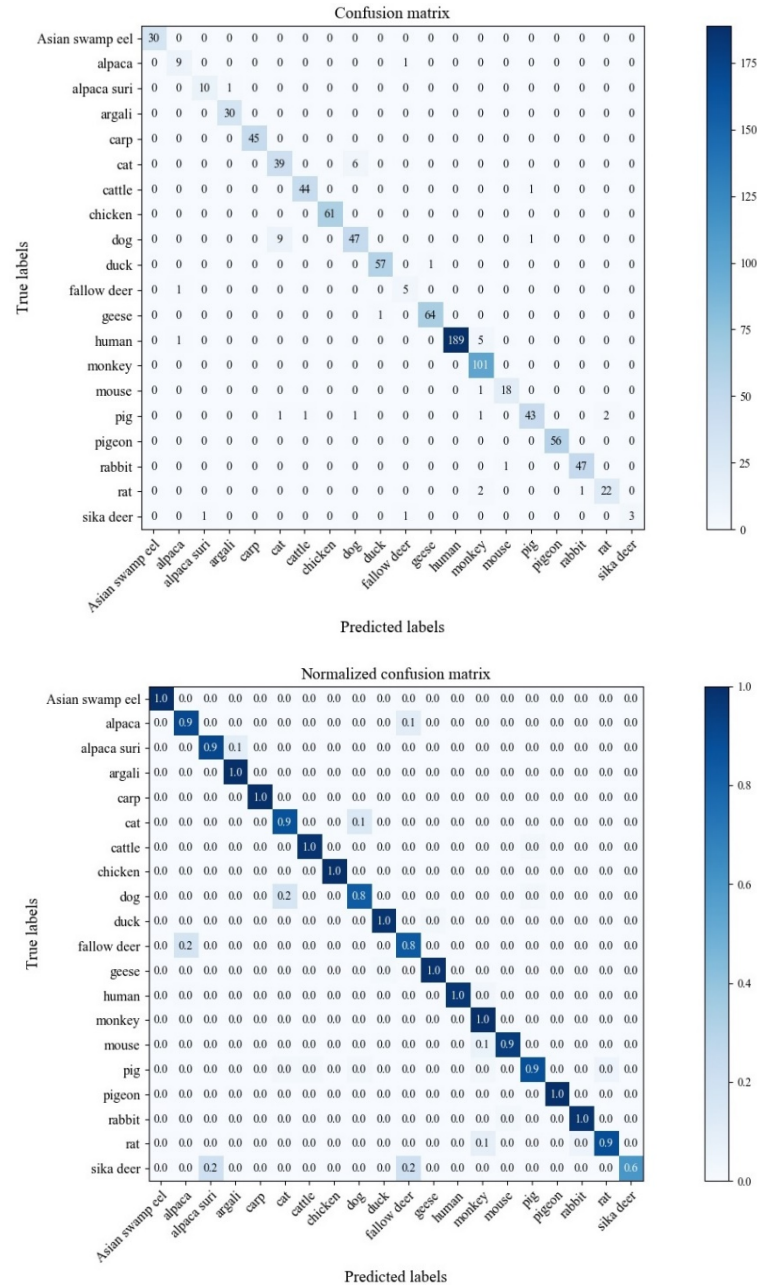


Fig. S1. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using simpleRNN cell.

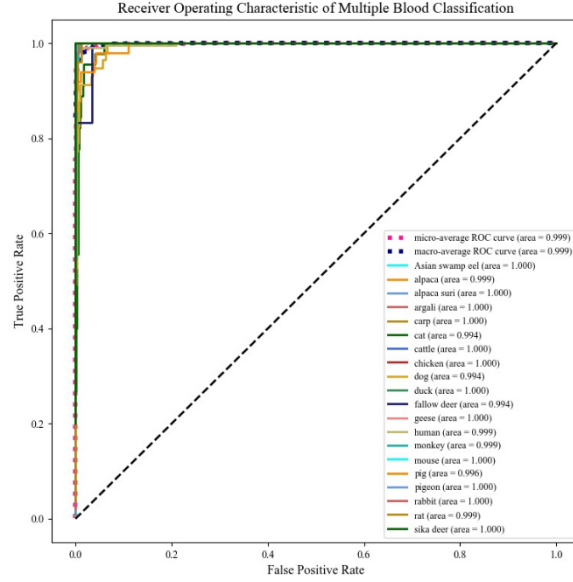


Fig. S2. ROC curve and AUC of multiple blood classification using simpleRNN cell.

Table S1. Classification report of simpleRNN model for blood species identification

	Precision	Recall	F1-score	Support
Asian swamp eel	1.000	1.000	1.000	30
alpaca	0.818	0.900	0.857	10
alpaca suri	0.909	0.909	0.909	11
argali	0.968	1.000	0.984	30
carp	1.000	1.000	1.000	45
cat	0.796	0.867	0.830	45
cattle	0.978	0.978	0.978	45
chicken	1.000	1.000	1.000	61
dog	0.870	0.825	0.847	57
duck	0.983	0.983	0.983	58
fallow deer	0.714	0.833	0.769	6
geese	0.985	0.985	0.985	65
human	1.000	0.969	0.984	195
monkey	0.918	1.000	0.957	101
mouse	0.947	0.947	0.947	19
pig	0.956	0.878	0.915	49
pigeon	1.000	1.000	1.000	56
rabbit	0.979	0.979	0.979	48
rat	0.917	0.880	0.898	25
sika deer	1.000	0.600	0.750	5
Accuracy			0.957	961
Macro avg	0.937	0.927	0.929	961
Weighted avg	0.959	0.957	0.957	961

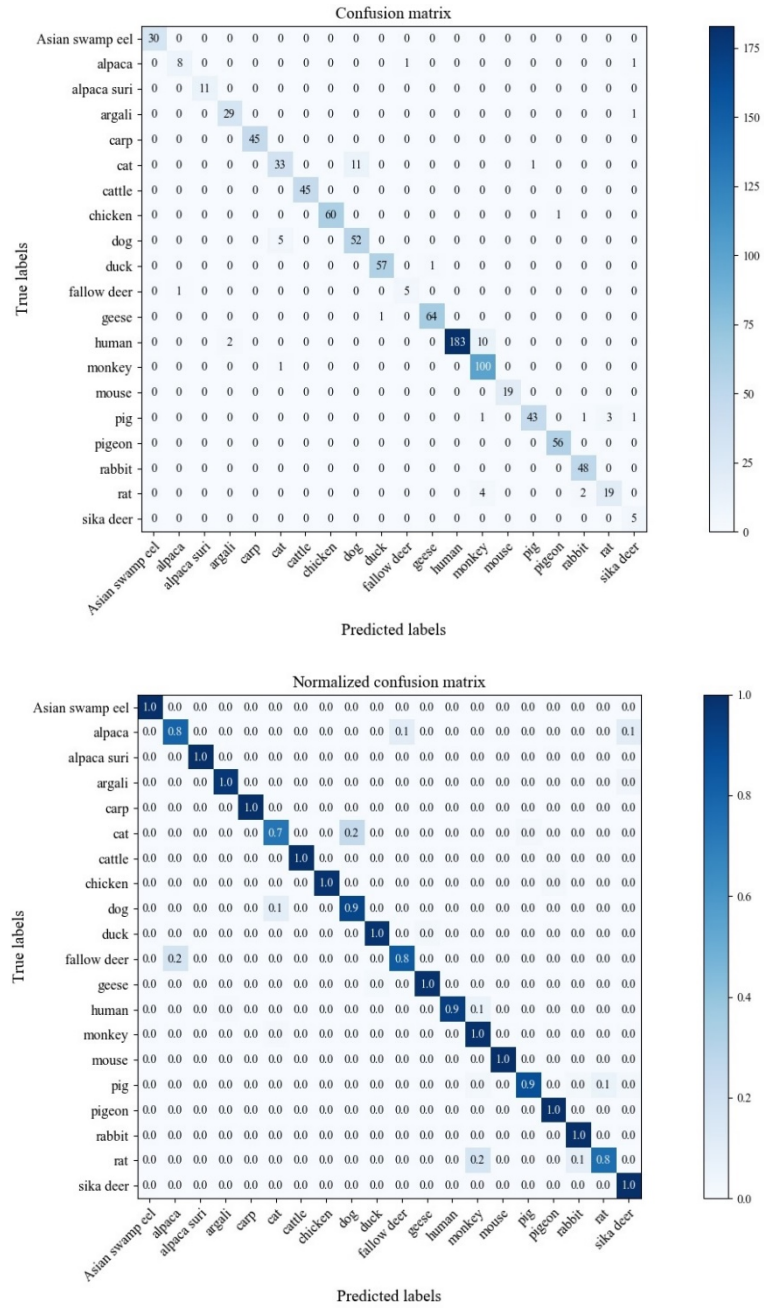


Fig. S3. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using GRU cell.

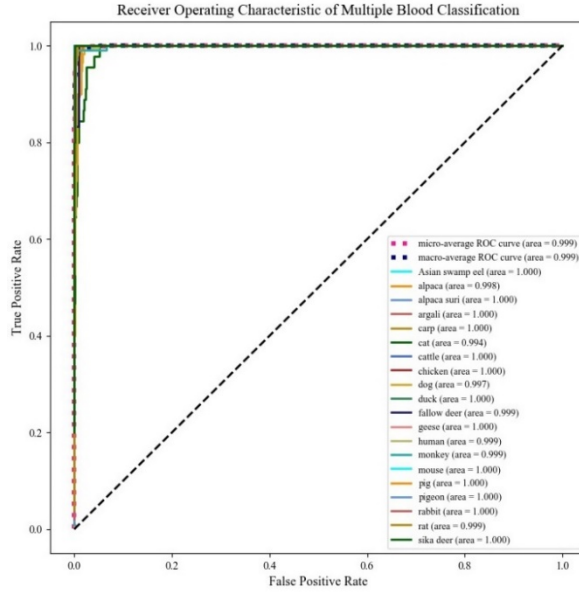


Fig. S4. ROC curve and AUC of multiple blood classification using GRU cell.

Table S2. Classification report of GRU model for blood specie identification

	Precision	Recall	F1-score	Support
Asian swamp eel	1.000	1.000	1.000	30
alpaca	0.889	0.800	0.842	10
alpaca suri	1.000	1.000	1.000	11
argali	0.935	0.967	0.951	30
carp	1.000	1.000	1.000	45
cat	0.846	0.733	0.786	45
cattle	1.000	1.000	1.000	45
chicken	1.000	0.984	0.992	61
dog	0.825	0.912	0.867	57
duck	0.983	0.983	0.983	58
fallow deer	0.833	0.833	0.833	6
geese	0.985	0.985	0.985	65
human	1.000	0.938	0.968	195
monkey	0.870	0.990	0.926	101
mouse	1.000	1.000	1.000	19
pig	0.977	0.878	0.925	49
pigeon	0.982	1.000	0.991	56
rabbit	0.941	1.000	0.970	48
rat	0.864	0.760	0.809	25
sika deer	0.625	1.000	0.769	5
Accuracy			0.949	961
Macro avg	0.928	0.938	0.930	961
Weighted avg	0.952	0.949	0.949	961

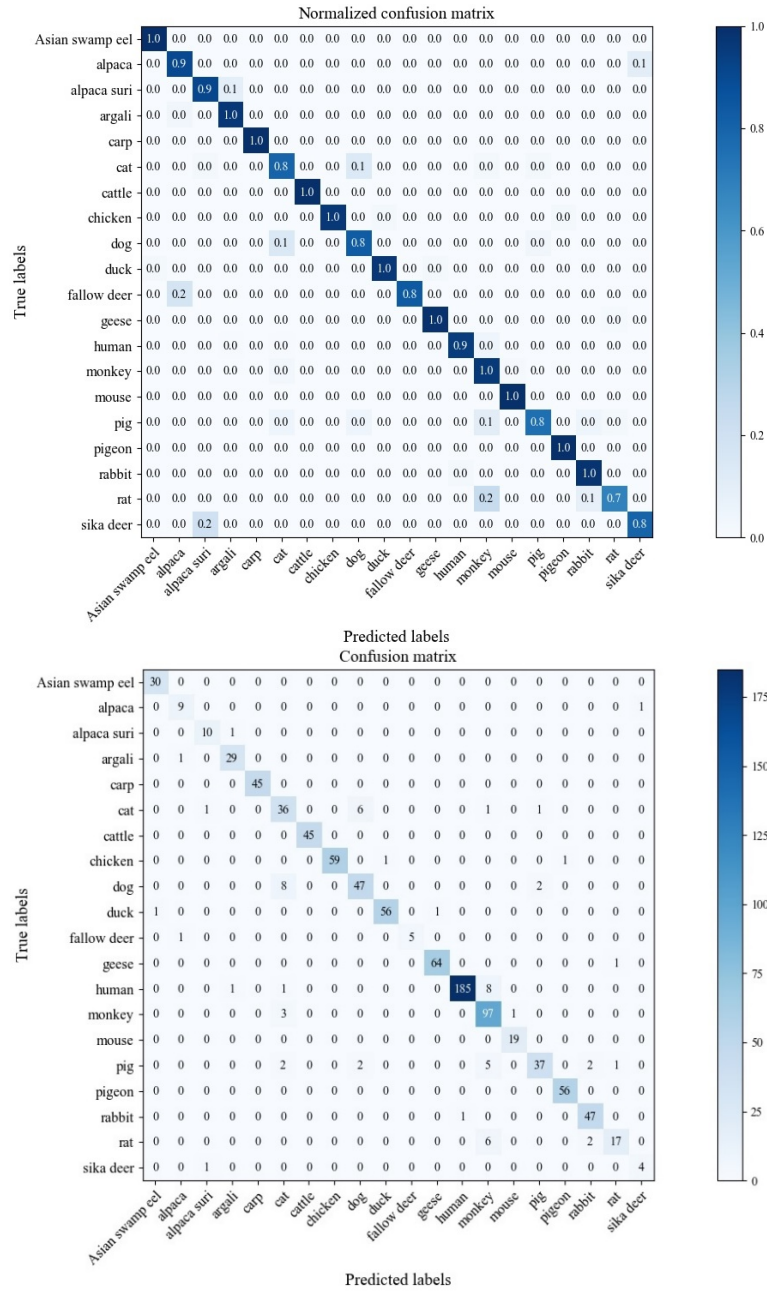


Fig. S5. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using LSTM cell.

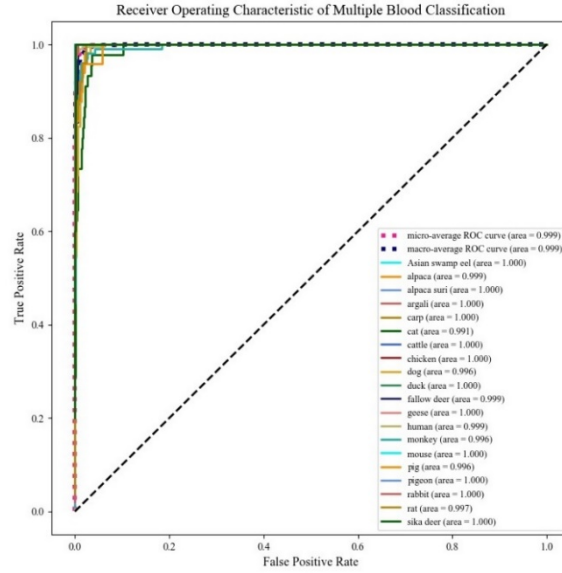


Fig. S6. ROC curve and AUC of multiple blood classification using LSTM cell.

Table S3. Classification report of LSTM model for blood specie identification

	Precision	Recall	F1-score	Support
Asian swamp eel	0.968	1.000	0.984	30
alpaca	0.818	0.900	0.857	10
alpaca suri	0.833	0.909	0.870	11
argali	0.935	0.967	0.951	30
carp	1.000	1.000	1.000	45
cat	0.720	0.800	0.758	45
cattle	1.000	1.000	1.000	45
chicken	1.000	0.967	0.983	61
dog	0.855	0.825	0.839	57
duck	0.982	0.966	0.974	58
fallow deer	1.000	0.833	0.909	6
geese	0.985	0.985	0.985	65
human	0.995	0.949	0.971	195
monkey	0.829	0.960	0.890	101
mouse	0.950	1.000	0.974	19
pig	0.925	0.755	0.831	49
pigeon	0.982	1.000	0.991	56
rabbit	0.922	0.979	0.949	48
rat	0.895	0.680	0.773	25
sika deer	0.800	0.800	0.800	5
Accuracy			0.933	961
Macro avg	0.920	0.914	0.914	961
Weighted avg	0.937	0.933	0.933	961

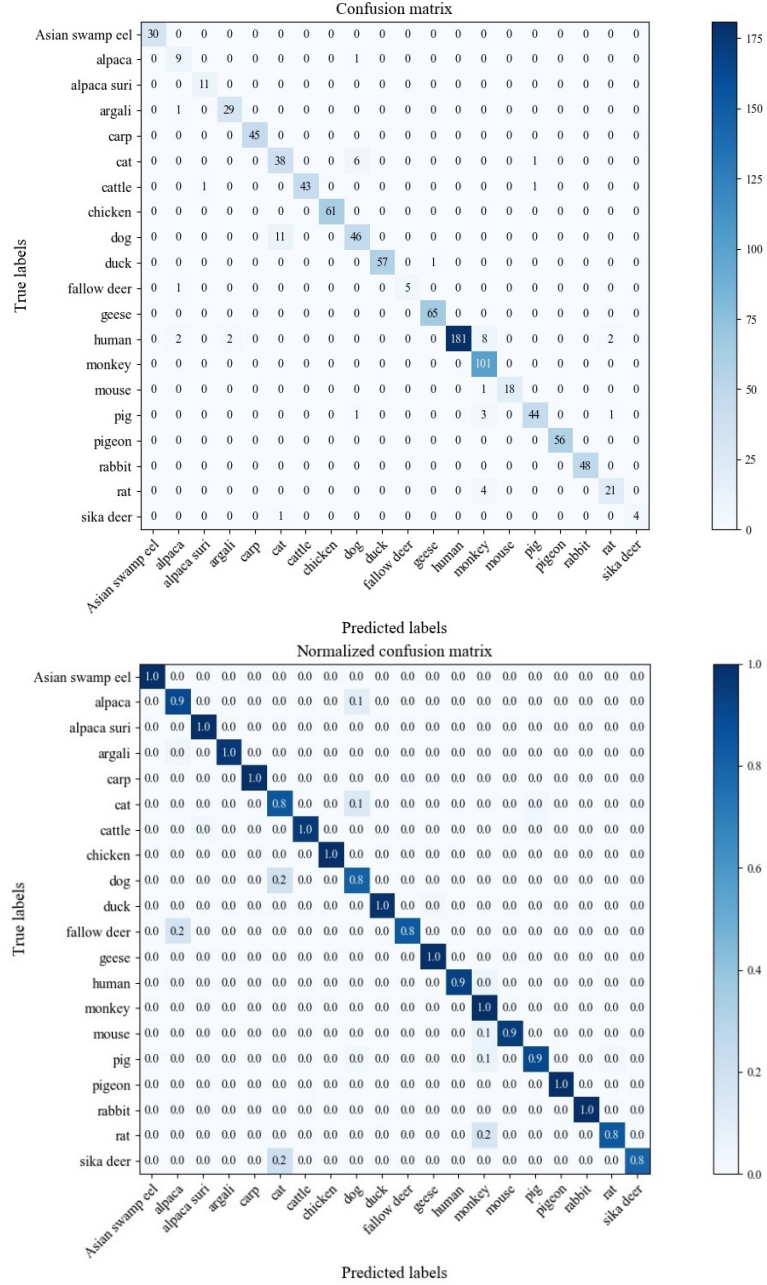


Fig. S7. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using bidirectional simpleRNN.

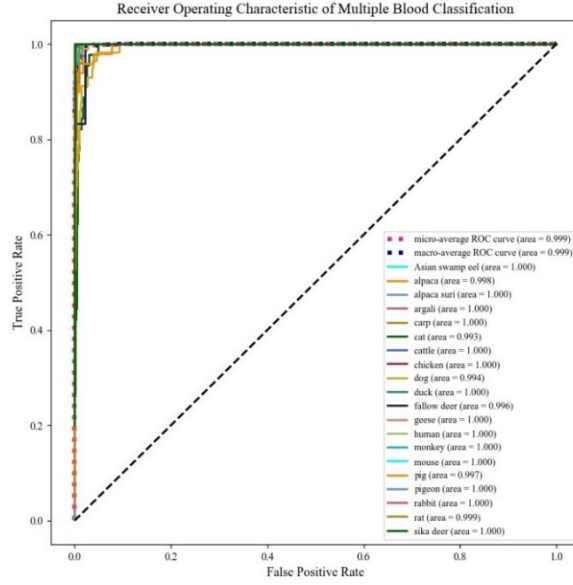


Fig. S8. ROC curve and AUC of multiple blood classification using bidirectional simpleRNN.

Table S4. Classification report of bidirectional SimpleRNN model for blood species identification

	Precision	Recall	F1-score	Support
Asian swamp eel	1.000	1.000	1.000	30
alpaca	0.692	0.900	0.783	10
alpaca suri	0.917	1.000	0.957	11
argali	0.935	0.967	0.951	30
carp	1.000	1.000	1.000	45
cat	0.760	0.844	0.800	45
cattle	1.000	0.956	0.977	45
chicken	1.000	1.000	1.000	61
dog	0.852	0.807	0.829	57
duck	1.000	0.983	0.991	58
fallow deer	1.000	0.833	0.909	6
geese	0.985	1.000	0.992	65
human	1.000	0.928	0.963	195
monkey	0.863	1.000	0.927	101
mouse	1.000	0.947	0.973	19
pig	0.957	0.898	0.926	49
pigeon	1.000	1.000	1.000	56
rabbit	1.000	1.000	1.000	48
rat	0.875	0.840	0.857	25
sika deer	1.000	0.800	0.889	5
Accuracy			0.949	961
Macro avg	0.942	0.935	0.936	961
Weighted avg	0.953	0.949	0.950	961

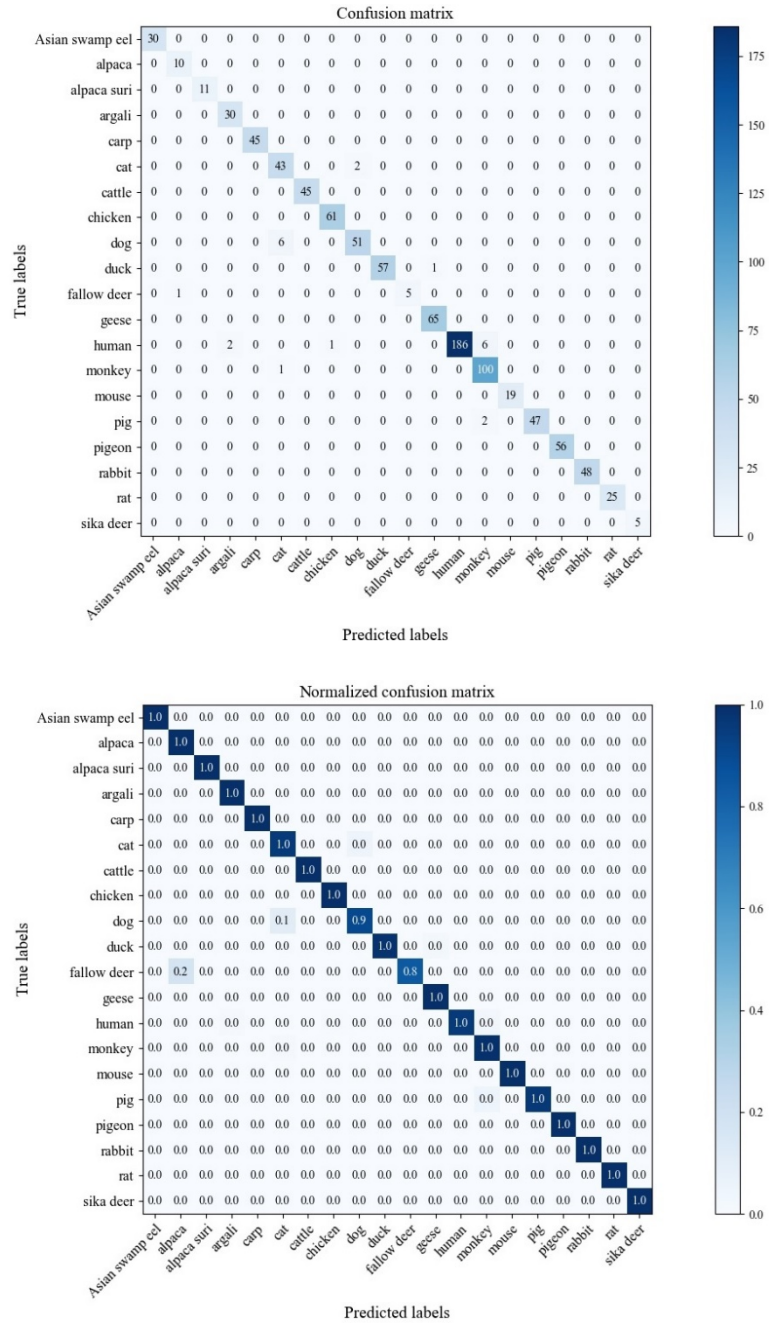


Fig. S9. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using bidirectional GRU.

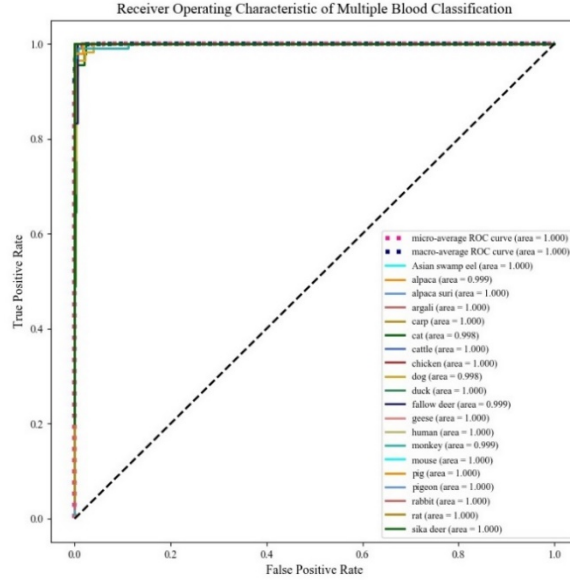


Fig. S10. ROC curve and AUC of multiple blood classification using bidirectional GRU.

Table S5. Classification report of bidirectional GRU model for blood species identification

	Precision	Recall	F1-score	Support
Asian swamp eel	1.000	1.000	1.000	30
alpaca	0.909	1.000	0.952	10
alpaca suri	1.000	1.000	1.000	11
argali	0.938	1.000	0.968	30
carp	1.000	1.000	1.000	45
cat	0.860	0.956	0.905	45
cattle	1.000	1.000	1.000	45
chicken	0.984	1.000	0.992	61
dog	0.962	0.895	0.927	57
duck	1.000	0.983	0.991	58
fallow deer	1.000	0.833	0.909	6
geese	0.985	1.000	0.992	65
human	1.000	0.954	0.976	195
monkey	0.926	0.990	0.957	101
mouse	1.000	1.000	1.000	19
pig	1.000	0.959	0.979	49
pigeon	1.000	1.000	1.000	56
rabbit	1.000	1.000	1.000	48
rat	1.000	1.000	1.000	25
sika deer	1.000	1.000	1.000	5
Accuracy			0.977	961
Macro avg	0.978	0.978	0.977	961
Weighted avg	0.978	0.977	0.977	961

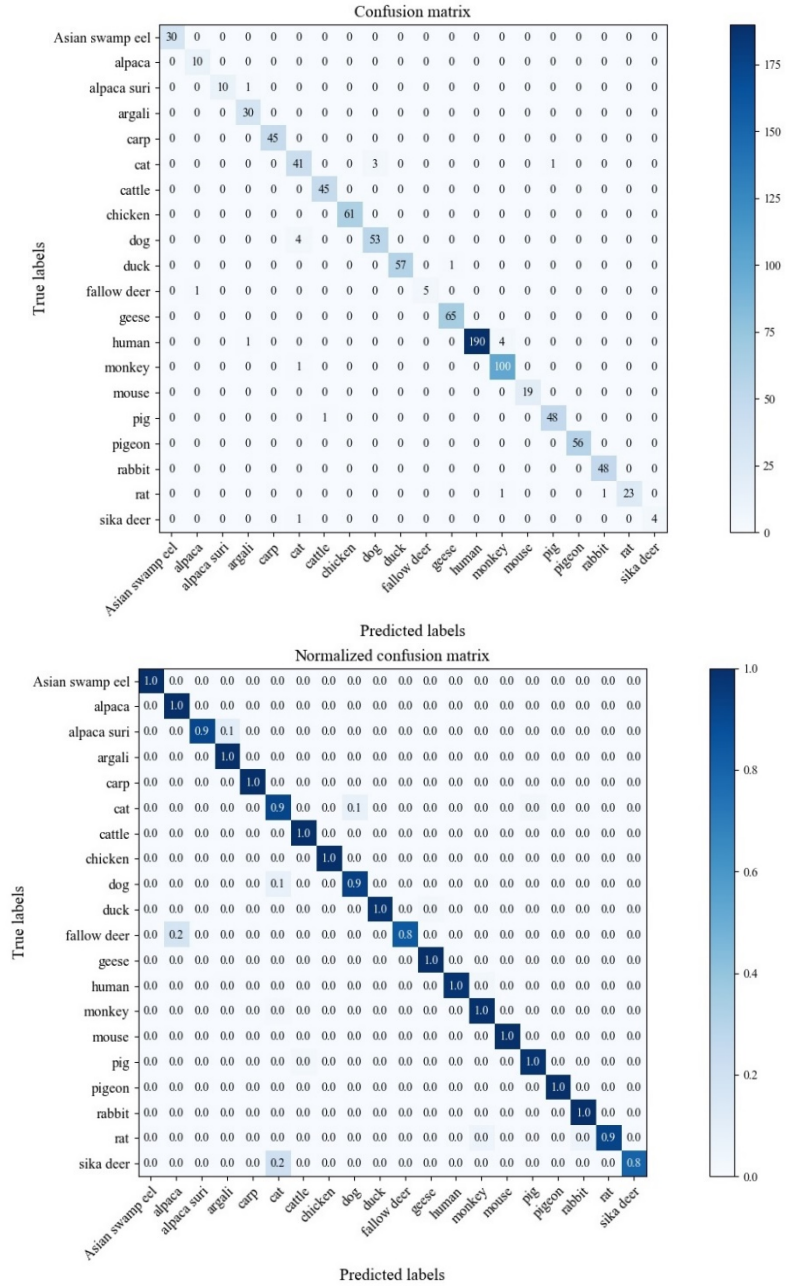


Fig. S11. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using bidirectional LSTM.

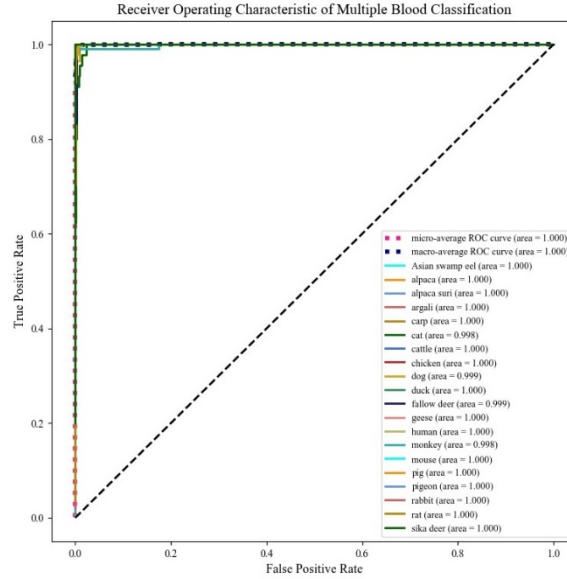


Fig. S12. ROC curve and AUC of multiple blood classification using bidirectional LSTM.

Table S6. Classification report of bidirectional LSTM model for blood specie identification

	Precision	Recall	F1-score	Support
Asian swamp eel	1.000	1.000	1.000	30
alpaca	0.909	1.000	0.952	10
alpaca suri	1.000	0.909	0.952	11
argali	0.938	1.000	0.968	30
carp	1.000	1.000	1.000	45
cat	0.872	0.911	0.891	45
cattle	0.978	1.000	0.989	45
chicken	1.000	1.000	1.000	61
dog	0.946	0.930	0.938	57
duck	1.000	0.983	0.991	58
fallow deer	1.000	0.833	0.909	6
geese	0.985	1.000	0.992	65
human	1.000	0.974	0.987	195
monkey	0.952	0.990	0.971	101
mouse	1.000	1.000	1.000	19
pig	0.980	0.980	0.980	49
pigeon	1.000	1.000	1.000	56
rabbit	0.980	1.000	0.990	48
rat	1.000	0.920	0.958	25
sika deer	1.000	0.800	0.889	5
Accuracy			0.978	961
Macro avg	0.977	0.962	0.968	961
Weighted avg	0.979	0.978	0.978	961

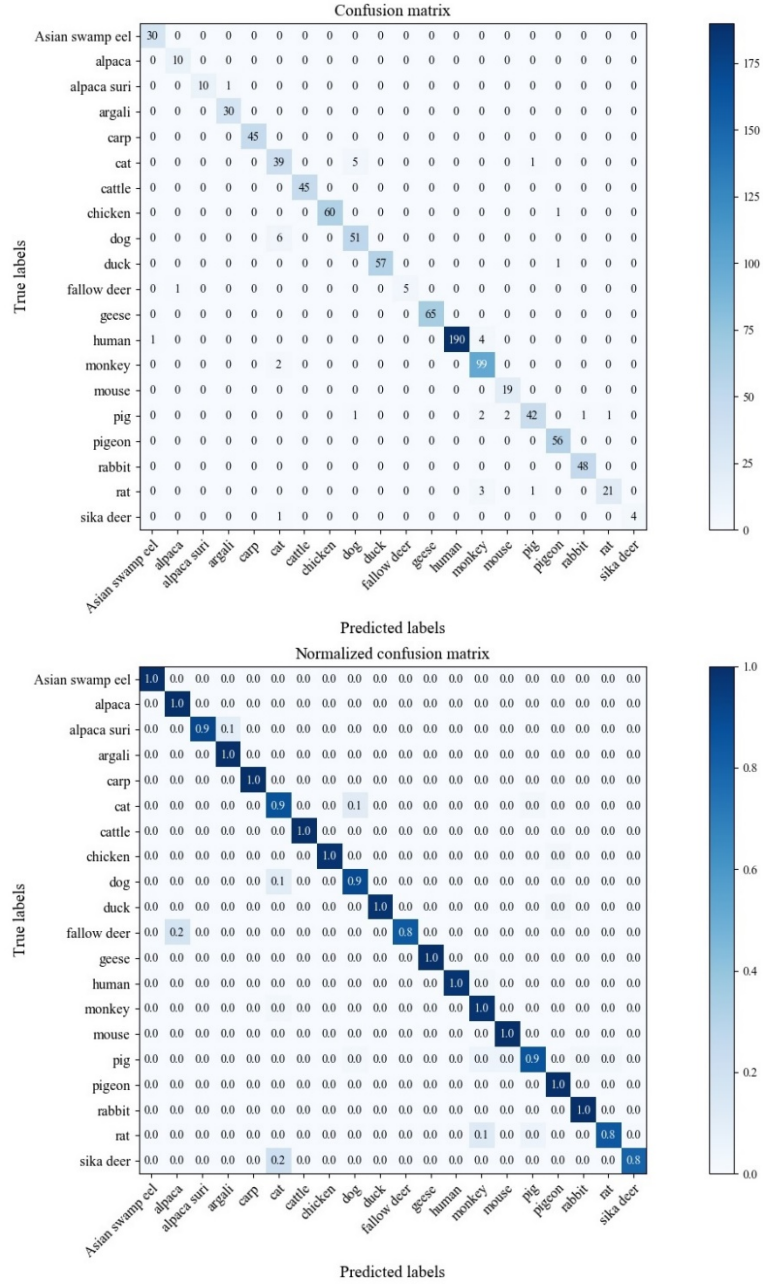


Fig. S13. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using CNN and GRU in series.

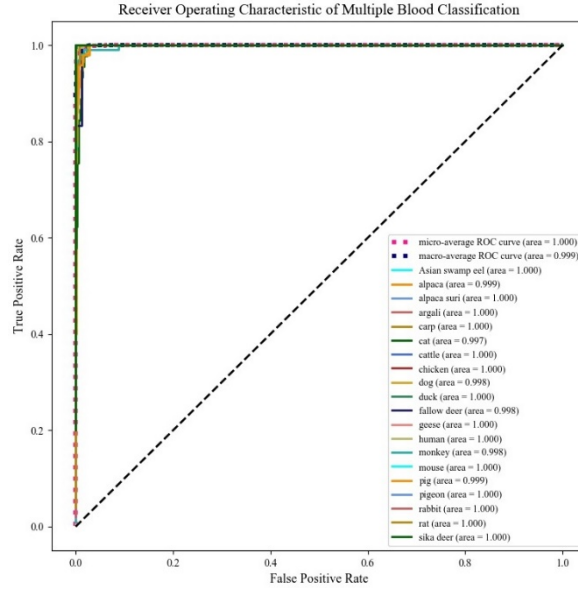


Fig. S14. ROC curve and AUC of multiple blood classification using CNN and GRU in series.

Table S7. Classification report of CNN-GRU in series model for blood specie identification

	Precision	Recall	F1-score	Support
Asian swamp eel	0.968	1.000	0.984	30
alpaca	0.909	1.000	0.952	10
alpaca suri	1.000	0.909	0.952	11
argali	0.968	1.000	0.984	30
carp	1.000	1.000	1.000	45
cat	0.812	0.867	0.839	45
cattle	1.000	1.000	1.000	45
chicken	1.000	0.984	0.992	61
dog	0.895	0.895	0.895	57
duck	1.000	0.983	0.991	58
fallow deer	1.000	0.833	0.909	6
geese	1.000	1.000	1.000	65
human	1.000	0.974	0.987	195
monkey	0.917	0.980	0.947	101
mouse	0.905	1.000	0.950	19
pig	0.955	0.857	0.903	49
pigeon	0.966	1.000	0.982	56
rabbit	0.980	1.000	0.990	48
rat	0.955	0.840	0.894	25
sika deer	1.000	0.800	0.889	5
Accuracy			0.964	961
Macro avg	0.961	0.946	0.952	961
Weighted avg	0.965	0.964	0.964	961

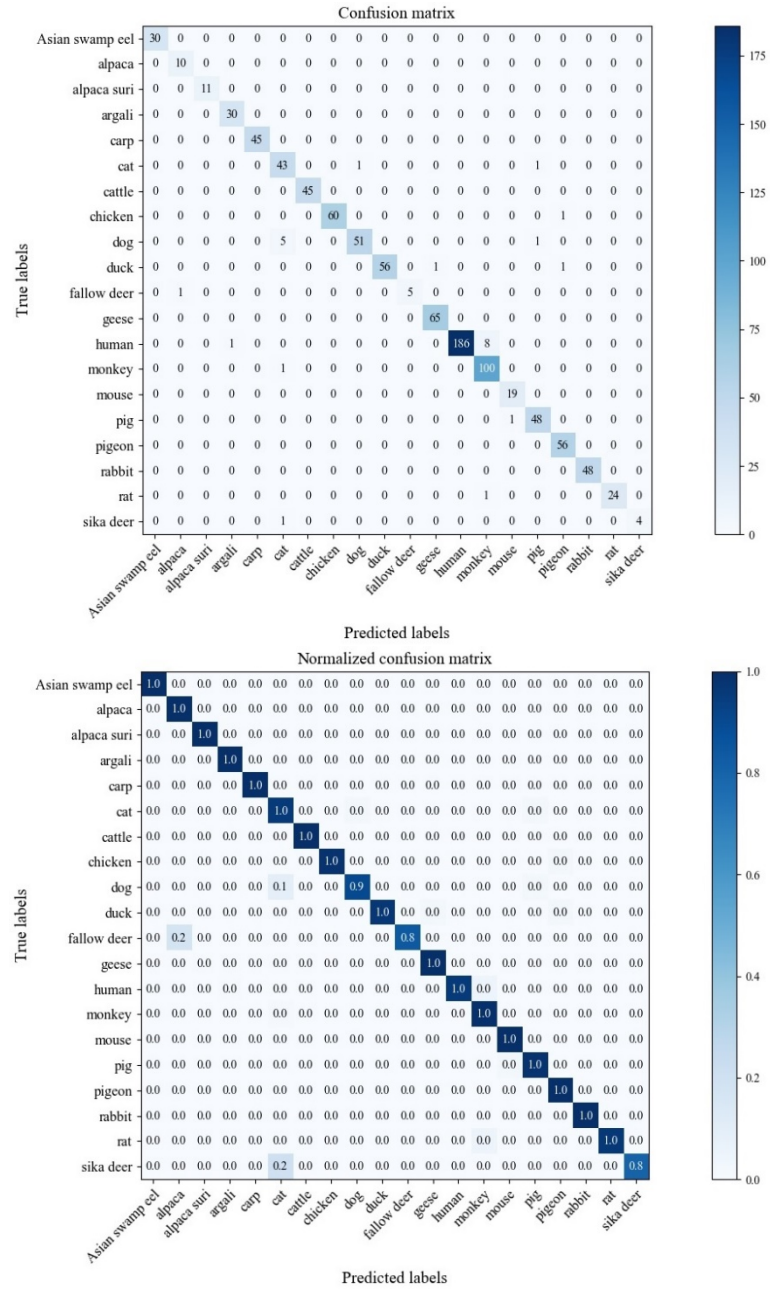


Fig. S15. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using CNN and GRU in parallel.

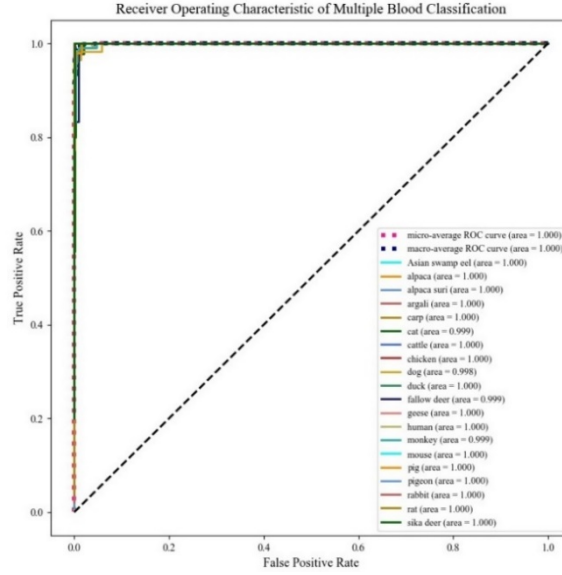


Fig. S16. ROC curve and AUC of multiple blood classification using CNN and GRU in parallel.

Table S8. Classification report of CNN-GRU in parallel model for blood specie identification

	Precision	Recall	F1-score	Support
Asian swamp eel	1.000	1.000	1.000	30
alpaca	0.909	1.000	0.952	10
alpaca suri	1.000	1.000	1.000	11
argali	0.968	1.000	0.984	30
carp	1.000	1.000	1.000	45
cat	0.860	0.956	0.905	45
cattle	1.000	1.000	1.000	45
chicken	1.000	0.984	0.992	61
dog	0.981	0.895	0.936	57
duck	1.000	0.966	0.982	58
fallow deer	1.000	0.833	0.909	6
geese	0.985	1.000	0.992	65
human	1.000	0.954	0.976	195
monkey	0.917	0.990	0.952	101
mouse	0.950	1.000	0.974	19
pig	0.960	0.980	0.970	49
pigeon	0.966	1.000	0.982	56
rabbit	1.000	1.000	1.000	48
rat	1.000	0.960	0.980	25
sika deer	1.000	0.800	0.889	5
Accuracy			0.974	961
Macro avg	0.975	0.966	0.969	961
Weighted avg	0.976	0.974	0.974	961

Table S9. Hyperparameter tuning of RNN model with GRU cell

Optimizer	Accuracy	Precision	Recall	F1-score
SGD	0.970	0.969	0.959	0.963
Rmsprop	0.940	0.906	0.941	0.919
Adagrad	0.830	0.717	0.798	0.746
Adadelta	0.964	0.956	0.962	0.958
Adam	0.951	0.936	0.952	0.942
Adamax	0.961	0.961	0.958	0.957
Nadam	0.852	0.811	0.825	0.805
Momentum	Accuracy	Precision	Recall	F1-score
0	0.959	0.953	0.956	0.952
0.2	0.963	0.930	0.954	0.940
0.4	0.964	0.943	0.958	0.949
0.6	0.967	0.958	0.965	0.960
0.8	0.972	0.969	0.964	0.965
0.9	0.972	0.972	0.964	0.966
Learning Rate	Accuracy	Precision	Recall	F1-score
0.0001	0.812	0.747	0.817	0.764
0.001	0.960	0.952	0.958	0.953
0.01	0.973	0.975	0.966	0.969
0.1	0.203	0.010	0.050	0.017
Loss	Accuracy	Precision	Recall	F1-score
Binary crossentropy	0.955	0.940	0.946	0.941
Categorical crossentropy	0.972	0.974	0.974	0.973
Cosine proximity	0.970	0.968	0.962	0.963
Kullback Leibler divergence	0.970	0.968	0.959	0.962
Mean squared error	0.901	0.843	0.897	0.859
Poisson	0.940	0.922	0.930	0.925
Categorical hing	0.972	0.974	0.963	0.967
Full Connection Layers	Accuracy	Precision	Recall	F1-score
64x64	0.969	0.949	0.958	0.952
64x128	0.959	0.934	0.944	0.937
64*256	0.976	0.968	0.960	0.963
64x512	0.965	0.962	0.960	0.959
128x64	0.960	0.924	0.943	0.931
128x128	0.961	0.938	0.945	0.939
128x256	0.968	0.951	0.967	0.957
128x512	0.960	0.949	0.954	0.946
256x64	0.968	0.961	0.962	0.961
256x128	0.960	0.945	0.948	0.945
256x256	0.958	0.954	0.953	0.951
256x512	0.963	0.939	0.950	0.942
512x64	0.958	0.952	0.945	0.944

512x128	0.958	0.941	0.935	0.936
512x256	0.960	0.945	0.946	0.943
512x512	0.958	0.944	0.944	0.942

SGD: Stochastic gradient descent

Adam: Adaptive moment estimation

RMSprop: Root Mean Square Prop

Nadam: Nesterov-accelerated adaptive moment estimation

Table S10. Optimal hyperparameters for GRU model of blood species classification

Hyperparameter	Default model	Optimized model
Optimizer	Adam	SGD
Learning rate	0.001	0.01
Parameter	beta1=0.9, beta2=0.999	Momentum=0.9
Loss	Categorical hinge	Categorical crossentropy
Full connection layers	512x512	64x256
Accuracy	0.951	0.976

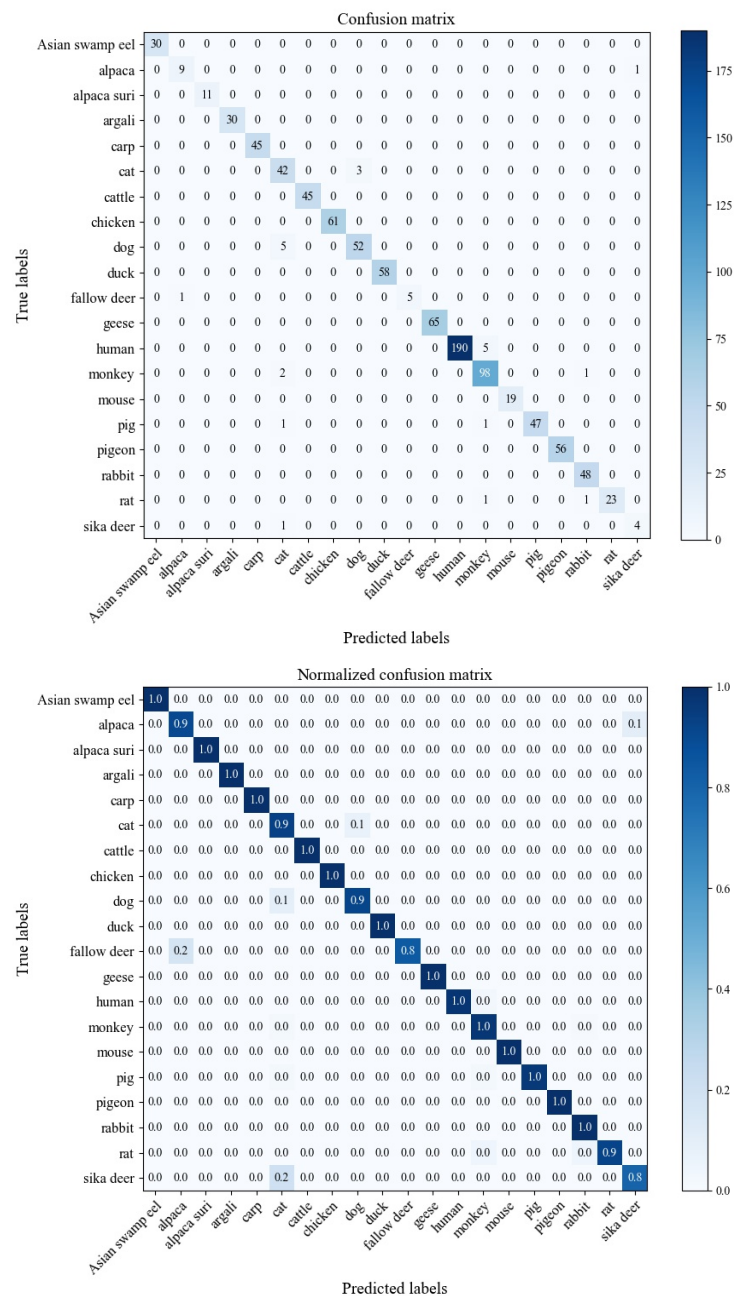


Fig. S17. Confusion matrix (a) and normalized confusion matrix (b) for multiple classification using optimized GRU model.

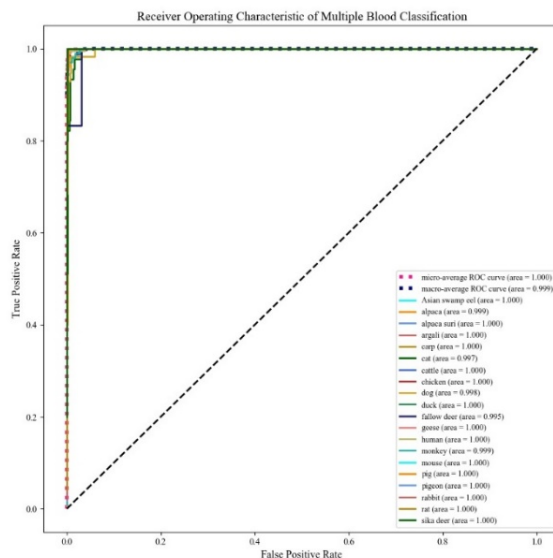


Fig. S18. ROC curve and AUC of multiple blood classification using optimized RNN model.

Table S11. Classification report of optimized GRU model for blood specie identification

	Precision	Recall	F1-score	Support
Asian swamp eel	1.000	1.000	1.000	30
alpaca	0.900	0.900	0.900	10
alpaca suri	1.000	1.000	1.000	11
argali	1.000	1.000	1.000	30
carp	1.000	1.000	1.000	45
cat	0.824	0.933	0.875	45
cattle	1.000	1.000	1.000	45
chicken	1.000	1.000	1.000	61
dog	0.945	0.912	0.929	57
duck	1.000	1.000	1.000	58
fallow deer	1.000	0.833	0.909	6
geese	1.000	1.000	1.000	65
human	1.000	0.974	0.987	195
monkey	0.933	0.970	0.951	101
mouse	1.000	1.000	1.000	19
pig	1.000	0.959	0.979	49
pigeon	1.000	1.000	1.000	56
rabbit	0.960	1.000	0.980	48
rat	1.000	0.920	0.958	25
sika deer	0.800	0.800	0.800	5
Accuracy			0.976	961
Macro avg	0.968	0.960	0.963	961
Weighted avg	0.977	0.976	0.976	961