

Table S1. Parameters used for training machine learning models.

Model	Parameter	Description	Range
ANN	hidden_size	Number of neurons in the hidden layer	2~100
	learning_rate	Change rate of weight in the training process	0.0001~1
	n_estimators	Number of trees in the random forest	5~200
RF	max_depth	Maximum number of splitting iterations	2~20
	min_samples_leaf	Minimum number of samples for end nodes	2~10
	min_samples_split	The minimum number of samples in every leaf node	2~20
DT	max_depth	Maximum number of splitting iterations in a single tree	2~20
	C_value	Normalized parameters used for controlling model complexity	0.001~200
LR	max_iter	Maximum number of iterations at run time	100~1000

Table S2. Optimal parameters of ANN models derived from grid-search training process.

Training dataset	hidden_size	learning_rate	Accuracy of 10-fold validation
Fra_Lab1	60	0.3501	0.8471
Fra_Lab2	40	0.0501	0.8726
Fra_Lab3	40	0.0501	0.8558
Fra_Lab4	60	0.5501	0.8511
Fra_Lab5	60	0.2501	0.8638
Fra_Lab6	20	0.8501	0.8475
Fra_Lab7	100	0.1501	0.8888
Fra_Lab8	40	0.1501	0.8475
Fra_Lab9	80	0.8001	0.8813
Fra_Lab10	20	0.3501	0.8679
NoFra_Lab1	60	0.0501	0.8382
NoFra_Lab2	100	0.6501	0.8639
NoFra_Lab3	40	0.1001	0.8558
NoFra_Lab4	20	0.2001	0.8509
NoFra_Lab5	80	0.0501	0.8426
NoFra_Lab6	60	0.3001	0.8676
NoFra_Lab7	20	0.0501	0.8806
NoFra_Lab8	20	0.1501	0.8601
NoFra_Lab9	80	0.1001	0.8678
NoFra_Lab10	20	0.1001	0.8685

Training datasets listed in the first column correspond to the data files in the following path:
 \Supplementary Materials\Code\6_Machine-Learning\ANN_Fra\TrainDataset and \Supplementary
 Materials\Code\6_Machine-Learning\ANN_NoFra\TrainDataset.

Table S3. Optimal parameters of RF models derived from grid-search training process.

Training dataset	n_estimators	max_depth	min_samples_leaf	Accuracy of 10-fold validation
Fra_Lab1	5	10	6	0.8683
Fra_Lab2	150	10	10	0.8725
Fra_Lab3	5	5	4	0.8764
Fra_Lab4	5	10	8	0.8891
Fra_Lab5	100	10	4	0.8594
Fra_Lab6	5	2	4	0.8721
Fra_Lab7	150	5	8	0.8645
Fra_Lab8	150	10	2	0.8766
Fra_Lab9	100	2	2	0.873
Fra_Lab10	150	2	2	0.8723
NoFra_Lab1	50	5	8	0.8467
NoFra_Lab2	5	2	8	0.8728
NoFra_Lab3	50	10	2	0.8587
NoFra_Lab4	200	10	2	0.8935
NoFra_Lab5	100	2	2	0.8679
NoFra_Lab6	50	15	2	0.8719
NoFra_Lab7	150	5	2	0.8766
NoFra_Lab8	150	10	2	0.8551
NoFra_Lab9	5	2	4	0.8603
NoFra_Lab10	100	10	2	0.8803

Training datasets listed in the first column correspond to the data files in the following path:
 \Supplementary Materials\Code\6_Machine-Learning\RF_Fra\TrainDataset and \Supplementary
 Materials\Code\6_Machine-Learning\RF_NoFra\TrainDataset.

Table S4. Optimal parameters of DT models derived from grid-search training process.

Training dataset	min_samples_split	max_depth	Accuracy of 10-fold validation
Fra_Lab1	8	5	0.8562
Fra_Lab2	17	8	0.8382
Fra_Lab3	2	2	0.8643
Fra_Lab4	5	11	0.817
Fra_Lab5	2	8	0.8632
Fra_Lab6	14	8	0.8261
Fra_Lab7	2	2	0.8511
Fra_Lab8	2	2	0.8429
Fra_Lab9	11	5	0.8386
Fra_Lab10	17	5	0.8304
NoFra_Lab1	2	2	0.8391
NoFra_Lab2	14	8	0.8263
NoFra_Lab3	2	2	0.8643
NoFra_Lab4	17	8	0.8339
NoFra_Lab5	20	5	0.8422
NoFra_Lab6	2	2	0.8216
NoFra_Lab7	2	5	0.8551
NoFra_Lab8	2	2	0.8429
NoFra_Lab9	11	8	0.8259
NoFra_Lab10	2	2	0.8303

Training datasets listed in the first column correspond to the data files in the following path:
 \Supplementary Materials\Code\6_Machine-Learning\DT_Fra\TrainDataset and \Supplementary
 Materials\Code\6_Machine-Learning\DT_NoFra\TrainDataset.

Table S5. Optimal parameters of LR models derived from grid-search training process.

Training dataset	C_value	max_iter	Accuracy of 10-fold validation
Fra_Lab1	20	100	0.8389
Fra_Lab2	10	100	0.8382
Fra_Lab3	10	100	0.8473
Fra_Lab4	30	100	0.8551
Fra_Lab5	10	100	0.8683
Fra_Lab6	10	100	0.8469
Fra_Lab7	20	100	0.8761
Fra_Lab8	20	100	0.8433
Fra_Lab9	10	100	0.8431
Fra_Lab10	10	100	0.8391
NoFra_Lab1	10	100	0.8375
NoFra_Lab2	20	100	0.8507
NoFra_Lab3	40	100	0.8428
NoFra_Lab4	10	100	0.8252
NoFra_Lab5	10	100	0.8683
NoFra_Lab6	10	100	0.8373
NoFra_Lab7	10	100	0.8803
NoFra_Lab8	10	100	0.8301
NoFra_Lab9	10	100	0.8594
NoFra_Lab10	70	100	0.8303

Training datasets listed in the first column correspond to the data files in the following path:
 \Supplementary Materials\Code\6_Machine-Learning\LR_Fra\TrainDataset and \Supplementary
 Materials\Code\6_Machine-Learning\LR_NoFra\TrainDataset.