

S1 Table Confusion matrix summary from the models built with Accuracy as a performance metric.

Model	Confusion matrix metrics				
	TP (True positives)	FN (False Negatives)	TN (True Negatives)	FP (False positives)	Detection rate (DR)
PLS-DA	26	8	62	10	0.245
SVM linear	23	11	58	14	0.217
SVM poly	21	13	63	9	0.198
SVM radial	28	6	56	16	0.264
RF	16	18	72	0	0.151
	Sensitivity (TPR)	Miss rate (FNR)	Specificity (TNR)	Fall out rate (FPR)	Diagnostic odd ratio (DOR)
PLS-DA	0.865	0.235	0.861	0.139	20.150
SVM linear	0.676	0.324	0.806	0.194	8.662
SVM poly	0.618	0.382	0.875	0.125	11.308
SVM radial	0.824	0.176	0.778	0.222	16.333
RF	0.471	0.529	1.000	0.000	-
	Precision (PPV)	False discovery rate (FDR)	Negative prediction (NPV)	False omission rate (FOR)	F ₁ -score
PLS-DA	0.722	0.278	0.886	0.114	0.743
SVM linear	0.622	0.378	0.841	0.159	0.648
SVM poly	0.700	0.300	0.829	0.171	0.656
SVM radial	0.636	0.364	0.903	0.097	0.718
RF	1.000	0.000	0.800	0.200	0.640
	Accuracy (Acc)	Balanced Accuracy	Pr(e)	Cohen's Kappa	MCM
PLS-DA	0.830	0.813	0.558	0.616	0.617
SVM linear	0.764	0.741	0.554	0.471	0.472
SVM poly	0.792	0.746	0.578	0.508	0.510
SVM radial	0.792	0.801	0.530	0.558	0.570
RF	0.830	0.735	0.625	0.547	0.614

The abbreviature MCC signifies Matthews correlation coefficient and Pr(e) means Expected random agreement.