

Independent Testing Performance

1 Performance Plots

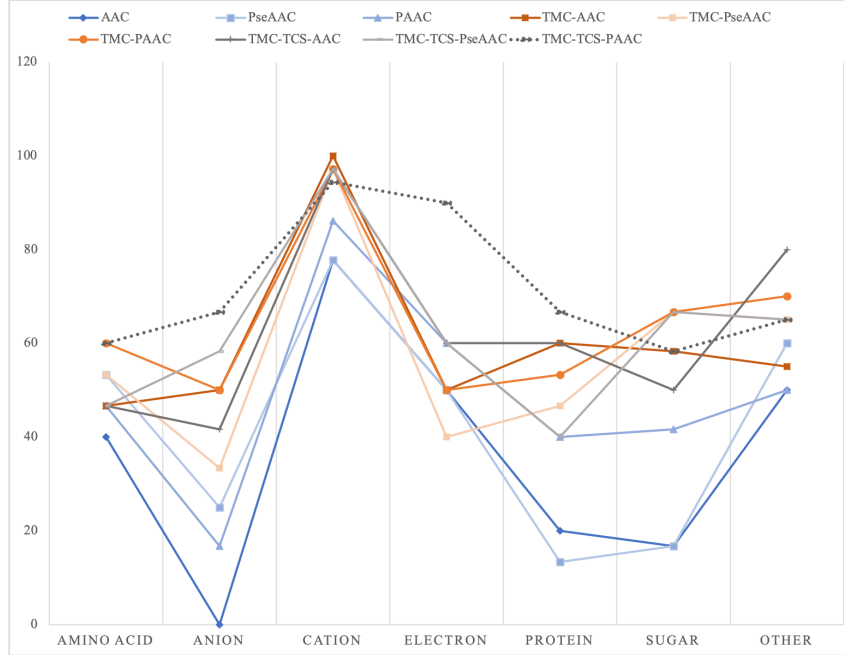


Figure 1: Sensitivity of different methods on different classes

The dotted line represents the performance of TranCEP, the TMC-TCS-PAAC method.

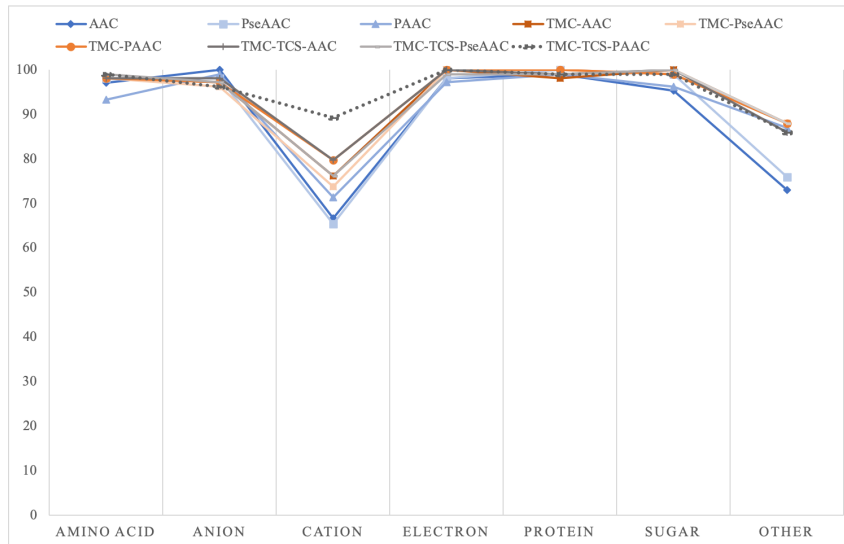


Figure 2: Specificity of different methods on different classes

The dotted line represents the performance of TranCEP, the TMC-TCS-PAAC method.

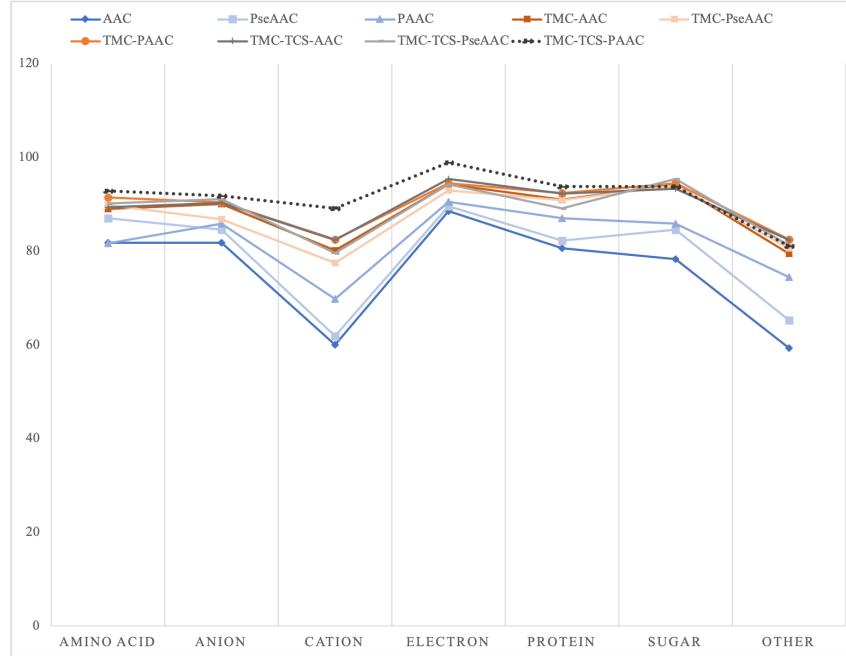


Figure 3: Accuracy of different methods on different classes

The dotted line represents the performance of TranCEP, the TMC-TCS-PAAC method.

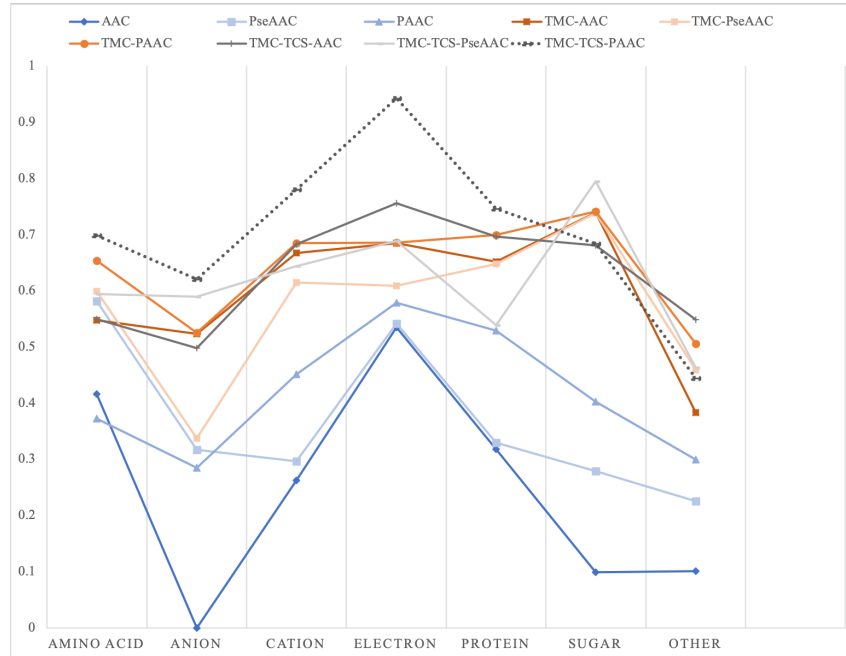


Figure 4: MCC of different methods on different classes

The dotted line represents the performance of TranCEP, the TMC-TCS-PAAC method.

2 Confusion matrix

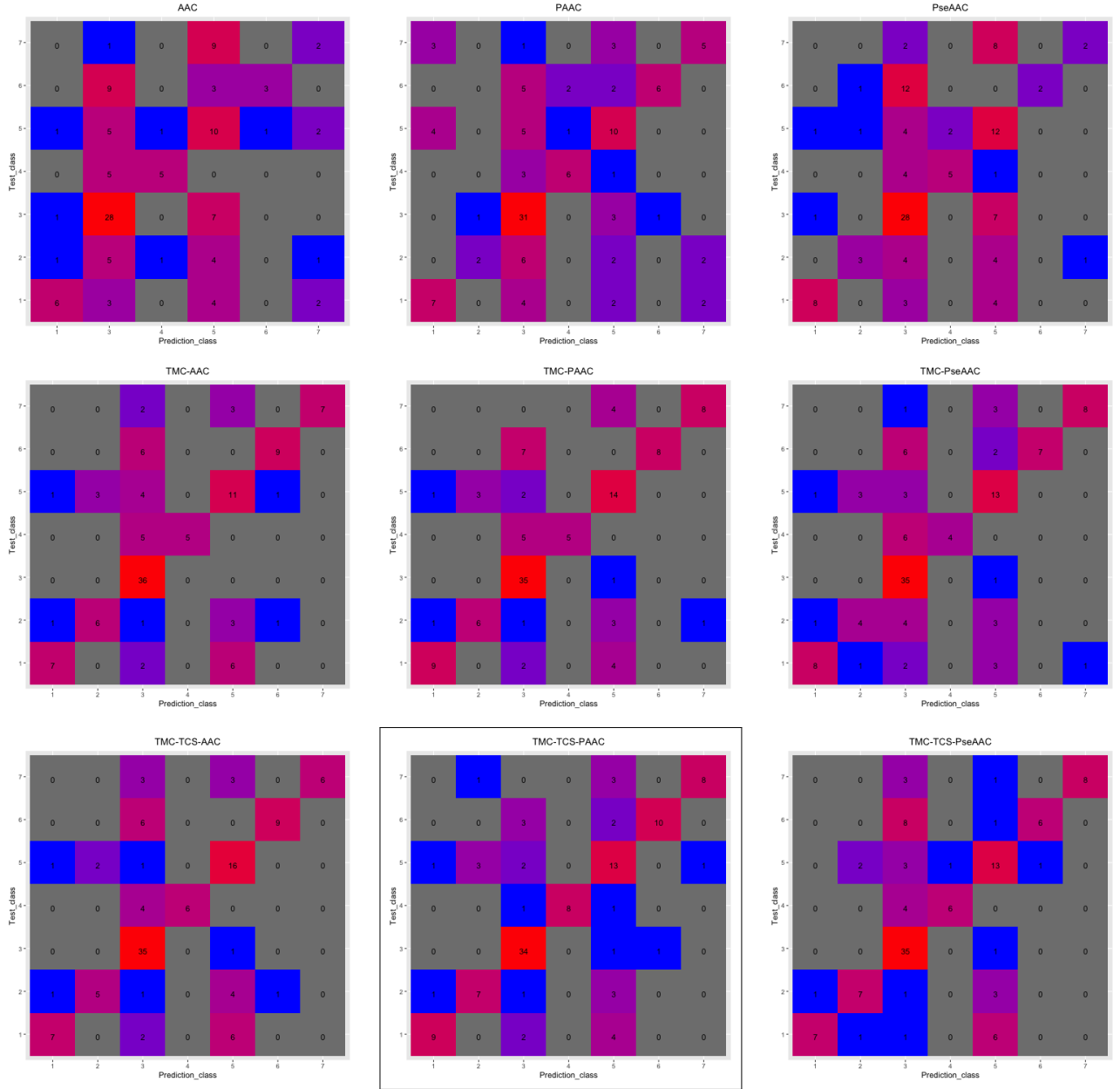


Figure 5: Confusion matrices

This figure presents the number of proteins in an actual substrate class that are predicted by different SVM models with different methods. The bordered matrix indicates the proposed tool prediction. The class can belong to one of the following seven categories (ordered alphabetically): [1] amino [2] anion [3] cation [4] electron [5] other [6] protein [7] sugar.

3 Protein compositions

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	97.14	40.00	81.82	0.42
Anion	100.00	0.00	81.82	
Cation	66.67	77.78	60.00	0.26
Electron	98.18	50.00	88.53	0.54
Protein	99.05	20.00	80.60	0.32
Sugar	95.37	16.67	78.26	0.10
Other	73.00	50.00	59.34	0.10
Overall			45.00	

Table 1: AAC independant testing performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	93.33	46.67	81.71	0.37
Anion	99.07	16.67	85.90	0.28
Cation	71.43	86.11	69.79	0.45
Electron	97.27	60.00	90.54	0.58
Protein	99.05	40.00	87.01	0.53
Sugar	96.30	41.67	85.90	0.40
Other	87.00	50.00	74.44	0.30
Overall			55.83	0.42

Table 2: PAAC independant testing performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.09	53.33	86.96	0.58
Anion	98.15	25.00	84.51	0.32
Cation	65.48	77.78	61.86	0.30
Electron	98.18	50.00	89.55	0.54
Protein	100.00	13.33	82.19	0.33
Sugar	99.07	16.67	84.51	0.28
Other	76.00	60.00	65.22	0.23
Overall			50.00	0.37

Table 3: PseAAC independant testing performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.09	46.67	89.01	0.55
Anion	97.22	50.00	90.00	0.52
Cation	76.19	100.00	80.20	0.67
Electron	100.00	50.00	94.19	0.68
Protein	98.09	60.00	91.01	0.65
Sugar	100.00	58.33	94.19	0.74
Other	88.00	55.00	79.41	0.38
Overall			67.50	0.60

Table 4: TMC-AAC independant testing performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.09	60.00	91.40	0.65
Anion	97.22	50.00	90.43	0.53
Cation	79.76	97.22	82.52	0.69
Electron	100.00	50.00	94.44	0.69
Protein	100.00	53.33	92.39	0.70
Sugar	99.07	66.67	94.44	0.74
Other	88.00	70.00	82.52	0.51
Overall			70.83	0.64

Table 5: TMC-PAAC independant testing performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.09	53.33	89.77	0.60
Anion	96.30	33.33	86.81	0.34
Cation	73.81	97.22	77.45	0.61
Electron	100.00	40.00	92.94	0.61
Protein	100.00	46.67	90.81	0.65
Sugar	99.07	66.67	94.05	0.74
Other	88.00	65.00	80.61	0.46
Overall			65.83	0.57

Table 6: TMC-PseAAC independant testing performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.09	46.67	89.36	0.55
Anion	98.15	41.67	90.32	0.50
Cation	79.76	97.22	82.35	0.68
Electron	100.00	60.00	95.45	0.76
Protein	99.05	60.00	92.31	0.70
Sugar	100.00	50.00	93.33	0.68
Other	86.00	80.00	82.35	0.55
Overall			70.00	0.63

Table 7: TMC-TCS-AAC independant testing performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.10	60.00	91.75	0.66
Anion	96.30	58.33	90.82	0.56
Cation	89.29	94.44	89.00	0.78
Electron	100.00	80.00	97.80	0.88
Protein	99.07	66.67	93.68	0.75
Sugar	99.07	66.67	94.68	0.74
Other	86.00	65.00	80.91	0.44
Overall			74.17	0.69

Table 8: TMC-TCS-PAAC independant testing performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	99.05	46.67	90.11	0.59
Anion	97.22	58.33	91.11	0.59
Cation	76.19	97.22	79.61	0.64
Electron	99.09	60.00	94.25	0.69
Protein	99.05	40.00	89.13	0.54
Sugar	100.00	66.67	95.35	0.80
Other	88.00	65.00	81.19	0.46
Overall			68.33	0.62

Table 9: TMC-TCS-PseAAC independant testing performance