

**Table S4.** Performances of the optimized RF and SVM models with MOE descriptors on the external validation set.

<b>Descriptors</b>	<b>Models</b>	<b>Accuracy %</b>	<b>Sensitivity %</b>	<b>Specificity %</b>	<b>MCC %</b>
15 MOE	RF	83.16	86.66	78.65	67.36
	SVM	82.49	86.76	76.97	65.89
20 MOE	RF	83.39	86.56	79.30	68.27
	SVM	82.09	86.26	76.71	68.11
36 MOE	RF	83.95	87.06	79.95	69.47
	SVM	82.66	87.36	76.58	66.52
170 MOE	RF	84.18	87.96	79.30	70.85
	SVM	84.75	88.47	79.95	70.32