

Detailed results for polymer classification

Table 1: Performance metrics of CNN-KAN and simple CNN for polymer classification dataset. All results are presented as %, except for the standard deviation, which is expressed in percentage points.

Results for CNN-KAN architecture						
	Train dataset			Test dataset		
Trial no	acc.	spec.	rec.	acc.	spec.	rec.
1	94.71	98.93	94.56	95.17	99.07	95.57
2	94.54	98.9	94.39	94.33	98.9	94.81
3	98.75	99.75	98.76	97.83	99.58	97.79
4	93.83	98.76	93.66	93.33	98.69	93.94
5	99.75	99.95	99.75	99.17	99.83	99.19
6	89.92	97.98	89.75	91.33	98.29	91.84
7	98.71	99.74	98.69	98.5	99.71	98.55
8	95.62	99.12	95.5	95.17	99.07	95.55
9	98.71	99.74	98.69	98.5	99.71	98.55
10	83.0	96.61	82.96	82.0	96.34	82.15
Avg.	94.75	98.95	94.67	94.53	98.92	94.79
Std. Dev.	4.9	0.97	4.9	4.8	0.98	4.8

Results for simple CNN architecture						
	Train dataset			Test dataset		
Trial no	acc.	spec.	rec.	acc.	spec.	rec.
1	83.0	96.61	82.96	82.0	96.34	82.15
2	77.38	95.48	77.15	76.33	95.24	77.15
3	83.17	96.65	83.12	82.83	96.51	82.97
4	83.12	96.64	83.08	82.17	96.37	82.36
5	94.38	98.87	94.21	94.0	98.82	94.55
6	94.75	98.94	94.59	94.5	98.94	95.01
7	99.79	99.96	99.79	99.33	99.87	99.33
8	98.92	99.78	98.9	99.0	99.8	98.98
9	96.12	99.22	96.01	96.0	99.23	96.35
10	78.12	95.63	77.93	77.67	95.49	78.35
Avg.	88.87	97.78	88.77	88.38	97.66	88.72
Std. Dev.	8.3	1.6	8.3	8.5	1.7	8.4

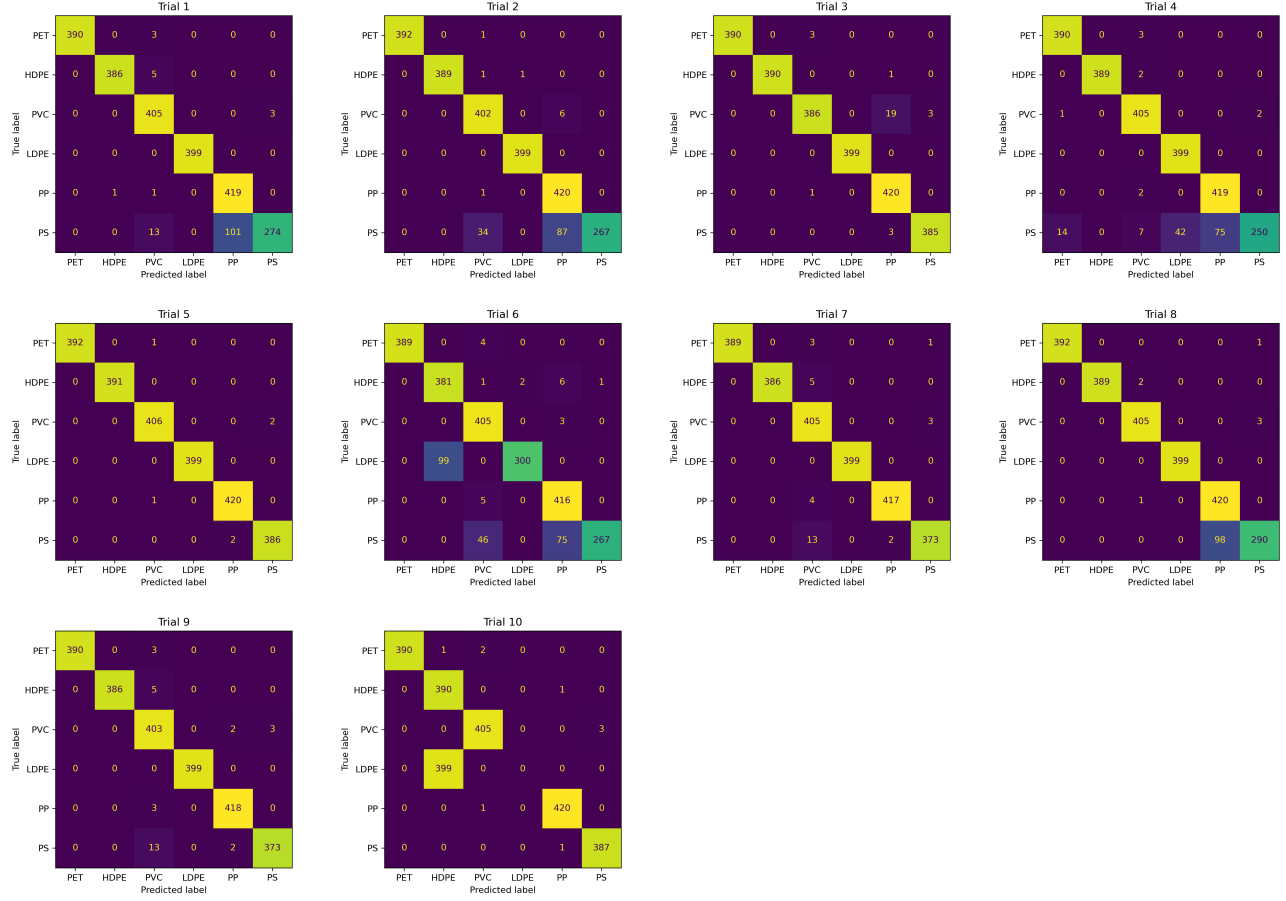


Figure 1: Confusion matrices for the CNN-KAN architecture on the training set.

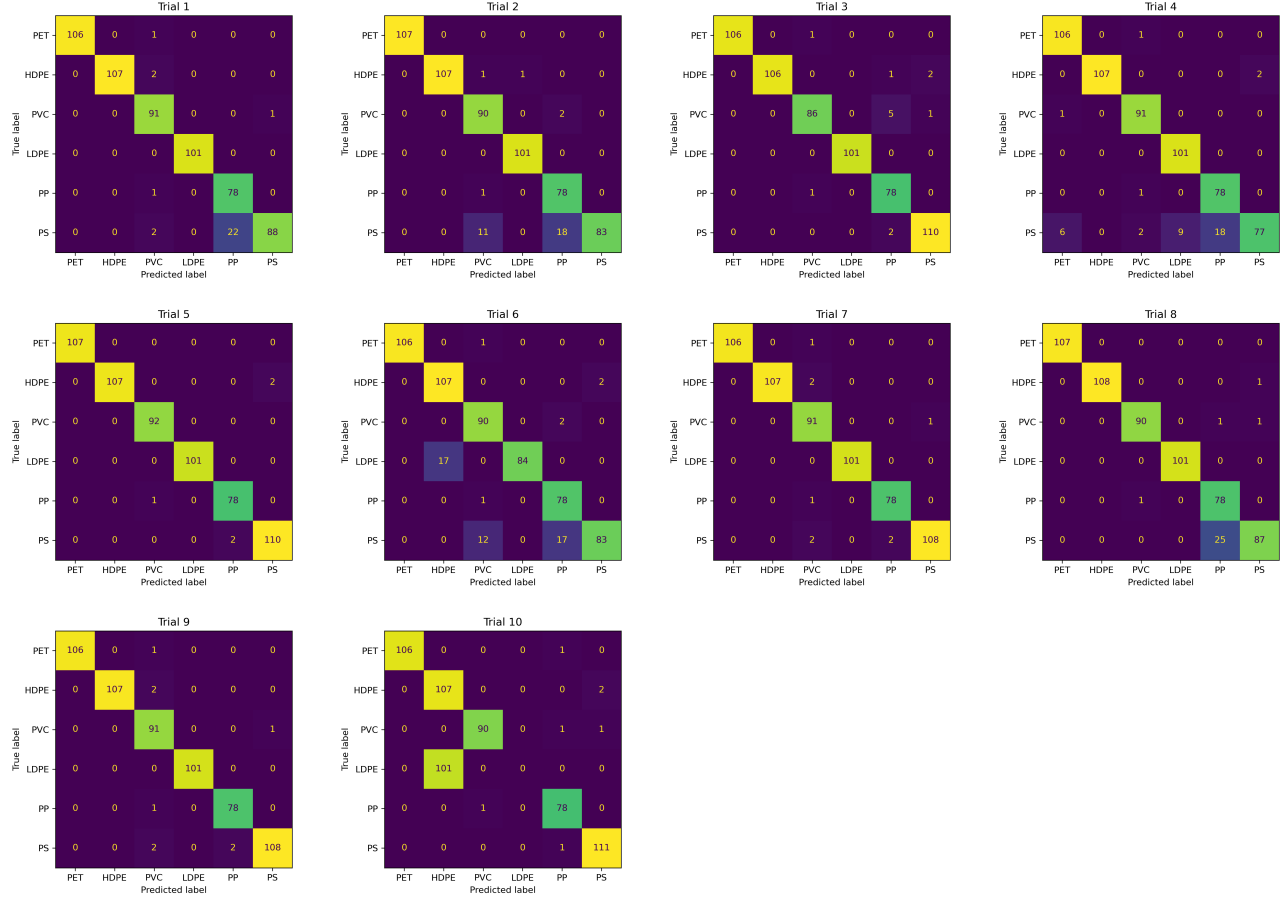


Figure 2: Confusion matrices for the CNN-KAN architecture on the test set.

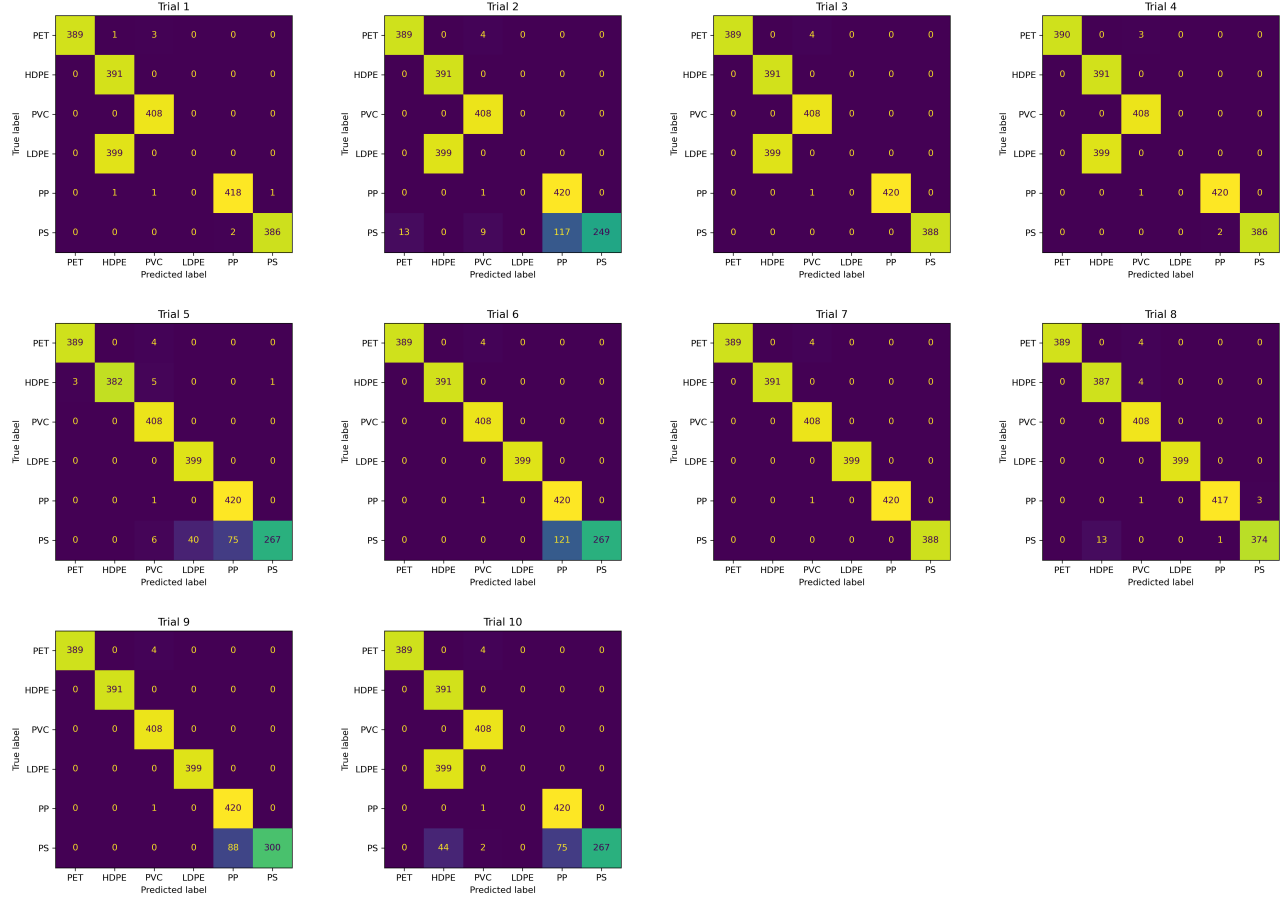


Figure 3: Confusion matrices for the simple CNN architecture on the training set.

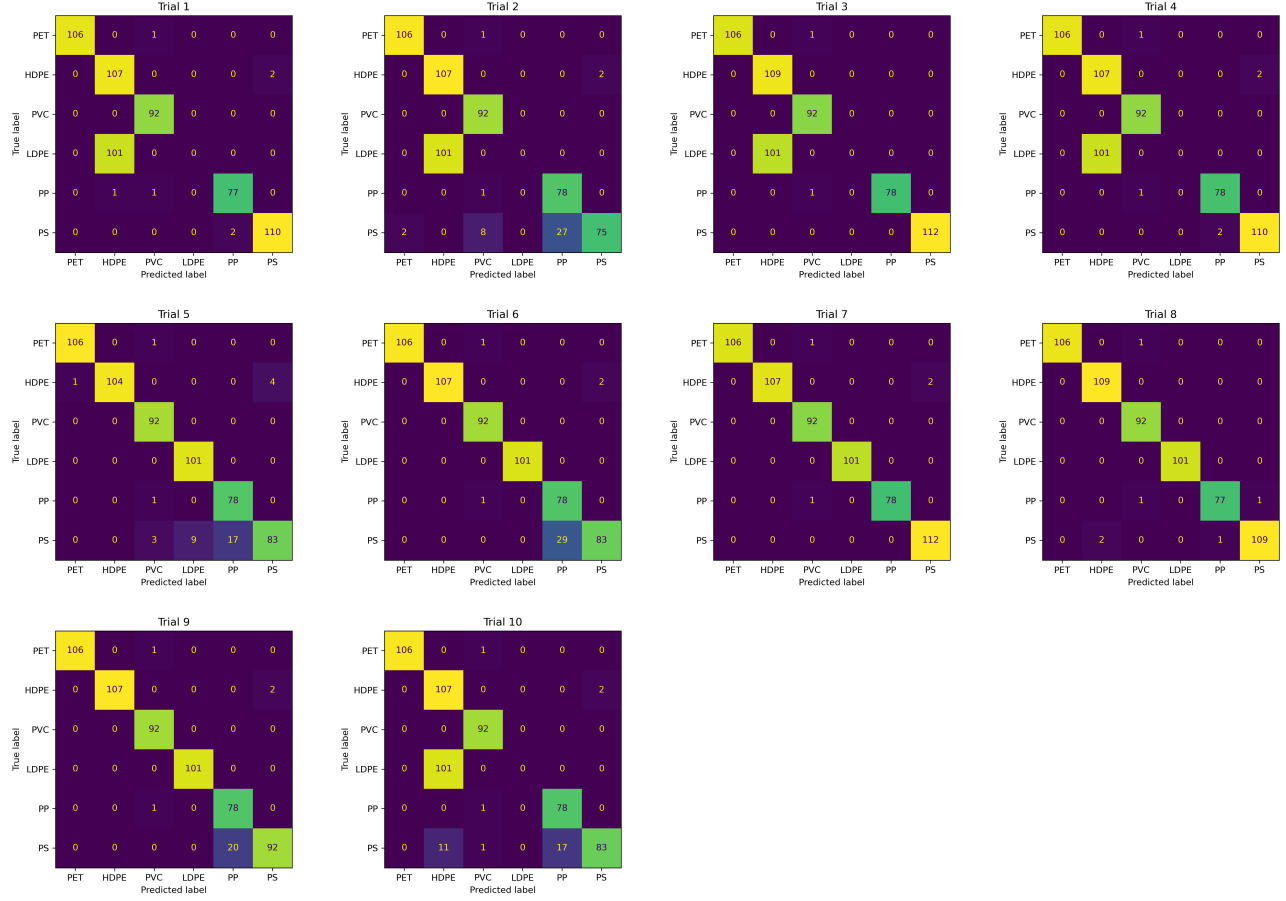


Figure 4: Confusion matrices for the simple CNN architecture on the test set.