

Table S3. Parameters of the optimized best RF and SVM models.

Best models	15 MOE +7 IE descriptors	20 MOE +7 IE descriptors	36 MOE +7 IE descriptors	170 MOE +7 IE descriptors
RF <i>n</i>tree	250	300	275	275
RF <i>m</i>try	7	7	11	9
SVM Cost	8	4	8	4
SVM Sigma	0.0452	0.0348	0.0203	0.0036