

**Table S1.** Optimized hyperparameters for the ML algorithms applied to the *M. canis* dataset.

<b>model_name</b>	RF	SVC	GB	LR	KNN
<b>preprocess_fn</b>	baug10	baug10	baug10	baug10	baug10
<b>model</b>	bootstrap=True ccp_alpha=0.0 class_weight=None criterion='gini' max_depth=None max_features='auto' max_leaf_nodes=None max_samples=None min_impurity_decrease=0.0 min_impurity_split=None min_samples_leaf=1 min_samples_split=2 min_weight_fraction_leaf=0.0 n_estimators=2 n_jobs=None oob_score=False random_state=None verbose=0 warm_start=False	C=0.1 break_ties=False cache_size=200 class_weight=None coef0=0.0 decision_function_shape='ovr' degree=3 gamma='scale' kernel='linear' max_iter=-1 probability=False random_state=None shrinking=True tol=0.001 verbose=False	ccp_alpha=0.0 criterion='friedman_mse' init=None learning_rate=0.1 loss='deviance' max_depth=3 max_features='log2' max_leaf_nodes=None min_impurity_decrease=0.0 min_impurity_split=None min_samples_leaf=1 min_samples_split=2 min_weight_fraction_leaf=0.0 n_estimators=7 n_iter_no_change=None presort='deprecated' random_state=None subsample=1.0 tol=0.0001 validation_fraction=0.1 verbose=0 warm_start=False	C=0.1 class_weight=None dual=False fit_intercept=True intercept_scaling=1 l1_ratio=None max_iter=100 multi_class='auto' n_jobs=None penalty='l2' random_state=None solver='lbfgs' tol=0.0001 verbose=0 warm_start=False	algorithm='auto' leaf_size=30 metric='minkowski' metric_params=None n_jobs=None n_neighbors=1 p=2 weights='uniform'
<b>threshold</b>	20	20	20	20	20
<b>component_min</b>	0	0	0	0	0
<b>kfold</b>	5	5	5	5	5
<b>pc</b>	0	0	0	0	0
<b>mcc_cv</b>	0.84	0.77	0.77	0.774	0.66
<b>acc_cv</b>	0.95	0.93	0.93	0.937	0.88
<b>mcc_fit</b>	1	0.95	0.95	0.952	1
<b>acc_fit</b>	1	0.98	0.98	0.989	1
<b>pca</b>					
<b>idx</b>	36531	36339	36434	36699	36692

**Table S2.** Optimized hyperparameters for the ML algorithms applied to the *M. gypseum* dataset.

<b>model_name</b>	SVC	LR	GB	RF	KNN
<b>preprocess_fn</b>	baug10	baug10	baug10	baug10	baug10
<b>model</b>	C=0.1 break_ties=False cache_size=200 class_weight=None coef0=0.0 decision_function_shape='ovr' degree=3 gamma='scale' kernel='linear' max_iter=-1 probability=False random_state=None shrinking=True tol=0.001 verbose=False	C=0.1 class_weight=None dual=False fit_intercept=True intercept_scaling=1 l1_ratio=None max_iter=100 multi_class='auto' n_jobs=None penalty='l2' random_state=None solver='lbfgs' tol=0.0001 verbose=0 warm_start=False	ccp_alpha=0.0 criterion='friedman_mse' init=None learning_rate=0.01 loss='deviance' max_depth=3 max_features=10 max_leaf_nodes=None min_impurity_decrease=0.0 min_impurity_split=None min_samples_leaf=1 min_samples_split=2 min_weight_fraction_leaf=0.0 n_estimators=10 n_iter_no_change=None presort='deprecated' random_state=None subsample=1.0 tol=0.0001 validation_fraction=0.1 verbose=0 warm_start=False	(bootstrap=True ccp_alpha=0.0 class_weight='balanced' criterion='gini' max_depth=9 max_features='auto' max_leaf_nodes=None max_samples=None min_impurity_decrease=0.0 min_impurity_split=None min_samples_leaf=1 min_samples_split=2 min_weight_fraction_leaf=0.0 n_estimators=5 n_jobs=None oob_score=False random_state=None verbose=0 warm_start=False	algorithm='auto' leaf_size=30 metric='minkowski' metric_params=None n_jobs=None n_neighbors=1 p=2 weights='uniform'
<b>threshold</b>	30	30	30	30	30
<b>component_min</b>	0	0	0	0	0
<b>kfold</b>	5	5	5	5	5
<b>pc</b>	0	0	0	0	0
<b>mcc_cv</b>	0.80	0.80	0.75	0.69	0.61
<b>acc_cv</b>	0.94	0.93	0.92	0.90	0.86
<b>mcc_fit</b>	0.95	1	0.45	1	1
<b>acc_fit</b>	0.98	1	0.64	1	1
<b>pca</b>					
<b>idx</b>	36339	36699	36485	36586	36692