Supplemental data

## Article

## Machine Learning Models Identify Molecules Active Against the Ebola Virus *In Vitro*

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**Supplemental data S1. Pseudotype bayesian model**

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| |  | | --- | | ROC score is 0.847 (leave-one-out). Best cutoff for this model is 0.812. | |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | **5-Fold Cross-Validation Result** | | | | | | | | | | | **Model Name** | **ROC Score** | **ROC Rating** | **True Positive** | **False Negative** | **False Positive** | **True Negative** | **Sensitivity** | **Specificity** | **Concordance** | | Ebola pseudoviral N868 | 0.846 | Good | 39 | 2 | 176 | 651 | 0.951 | 0.787 | 0.795 | | | C:\Users\sean\Documents\Discovery Studio\Results\CreateBayesianModel_2014_10_15_193044_538\Output\Report\images\image4602195027874986580.png  Leave out 50% x 100 fold cross validation   |  |  |  |  |  | | --- | --- | --- | --- | --- | | External\_ROC\_Score | Internal\_ROC\_Score | Concordance | Specificity | Sensitivity | | 0.82 | 0.82 | 79.98 | 80.52 | 68.90 | | 0.05 | 0.04 | 7.60 | 8.39 | 12.40 | | | |

**Supplemental data S2. EBOV replication Bayesian**

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| --- | --- |
| |  | | --- | | ROC score is 0.858 (leave-one-out). Best cutoff for this model is 6.770. See ModelDescription.html for more detailed information about this model. | |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | **5-Fold Cross-Validation Result** | | | | | | | | | | | **Model Name** | **ROC Score** | **ROC Rating** | **True Positive** | **False Negative** | **False Positive** | **True Negative** | **Sensitivity** | **Specificity** | **Concordance** | | Ebola EBOV rep N868 USES CHLOROQUINE AND TOREMIFENE | 0.867 | Good | 19 | 1 | 239 | 609 | 0.950 | 0.718 | 0.724 | | |  | | |

Leave out 50% x 100 fold cross validation

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| External\_ROC\_Score | Internal\_ROC\_Score | Concordance | Specificity | Sensitivity |
| 0.84 | 0.85 | 75.66 | 75.81 | 67.67 |
| 0.05 | 0.05 | 13.57 | 14.26 | 21.07 |

**Supplemental Data S3. SVM output file for Pseudotype model**

FitSummary

Call:

svm(formula = form, data = xy, type = type, kernel = tolower("Radial"),

gamma = gamma, cost = cost, probability = prob, fitted = TRUE,

epsilon = epsilon, nu = nu, coef0 = coef0, degree = degree, scale = TRUE)

Parameters:

SVM-Type: C-classification

SVM-Kernel: radial

cost: 2

gamma: 0.007352941

Number of Support Vectors: 307

( 266 41 )

Number of Classes: 2

Levels:

0 1

Cross-validation results (5-fold):

Gamma Cost ROC Score Best

1 0.007353 1 0.7538

2 0.007353 2 0.7598 \*\*\*

Contingency Table (best CV model):

Predicted

Actual 0 1

0 823 4

1 41 0

All-data model results (non-cross-validated):

Settings used:

Gamma Cost

0.007352941 2

ROC Score: 0.9997

Contingency Table (all-data model):

Predicted

Actual 0 1

0 827 0

1 13 28

FitPlot

Binary Property

**Supplemental Data S4. SVM output file for EBOV replication model**

FitSummary

Call:

svm(formula = form, data = xy, type = type, kernel = tolower("Radial"),

gamma = gamma, cost = cost, probability = prob, fitted = TRUE,

epsilon = epsilon, nu = nu, coef0 = coef0, degree = degree, scale = TRUE)

Parameters:

SVM-Type: C-classification

SVM-Kernel: radial

cost: 2

gamma: 0.007352941

Number of Support Vectors: 222

( 202 20 )

Number of Classes: 2

Levels:

0 1

Cross-validation results (5-fold):

Gamma Cost ROC Score Best

1 0.007353 1 0.7235

2 0.007353 2 0.7263 \*\*\*

Contingency Table (best CV model):

Predicted

Actual 0 1

0 845 3

1 20 0

All-data model results (non-cross-validated):

Settings used:

Gamma Cost

0.007352941 2

ROC Score: 1

Contingency Table (all-data model):

Predicted

Actual 0 1

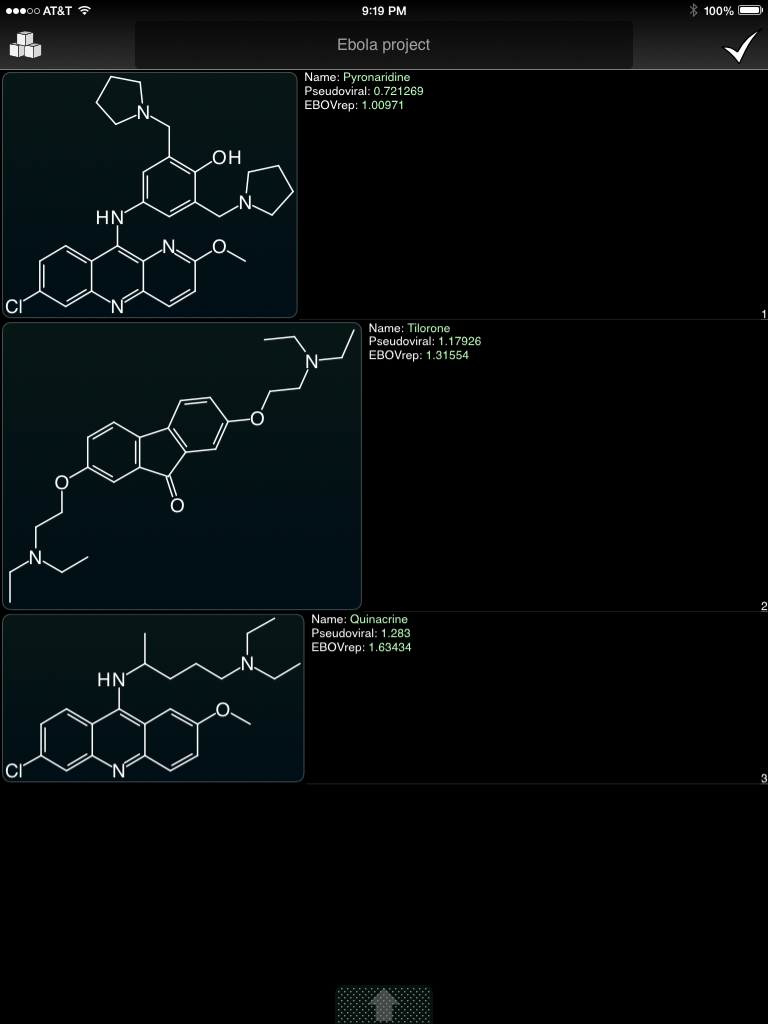
0 848 0

1 5 15

FitPlot

Binary Property

**Supplemental Data S6. Predictions for Ebola activity using Open Bayesian models in the MMDS app.** Higher scores are more likely to be active.

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**Supplemental Data S7. High content screening images illustrating inhibition of Ebola and cytotoxic concentration.**

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