

Leave-one-out Cross-Validation Performance

1 Performance Plots

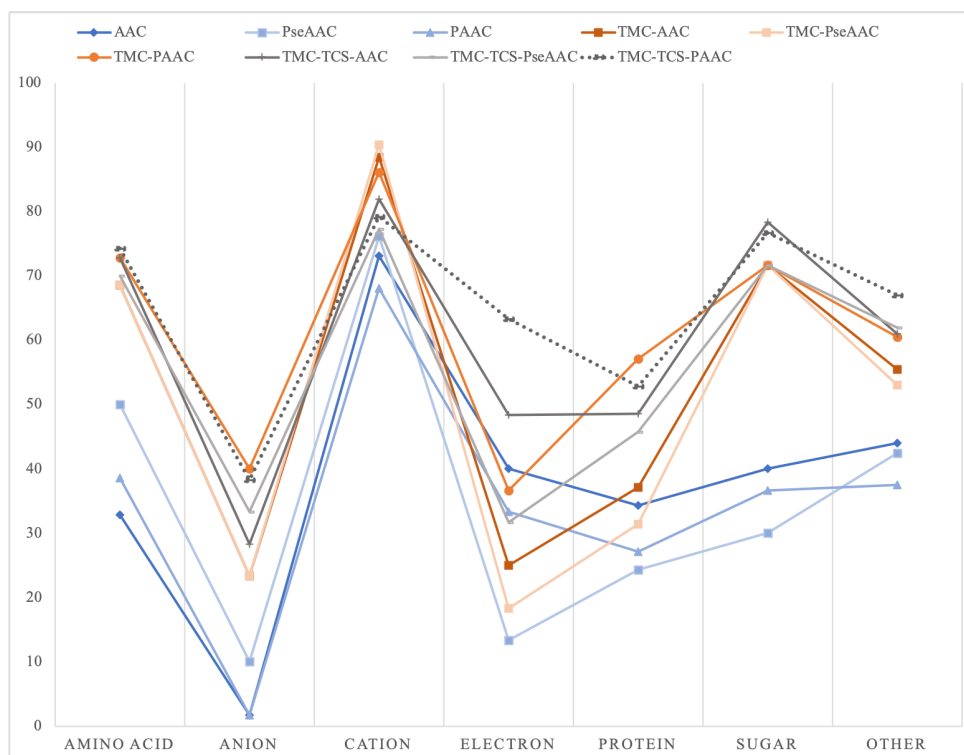


Figure 1: Sensitivity of different methods on different classes

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

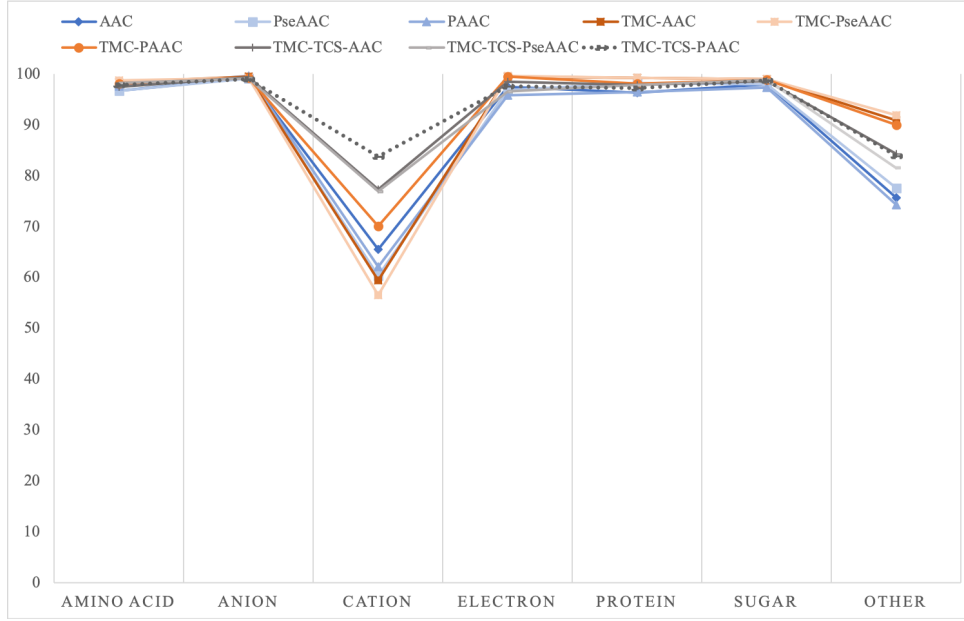


Figure 2: Specificity of different methods on different classes

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

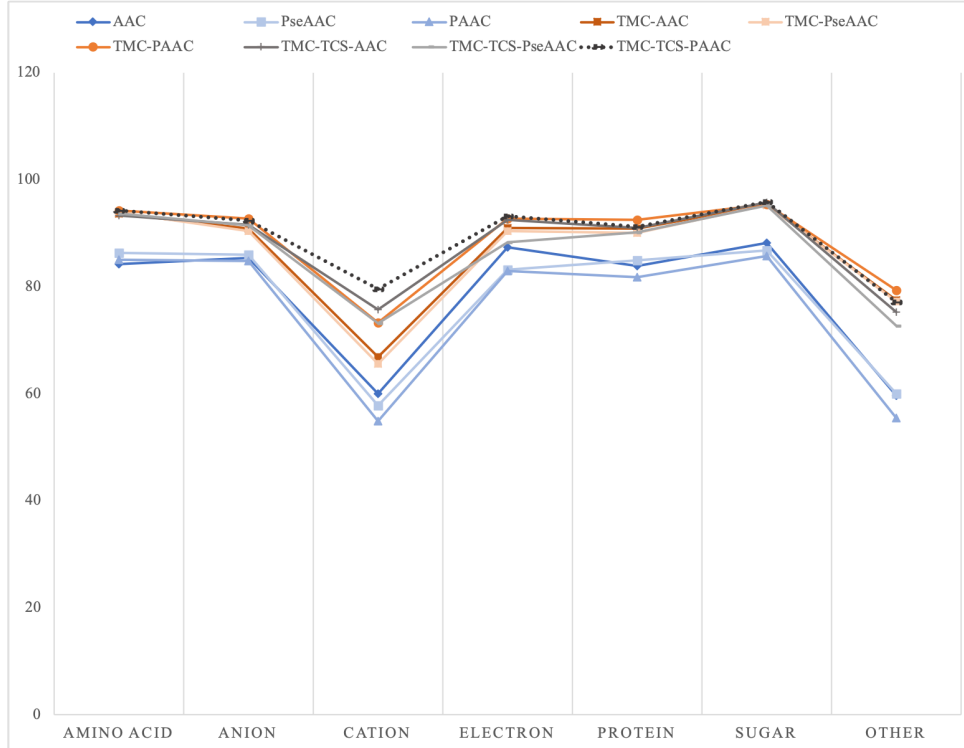


Figure 3: Accuracy of different methods on different classes

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

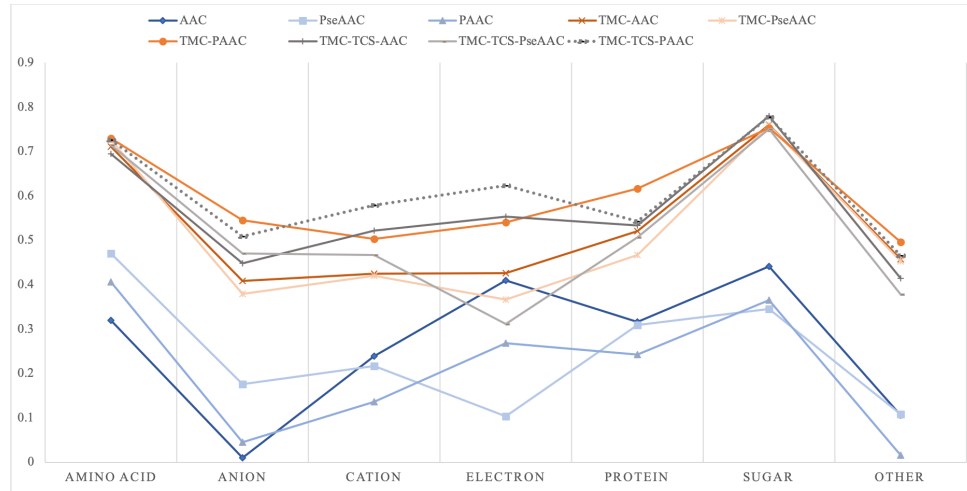


Figure 4: MCC of different methods on different classes

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

2 Protein compositions

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	96.76	32.86	84.23	0.32
Anion	99.31	1.67	85.39	0.01
Cation	65.58	73.08	60.03	0.24
Electron	97.50	40.00	87.38	0.41
Protein	96.34	34.29	83.86	0.32
Sugar	98.06	40.00	88.21	0.44
Other	75.69	44.00	59.65	0.11
Overall			47.95	0.26

Table 1: AAC LOOCV performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	97.61	38.57	85.04	0.41
Anion	99.72	1.67	84.83	0.04
Cation	62.12	68.08	54.91	0.14
Electron	95.83	33.33	82.97	0.27
Protein	96.48	27.14	81.78	0.24
Sugar	97.36	36.67	85.68	0.37
Other	74.31	37.50	55.45	0.02
Overall			43.72	0.21

Table 2: PAAC LOOCV performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	96.76	50.00	86.35	0.47
Anion	99.17	10.00	85.95	0.18
Cation	60.38	76.15	57.80	0.22
Electron	96.94	13.33	83.22	0.10
Protein	98.31	24.29	84.95	0.31
Sugar	98.06	30.00	86.76	0.34
Other	77.59	42.50	59.97	0.11
Overall			47.05	0.25

Table 3: PseAAC LOOCV performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.45	68.57	93.65	0.71
Anion	99.58	23.33	90.86	0.41
Cation	59.42	88.46	66.90	0.43
Electron	99.58	25.00	91.03	0.43
Protein	99.30	37.14	90.86	0.52
Sugar	99.03	71.67	95.30	0.76
Other	90.86	55.50	77.42	0.46
Overall			62.44	0.53

Table 4: TMC-AAC LOOCV performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.17	72.86	94.25	0.73
Anion	99.31	40.00	92.76	0.54
Cation	70.19	86.15	73.32	0.50
Electron	99.58	36.67	92.76	0.54
Protein	98.17	57.14	92.43	0.62
Sugar	98.89	71.67	95.45	0.75
Other	90.00	60.50	79.31	0.50
Overall			67.31	0.60

Table 5: TMC-PAAC LOOCV performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.73	68.57	93.92	0.73
Anion	99.31	23.33	90.38	0.38
Cation	56.54	90.39	65.62	0.42
Electron	99.72	18.33	90.38	0.37
Protein	99.30	31.43	90.04	0.47
Sugar	99.03	71.67	95.23	0.76
Other	91.90	53.00	77.26	0.45
Overall			61.41	0.51

Table 6: TMC-PseAAC LOOCV performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	97.47	72.86	93.27	0.70
Anion	99.44	28.33	91.61	0.45
Cation	77.31	81.92	75.66	0.52
Electron	98.47	48.33	92.43	0.55
Protein	97.89	48.57	90.96	0.53
Sugar	98.61	78.33	95.71	0.78
Other	84.31	61.00	75.22	0.41
Overall			65.77	0.56

Table 7: TMC-TCS-AAC LOOCV performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	97.89	74.29	94.20	0.73
Anion	99.03	38.33	92.41	0.51
Cation	83.85	79.23	79.53	0.58
Electron	97.64	63.33	93.22	0.62
Protein	97.32	52.86	91.16	0.54
Sugar	98.75	76.67	95.89	0.78
Other	83.97	67.00	77.12	0.47
Overall			68.72	0.60

Table 8: TMC-TCS-PAAC LOOCV performance

Class	Specificity	Sensitivity	Accuracy	MCC
Amino acid	98.31	70.00	93.67	0.71
Anion	99.17	33.33	91.39	0.47
Cation	76.92	77.31	73.16	0.47
Electron	96.67	31.67	88.25	0.31
Protein	97.89	45.71	90.20	0.51
Sugar	98.89	71.67	95.13	0.75
Other	81.55	62.00	72.73	0.38
Overall			62.56	0.51

Table 9: TMC-TCS-PseAAC LOOCV performance