Supplementary materials

Table S1 Summary of sample types, sources, quantities, and collection periods

Sample Type	Source /Preparation Method	Quantity	Collection Period
Fermentation broth	Cultured from Bacillus strains in YPDM medium	363	March–August 2024
Zaopei	Sorghum fermentation, extracted using 30% methanol	32	June–August 2024
Daqu	Wheat fermented and extracted with 30% methanol after grinding	175	June–August 2024
Baijiu	Distilled liquor with ~53% (v/v) ethanol content	17	June–August 2024

Table S2 Standard curve parameters for eight pyrazine compounds

Compounds	Retention time	Calibration Curve Equation	R^2	concentration range/(μg/L)
2-Methylpyrazine	3.49	Y=27409.2X+198.078	0.9994	16 - 835
2-Ethylpyrazine	6.79	Y=28599.8X+214.778	0.9991	14 - 833
2,5-Dimethylpyrazine	5.55	Y=43655.1X	0.9994	54 - 1916
2-Ethyl-6-methyl pyrazine	9.94	Y=47737.5X+247.142	0.9990	12 - 617
2,3,5-Trimethylpyrazine	6.31	Y=247898X+3720.12	0.9992	11 - 806
2,3-Diethylpyrazine	14.59	Y=17238.4X+3147.32	0.9995	16 - 797
2,3,5,6-Tetramethylpyrazine	4.89	Y=542602X+26740.2	0.9990	21 - 2808
2,3-Dimethyl-5-ethylpyrazine	11.61	Y=227727X+2597.54	0.9992	8 - 809

Table S3 Calculation results for the limits of detection (LOD) and limits of quantification (LOQ) of eight pyrazine compounds

Compounds	Concentration (μg/L)	S/N	LOD	LOQ
2-Methylpyrazine	15.668	108.760	0.432	1.441
2-Ethylpyrazine	14.319	66.880	0.642	2.141
2,5-Dimethylpyrazine	54.412	13.420	12.164	40.545
2-Ethyl-6-methyl pyrazine	8.474	66.380	0.383	1.277
2,3,5-Trimethylpyrazine	10.835	762.980	0.043	0.142
2,3-Diethylpyrazine	15.984	670.410	0.072	0.238
2,3,5,6-Tetramethylpyrazine	20.970	2992.690	0.021	0.070
2,3-Dimethyl-5-ethylpyrazine	8.005	11.270	2.131	7.103

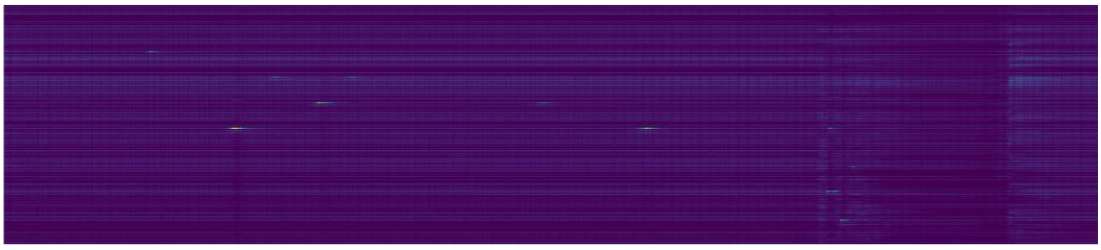
Table S4 Repeatability test results for eight pyrazine compounds

Compounds	Measurement value/(μg/L)						average value	RSD /(%)
	1	2	3	4	5	6		
2-Methylpyrazine	88.018	84.341	80.380	74.424	83.438	82.612	82.202	5.546
2-Ethylpyrazine	77.795	79.094	81.450	88.914	76.995	82.692	81.157	5.385
2,5-Dimethylpyrazine	194.613	194.090	196.083	197.243	195.611	196.573	195.702	0.608
2-Ethyl-6-methyl pyrazine	55.456	52.871	57.893	53.564	61.753	59.361	56.816	6.097
2,3,5-Trimethylpyrazine	84.450	80.435	82.194	80.409	78.419	79.918	80.971	2.580
2,3-Diethylpyrazine	85.779	87.801	89.031	89.060	87.578	92.225	88.579	2.431
2,3,5,6-Tetramethylpyrazine	195.806	204.374	199.380	195.919	199.962	204.880	200.053	1.969
2,3-Dimethyl-5-ethylpyrazine	70.874	70.925	71.589	73.604	72.372	72.779	72.024	1.509

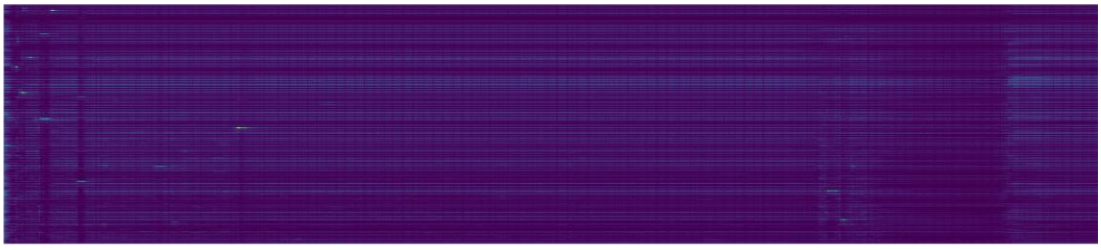
Table S5 Results of spiked recovery experiments for eight pyrazine compounds

Compounds	Measurement value/(μg/L)				average recovery rate /(%)	RSD/(%)
	Standard material	Test sample	Measured value 1	Measured value 2		
2-Methylpyrazine	834.854	ND	640.461	631.394	95.22	1.01
2-Ethylpyrazine	832.559	ND	684.652	676.635	102.19	0.83
2,5-Dimethylpyrazine	1915.502	ND	1487.645	1472.373	96.58	0.73
2-Ethyl-6-methyl pyrazine	616.969	ND	468.727	474.218	95.52	0.82
2,3,5-Trimethylpyrazine	805.883	215.243	794.935	788.652	96.11	0.56
2,3-Diethylpyrazine	803.002	ND	644.680	638.559	99.88	0.67
2,3,5,6-Tetramethylpyrazine	1808.207	742.877	2110.235	2134.783	105.64	0.82
2,3-Dimethyl-5-ethylpyrazine	809.059	ND	605.563	599.798	93.11	0.68

(A)



(B)



(C)

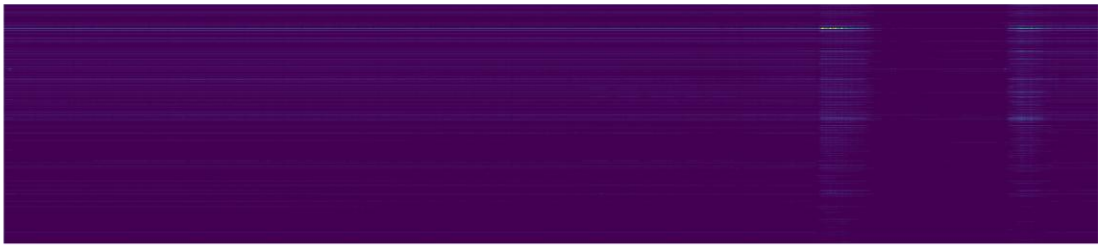


Fig. S1 Sample images after FastIMG process. All images will be resized to produce 224x224 pixel images. (A) standard curve sample (B) experimental sample (C) blank sample

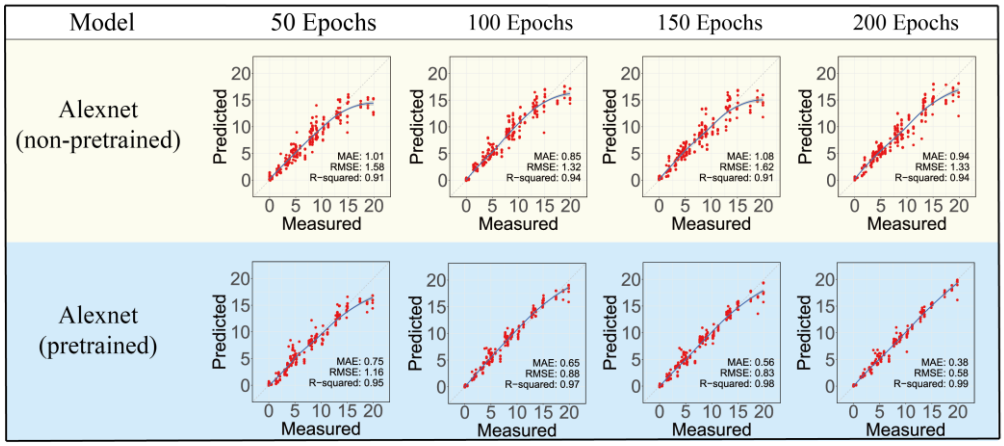


Fig. S2 The performance of Alexnet model with different epochs in prediction of the TTMP task.

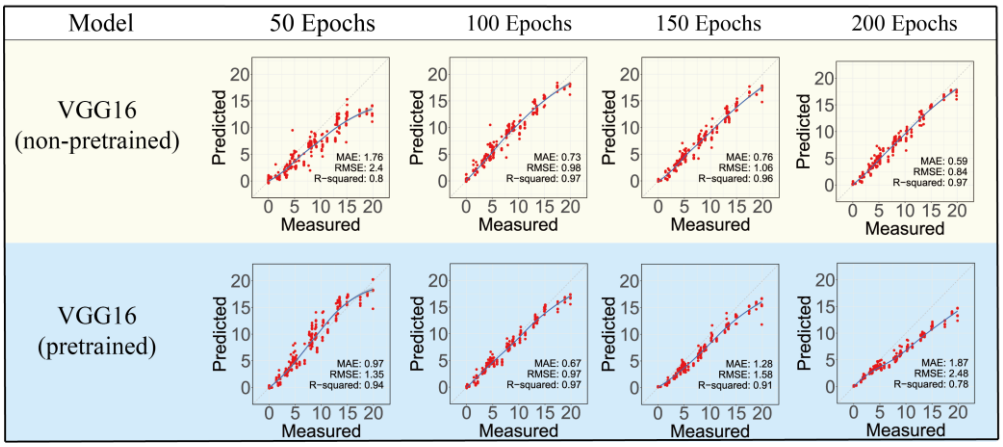


Fig. S3 The performance of VGG16 model with different epochs in prediction of the

TTMP task.

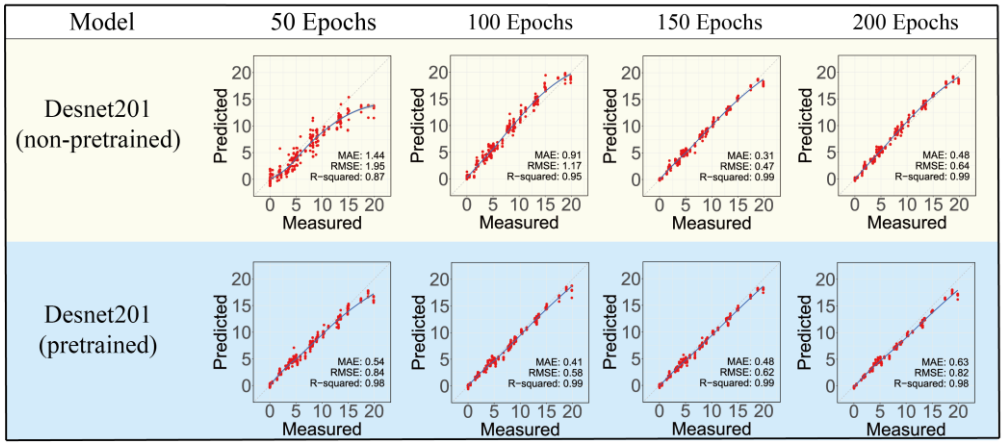


Fig. S4 The performance of Densnet201 model with different epochs in prediction of the TTMP task.

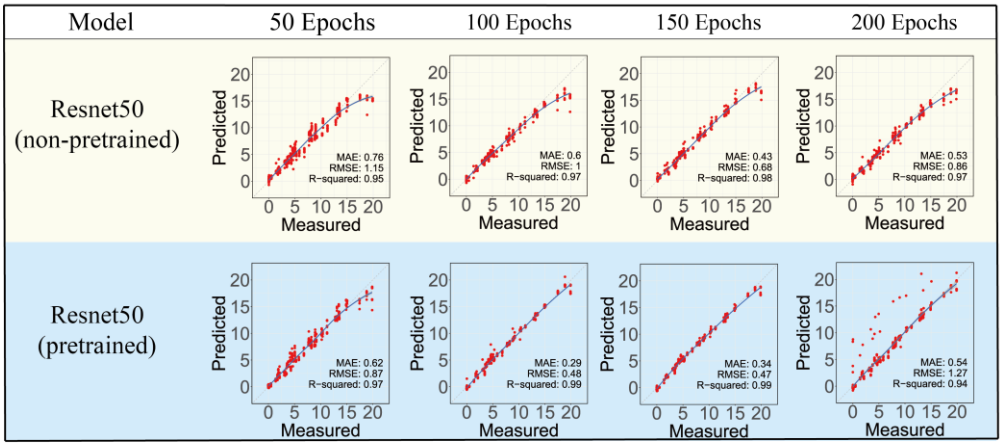


Fig. S5 The performance of Resnet50 model with different epochs in prediction of the TTMP task.

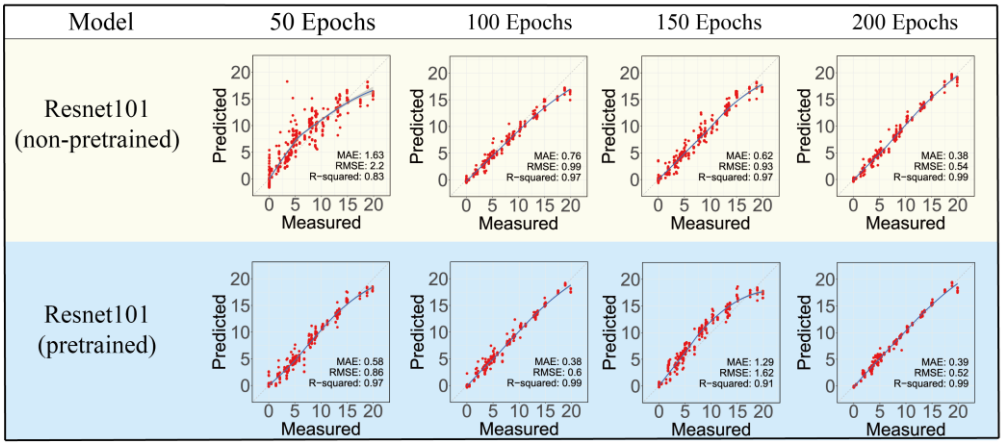


Fig. S6 The performance of Resnet101 model with different epochs in prediction of the TTMP task.

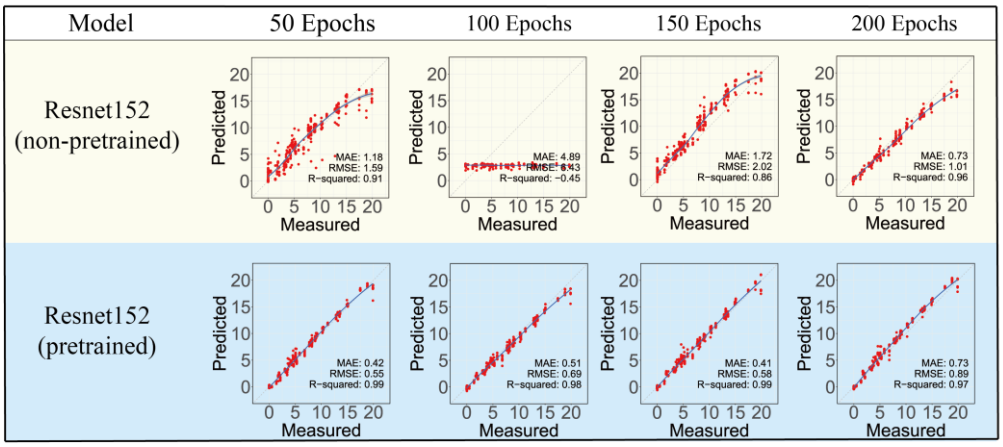


Fig. S7 The performance of Resnet152 model with different epochs in prediction of the TTMP task.

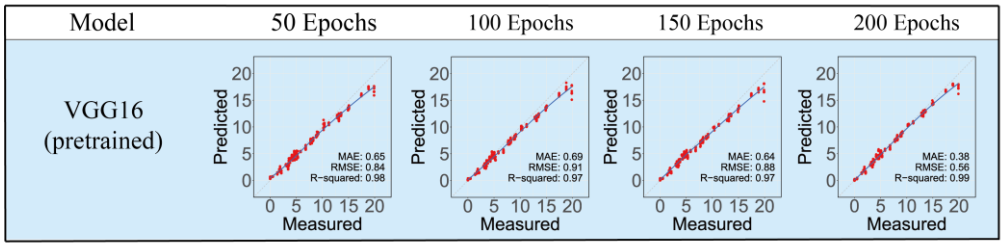


Fig. S8 The performance of Googlenet model with different epochs in prediction of the TTMP task.

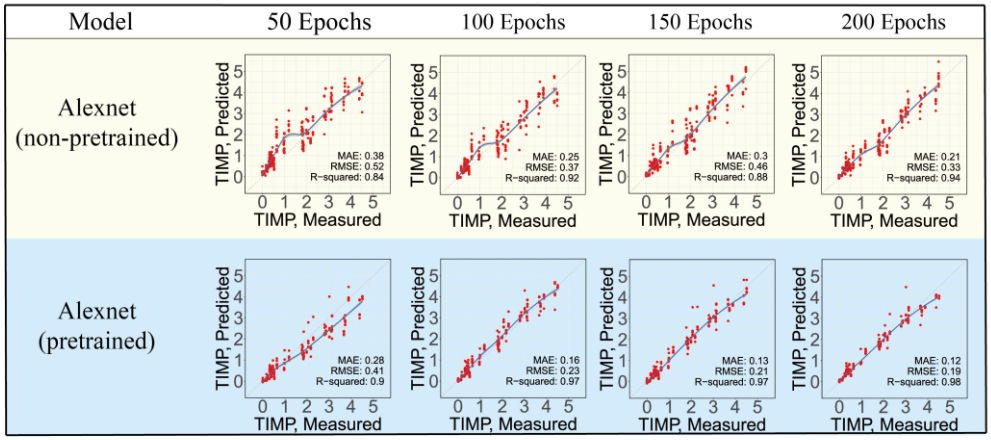


Fig. S9 The performance of Alexnet model with different epochs in prediction of the TIMP task.

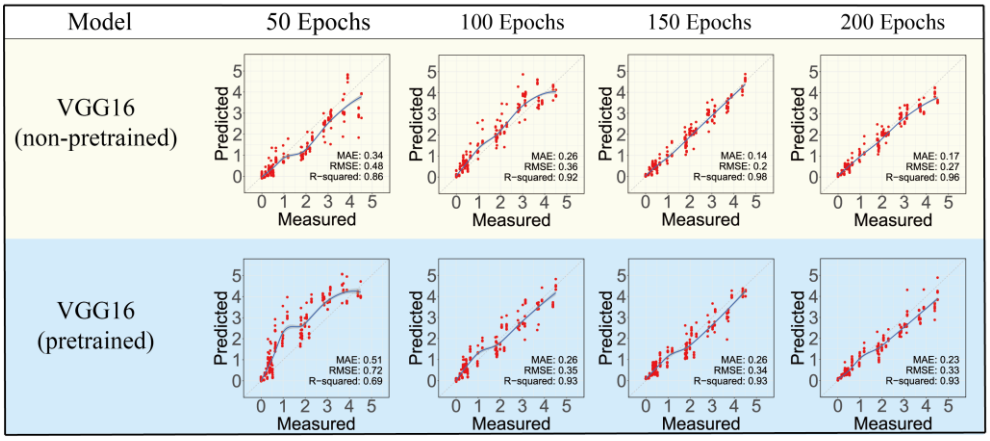


Fig. S110 The performance of VGG16 model with different epochs in prediction of the TIMP task.

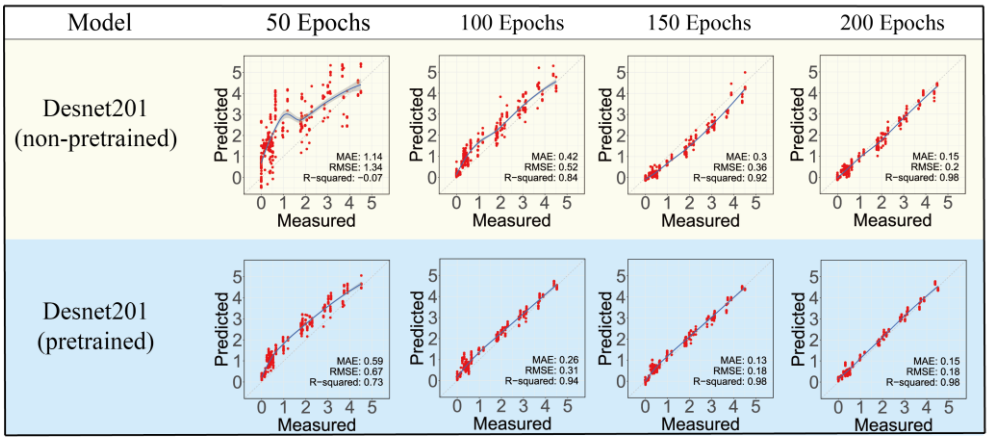


Fig. S11 The performance of Densnet201 model with different epochs in prediction of the TIMP task.

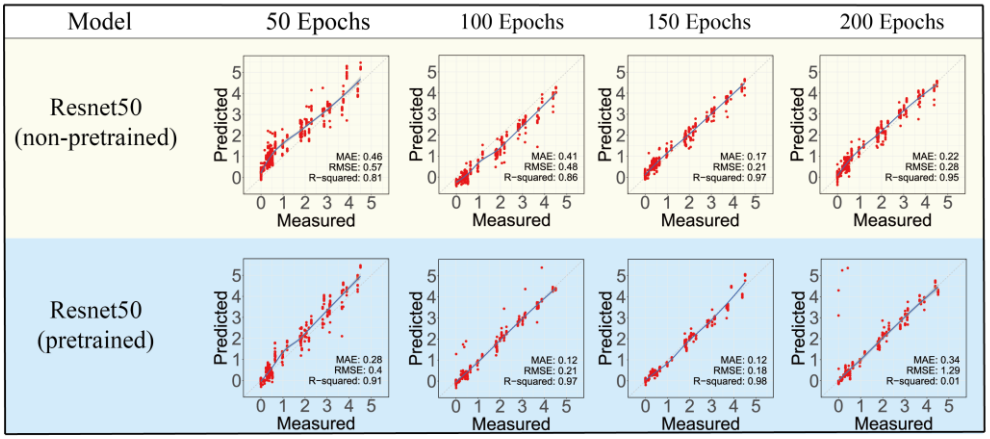


Fig. S12 The performance of Resnet50 model with different epochs in prediction of the TIMP task.

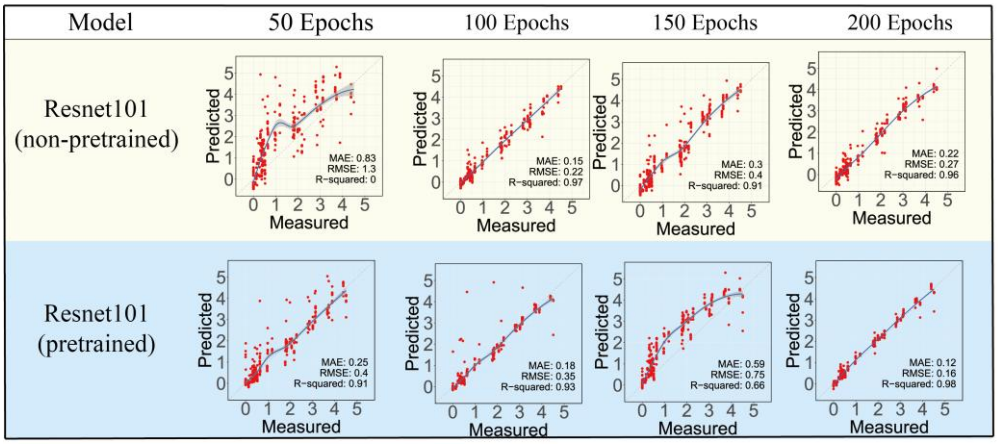


Fig. S13 The performance of Resnet101 model with different epochs in prediction of the TIMP task.

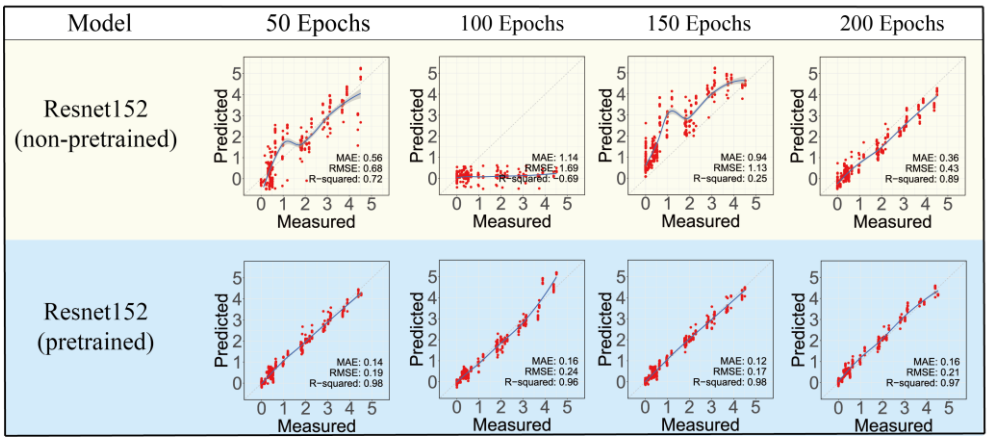


Fig. S14 The performance of Resnet152 model with different epochs in prediction of the TIMP task.

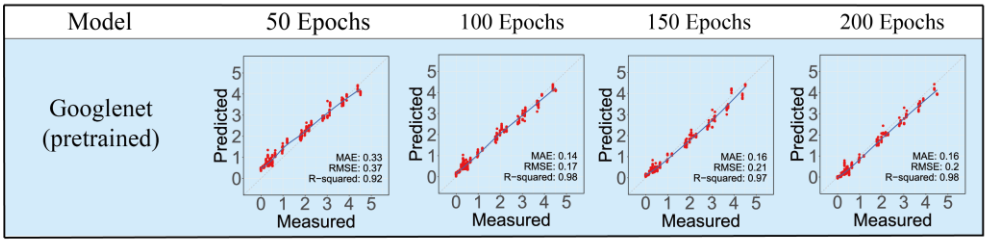


Fig. S15 The performance of Googlenet model with different epochs in prediction of the TIMP task.

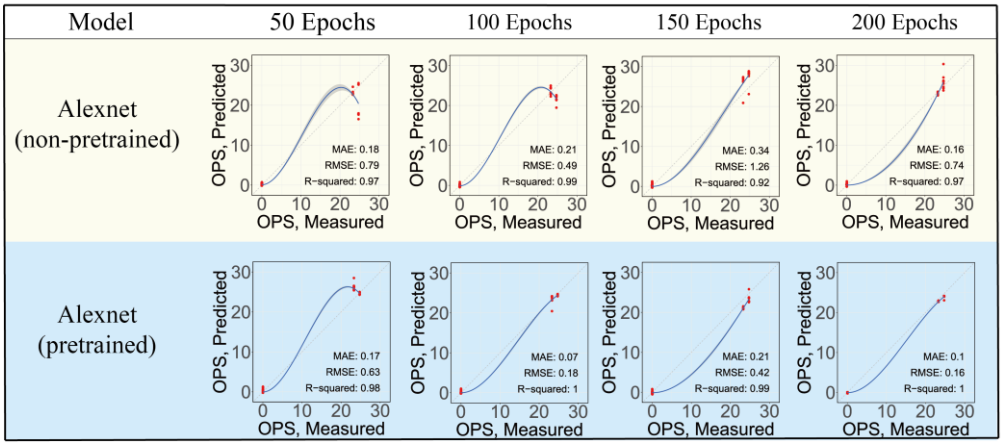


Fig. S16 The performance of Alexnet model with different epochs in prediction of the OPS task.

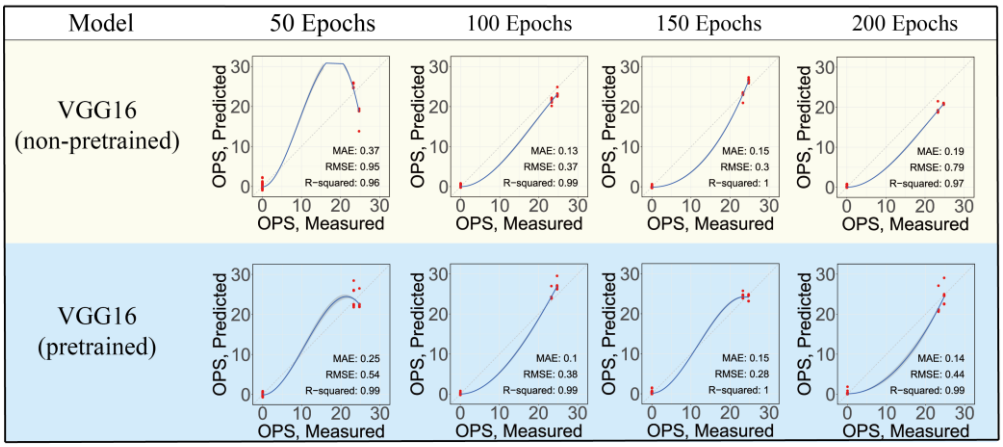


Fig. S17 The performance of VGG16 model with different epochs in prediction of the OPS task.

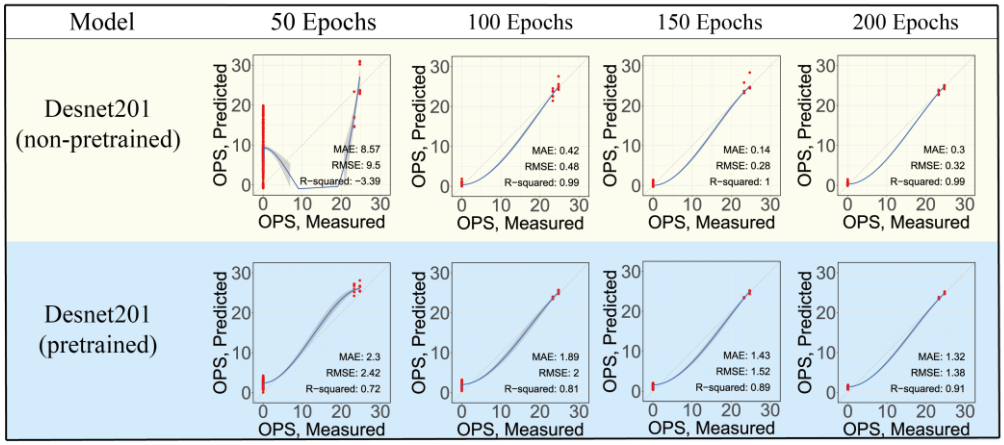


Fig. S18 The performance of Densnet201 model with different epochs in prediction of the OPS task.

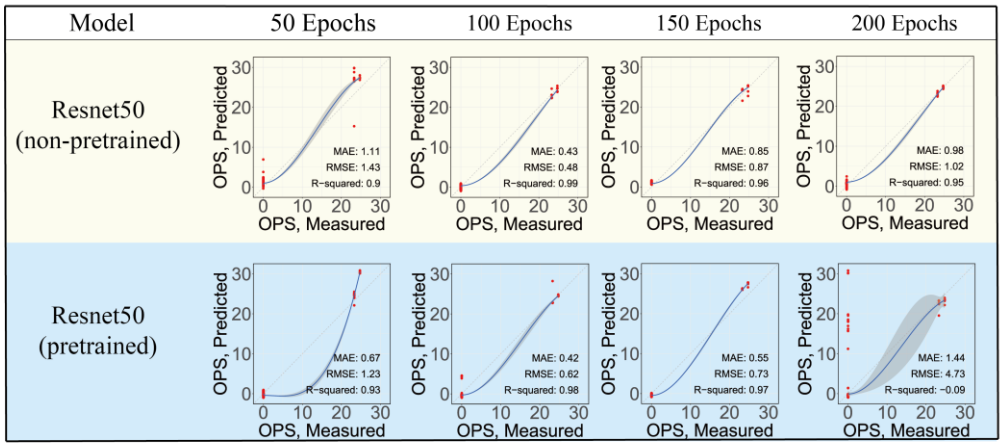


Fig. S19 The performance of Resnet50 model with different epochs in prediction of the OPS task.

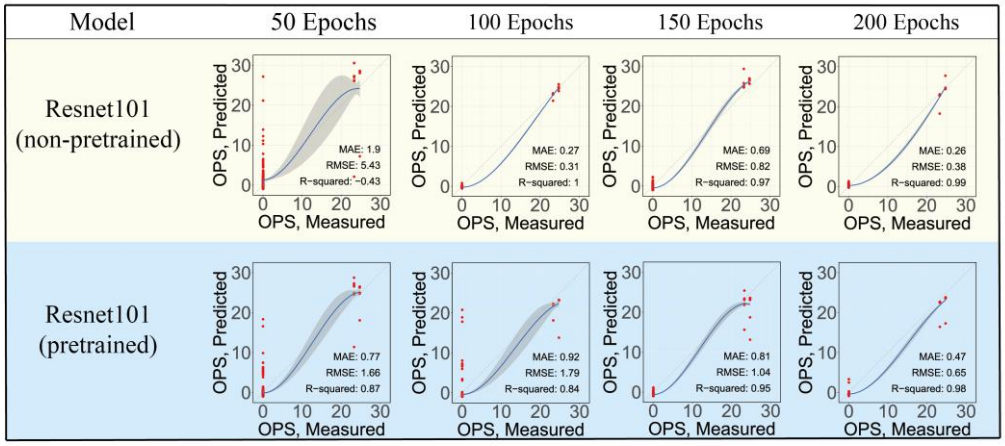


Fig. S20 The performance of Resnet101 model with different epochs in prediction of the OPS task.

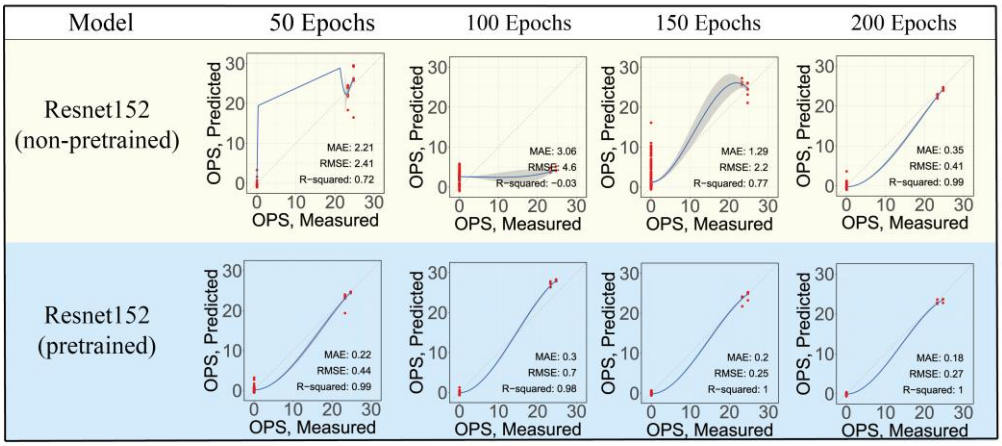


Fig. S21 The performance of Resnet152 model with different epochs in prediction of the OPS task.

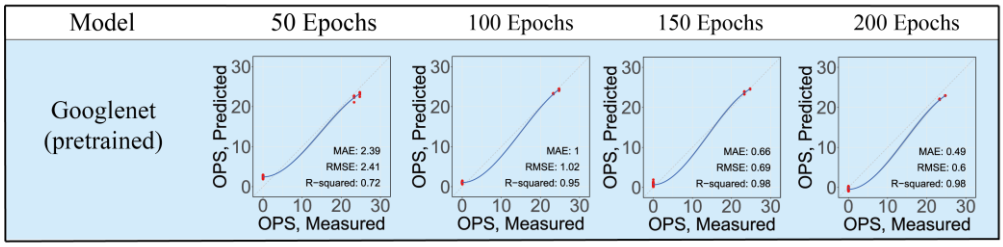


Fig. S22 The performance of Googlenet model with different epochs in prediction of the OPS task.

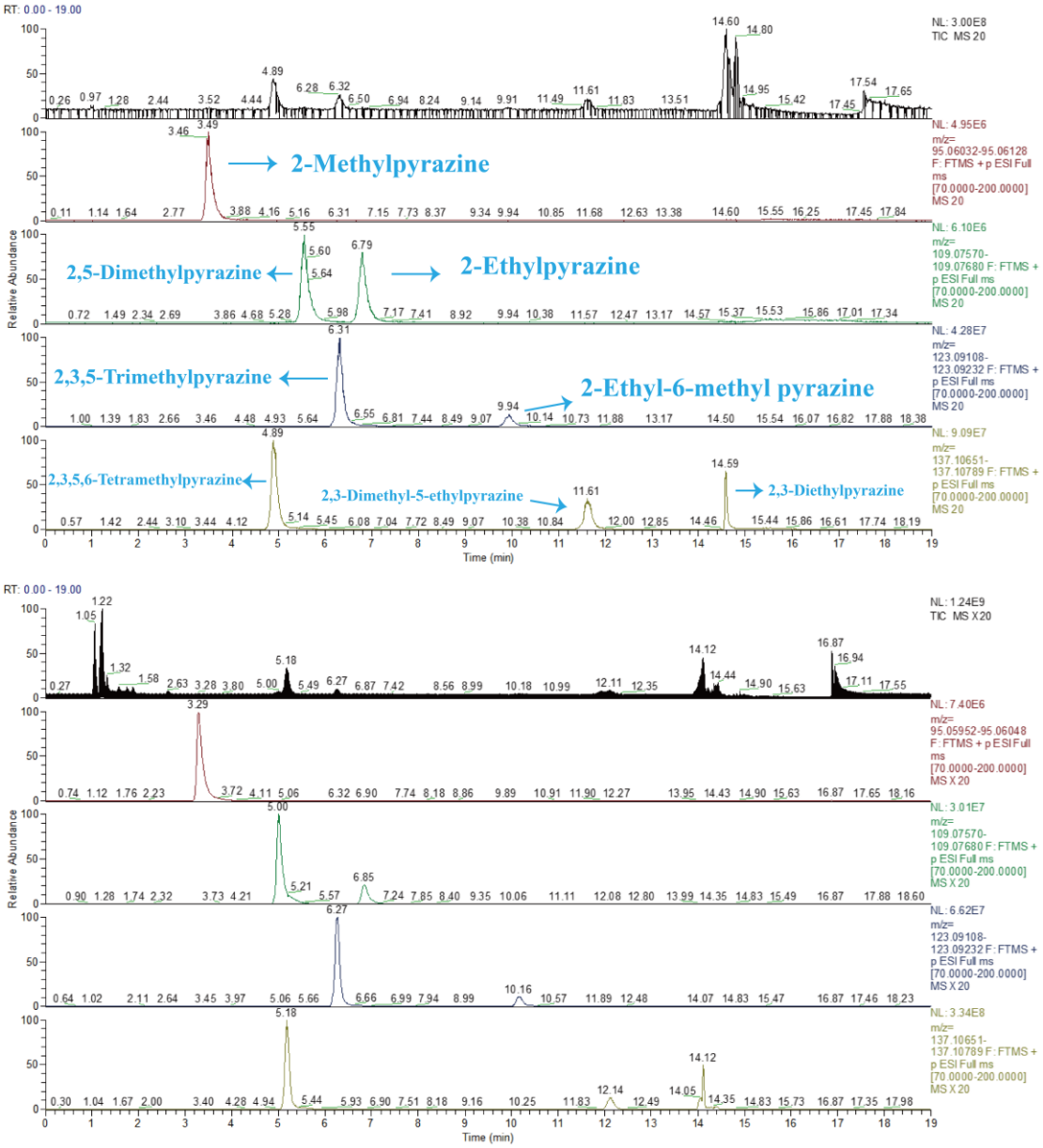


Fig. S23 Retention times of different pyrazines on old and new columns.

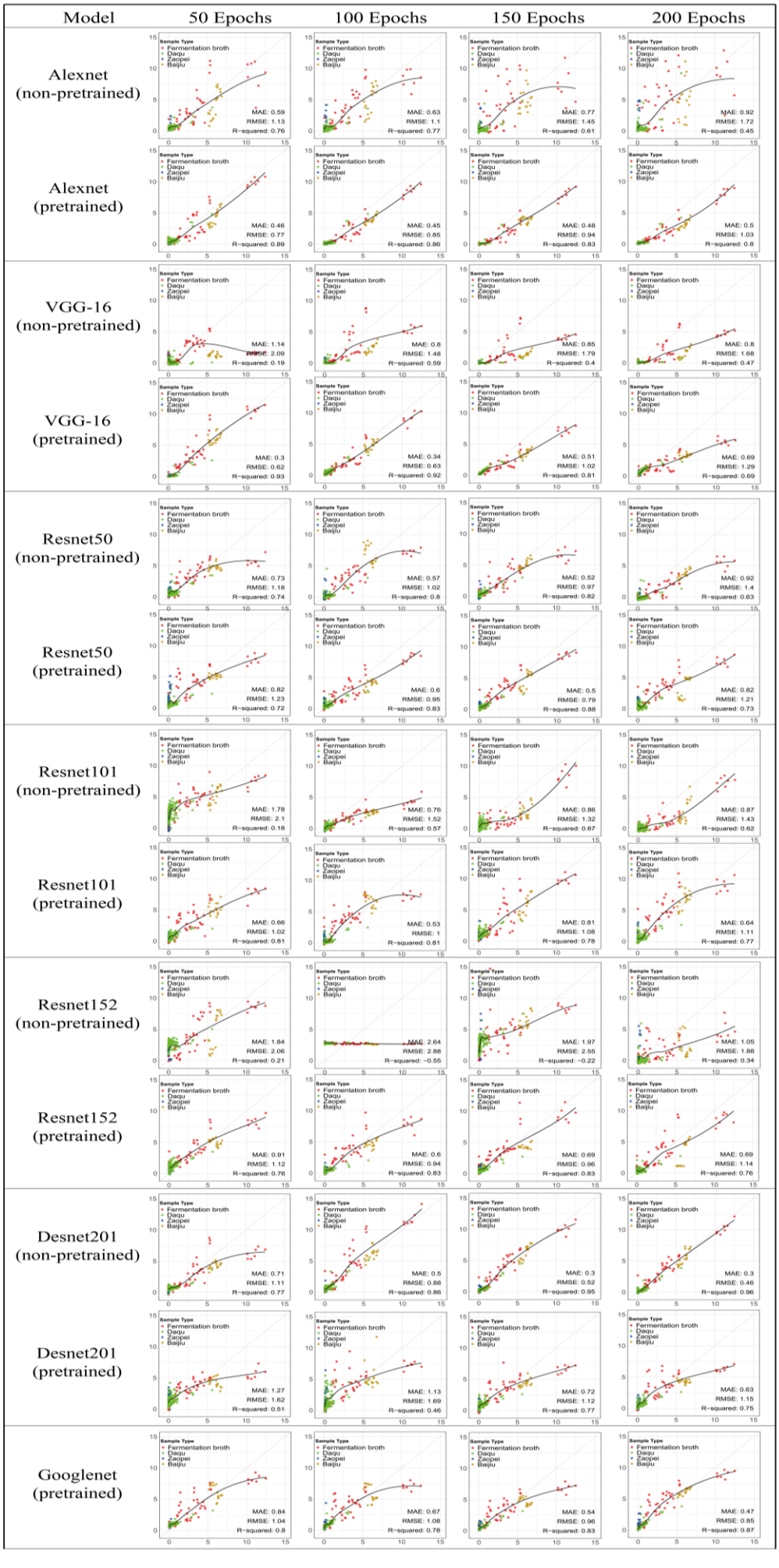

Model
50 Epochs
100 Epochs
150 Epochs
200 Epochs
Alexnet (non-pretrained)
MAE: 0.59 RMSE: 1.13 R-squared: 0.76
MAE: 0.63 RMSE: 1.1 R-squared: 0.77
MAE: 0.77 RMSE: 1.45 R-squared: 0.61
MAE: 0.92 RMSE: 1.72 R-squared: 0.45
Alexnet (pretrained)
MAE: 0.46 RMSE: 0.77 R-squared: 0.89
MAE: 0.45 RMSE: 0.85 R-squared: 0.86
MAE: 0.48 RMSE: 0.94 R-squared: 0.83
MAE: 0.5 RMSE: 1.03 R-squared: 0.8
VGG-16 (non-pretrained)
MAE: 1.14 RMSE: 2.09 R-squared: 0.19
MAE: 0.8 RMSE: 1.48 R-squared: 0.59
MAE: 0.85 RMSE: 1.79 R-squared: 0.4
MAE: 0.8 RMSE: 1.68 R-squared: 0.47
VGG-16 (pretrained)
MAE: 0.3 RMSE: 0.62 R-squared: 0.93
MAE: 0.34 RMSE: 0.63 R-squared: 0.92
MAE: 0.51 RMSE: 1.02 R-squared: 0.81
MAE: 0.69 RMSE: 1.29 R-squared: 0.69
Resnet50 (non-pretrained)
MAE: 0.73 RMSE: 1.18 R-squared: 0.74
MAE: 0.57 RMSE: 1.02 R-squared: 0.8
MAE: 0.52 RMSE: 0.97 R-squared: 0.82
MAE: 0.92 RMSE: 1.4 R-squared: 0.63
Resnet50 (pretrained)
MAE: 0.82 RMSE: 1.23 R-squared: 0.72
MAE: 0.6 RMSE: 0.95 R-squared: 0.83
MAE: 0.5 RMSE: 0.79 R-squared: 0.88
MAE: 0.82 RMSE: 1.21 R-squared: 0.73
Resnet101 (non-pretrained)
MAE: 1.78 RMSE: 2.1 R-squared: 0.18
MAE: 0.76 RMSE: 1.52 R-squared: 0.57
MAE: 0.86 RMSE: 1.32 R-squared: 0.67
MAE: 0.87 RMSE: 1.43 R-squared: 0.62
Resnet101 (pretrained)
MAE: 0.66 RMSE: 1.02 R-squared: 0.81
MAE: 0.53 RMSE: 1 R-squared: 0.81
MAE: 0.81 RMSE: 1.08 R-squared: 0.78
MAE: 0.64 RMSE: 1.11 R-squared: 0.77
Resnet152 (non-pretrained)
MAE: 1.84 RMSE: 2.06 R-squared: 0.21
MAE: 2.64 RMSE: 2.88 R-squared: −0.55
MAE: 1.97 RMSE: 2.55 R-squared: −0.22
MAE: 1.05 RMSE: 1.88 R-squared: 0.34
Resnet152 (pretrained)
MAE: 0.91 RMSE: 1.12 R-squared: 0.76
MAE: 0.6 RMSE: 0.94 R-squared: 0.83
MAE: 0.69 RMSE: 0.96 R-squared: 0.83
MAE: 0.69 RMSE: 1.14 R-squared: 0.76
Desnet201 (non-pretrained)
MAE: 0.71 RMSE: 1.11 R-squared: 0.77
MAE: 0.5 RMSE: 0.88 R-squared: 0.86
MAE: 0.3 RMSE: 0.52 R-squared: 0.95
MAE: 0.3 RMSE: 0.46 R-squared: 0.96
Desnet201 (pretrained)
MAE: 1.27 RMSE: 1.62 R-squared: 0.51
MAE: 1.13 RMSE: 1.69 R-squared: 0.46
MAE: 0.72 RMSE: 1.12 R-squared: 0.77
MAE: 0.63 RMSE: 1.15 R-squared: 0.75
Googlenet (pretrained)
MAE: 0.84 RMSE: 1.04 R-squared: 0.8
MAE: 0.67 RMSE: 1.08 R-squared: 0.78
MAE: 0.54 RMSE: 0.96 R-squared: 0.83
MAE: 0.47 RMSE: 0.85 R-squared: 0.87
Sample Type
Fermentation broth
Daqu
Zaopei
Baijiu

Fig. S24 The performance of deep learning models in prediction TTMP tasks with column replacement.

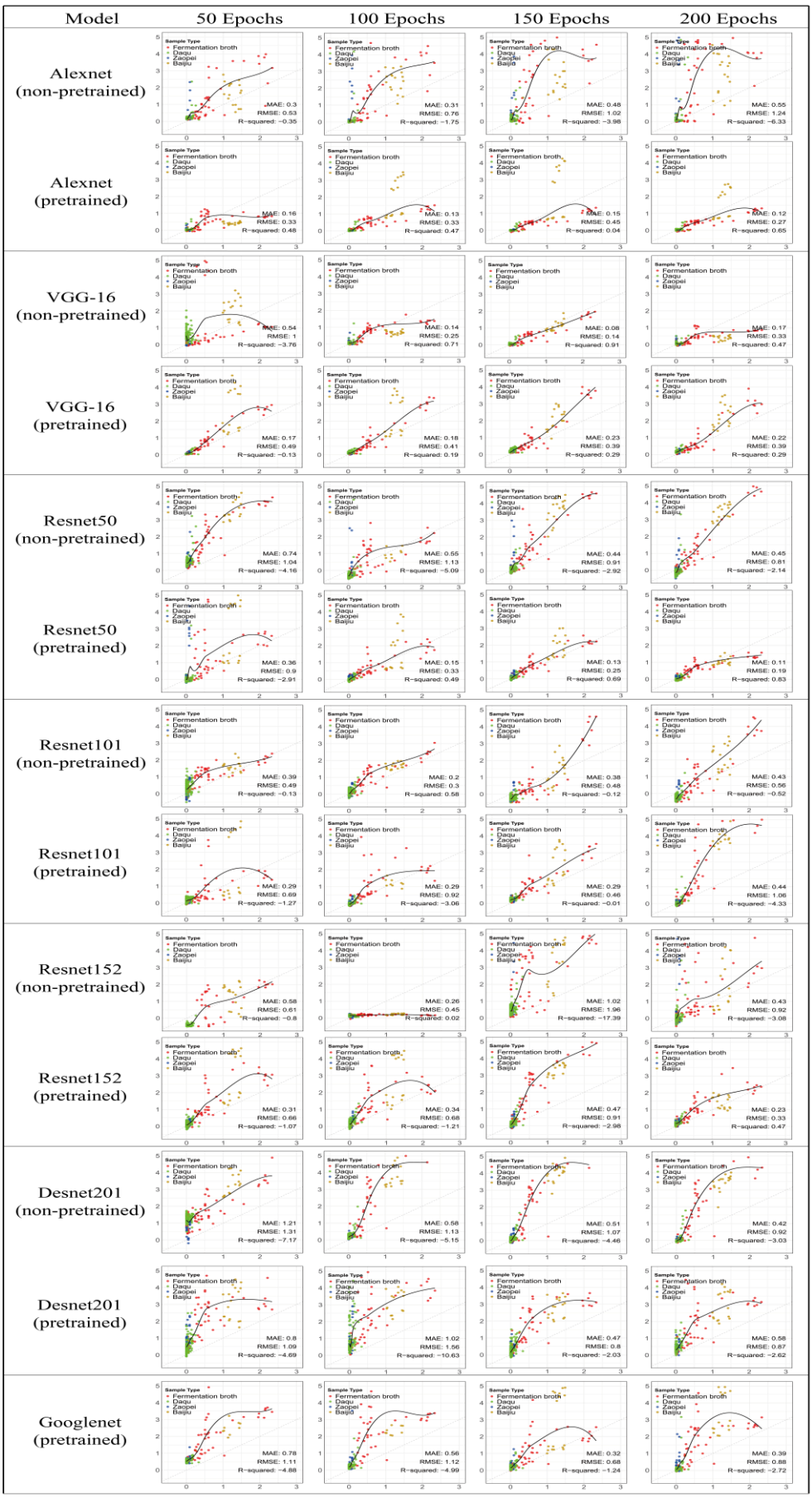

Model
50 Epochs
100 Epochs
150 Epochs
200 Epochs
Alexnet (non-pretrained)
Alexnet (pretrained)
VGG-16 (non-pretrained)
VGG-16 (pretrained)
Resnet50 (non-pretrained)
Resnet50 (pretrained)
Resnet101 (non-pretrained)
Resnet101 (pretrained)
Resnet152 (non-pretrained)
Resnet152 (pretrained)
Desnet201 (non-pretrained)
Desnet201 (pretrained)
Googlenet (pretrained)
Sample Type
Fermentation broth
Daqu
Zaopei
Baijiu

Fig. S25 The performance of deep learning models in prediction TIMP tasks with column replacement.

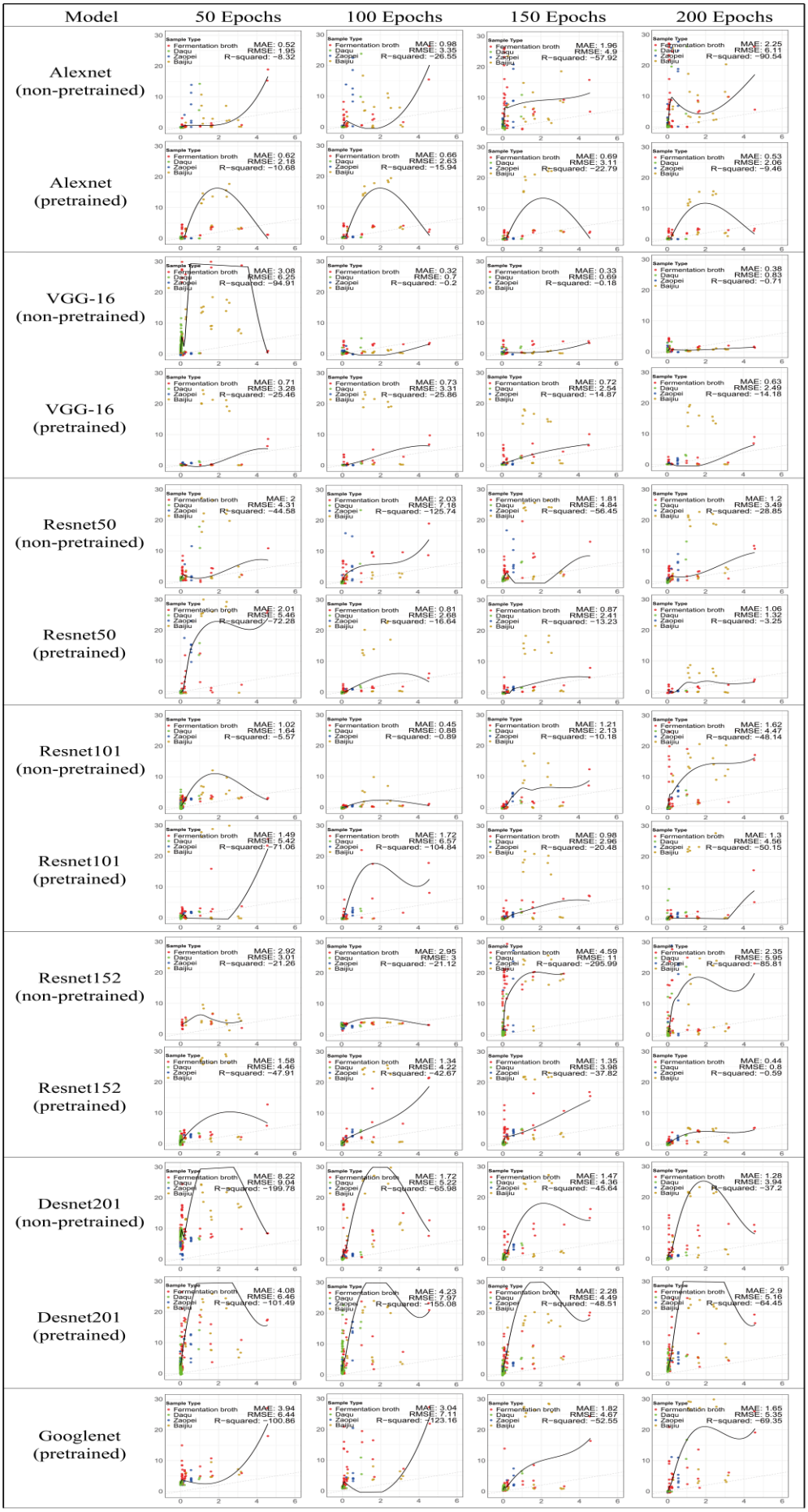

Model
50 Epochs
100 Epochs
150 Epochs
200 Epochs
Alexnet (non-pretrained)
Alexnet (pretrained)
VGG-16 (non-pretrained)
VGG-16 (pretrained)
Resnet50 (non-pretrained)
Resnet50 (pretrained)
Resnet101 (non-pretrained)
Resnet101 (pretrained)
Resnet152 (non-pretrained)
Resnet152 (pretrained)
Desnet201 (non-pretrained)
Desnet201 (pretrained)
Googlenet (pretrained)
Sample Type
Fermentation broth
Daqu
Zaopei
Baijiu
MAE: 0.52 RMSE: 1.95 R−squared: −8.32
MAE: 0.98 RMSE: 3.35 R−squared: −26.55
MAE: 1.96 RMSE: 4.9 R−squared: −57.92
MAE: 2.25 RMSE: 6.11 R−squared: −90.54
MAE: 0.62 RMSE: 2.18 R−squared: −10.68
MAE: 0.66 RMSE: 2.63 R−squared: −15.94
MAE: 0.69 RMSE: 3.11 R−squared: −22.79
MAE: 0.53 RMSE: 2.06 R−squared: −9.46
MAE: 3.08 RMSE: 6.25 R−squared: −94.91
MAE: 0.32 RMSE: 0.7 R−squared: −0.2
MAE: 0.33 RMSE: 0.69 R−squared: −0.18
MAE: 0.38 RMSE: 0.83 R−squared: −0.71
MAE: 0.71 RMSE: 3.28 R−squared: −25.46
MAE: 0.73 RMSE: 3.31 R−squared: −25.86
MAE: 0.72 RMSE: 2.54 R−squared: −14.87
MAE: 0.63 RMSE: 2.49 R−squared: −14.18
MAE: 2 RMSE: 4.31 R−squared: −44.58
MAE: 2.03 RMSE: 7.18 R−squared: −125.74
MAE: 1.81 RMSE: 4.84 R−squared: −56.45
MAE: 1.2 RMSE: 3.49 R−squared: −28.85
MAE: 2.01 RMSE: 5.46 R−squared: −72.28
MAE: 0.81 RMSE: 2.68 R−squared: −16.64
MAE: 0.87 RMSE: 2.41 R−squared: −13.23
MAE: 1.06 RMSE: 1.32 R−squared: −3.25
MAE: 1.02 RMSE: 1.64 R−squared: −5.67
MAE: 0.45 RMSE: 0.86 R−squared: −0.89
MAE: 1.21 RMSE: 2.13 R−squared: −10.18
MAE: 1.62 RMSE: 4.47 R−squared: −48.14
MAE: 1.49 RMSE: 5.42 R−squared: −71.06
MAE: 1.72 RMSE: 6.57 R−squared: −104.84
MAE: 0.98 RMSE: 2.96 R−squared: −20.48
MAE: 1.3 RMSE: 4.56 R−squared: −50.15
MAE: 2.92 RMSE: 3.01 R−squared: −21.26
MAE: 2.95 RMSE: 3 R−squared: −21.12
MAE: 4.59 RMSE: 11 R−squared: −295.99
MAE: 2.35 RMSE: 5.95 R−squared: −85.81
MAE: 1.58 RMSE: 4.46 R−squared: −47.91
MAE: 1.34 RMSE: 4.22 R−squared: −42.67
MAE: 1.35 RMSE: 3.98 R−squared: −37.82
MAE: 0.44 RMSE: 0.8 R−squared: −0.59
MAE: 8.22 RMSE: 9.04 R−squared: −199.78
MAE: 1.72 RMSE: 6.22 R−squared: −65.98
MAE: 1.47 RMSE: 4.36 R−squared: −45.64
MAE: 1.28 RMSE: 3.94 R−squared: −37.2
MAE: 4.08 RMSE: 6.46 R−squared: −101.49
MAE: 4.23 RMSE: 7.97 R−squared: −155.08
MAE: 2.28 RMSE: 4.49 R−squared: −48.51
MAE: 2.9 RMSE: 5.16 R−squared: −64.45
MAE: 3.94 RMSE: 6.44 R−squared: −100.86
MAE: 3.04 RMSE: 7.11 R−squared: −123.16
MAE: 1.82 RMSE: 4.67 R−squared: −52.55
MAE: 1.65 RMSE: 5.35 R−squared: −69.35

Fig. S226 The performance of deep learning models in prediction OPS tasks with column replacement.