

**Table S2.** Performances of preliminary RF models with the best MOE descriptors on the training set.

<b>Descriptors</b>	10 MOE	15 MOE	20 MOE	30 MOE	40 MOE
<b>Balanced accuracy %</b>	72.27	75.57	78.61	79.43	77.80
<b>Sensitivity %</b>	77.45	75.46	79.82	81.57	78.98
<b>Specificity %</b>	67.08	75.67	77.39	77.29	76.62