

Accurate Prediction for Antibody Resistance of Clinical HIV-1 Isolates

Reda Rawi¹, Raghvendra Mall², Chen-Hsiang Shen¹, S. Katie Farney¹, Andrea Shiakolas¹, Jing Zhou¹, Halima Bensmail², Tae-Wook Chun³, Nicole A. Doria-Rose¹, Rebecca M. Lynch⁴, John R. Mascola¹, Peter D. Kwong¹ & Gwo-Yu Chuang^{1*}

¹*Vaccine Research Center, National Institute of Allergy and Infectious Diseases, National Institutes of Health, Bethesda, 20892, MD, USA*

²*Qatar Computing Research Institute, Hamad Bin Khalifa University, Doha, 34110, Qatar*

³*Laboratory of Immunoregulation, National Institute of Allergy and Infectious Diseases, National Institutes of Health, Bethesda, 20892, MD, USA*

⁴*Department of Microbiology, Immunology and Tropical Medicine, George Washington University, Washington, DC, USA*

* Corresponding author: gwo-yu.chuang@nih.gov

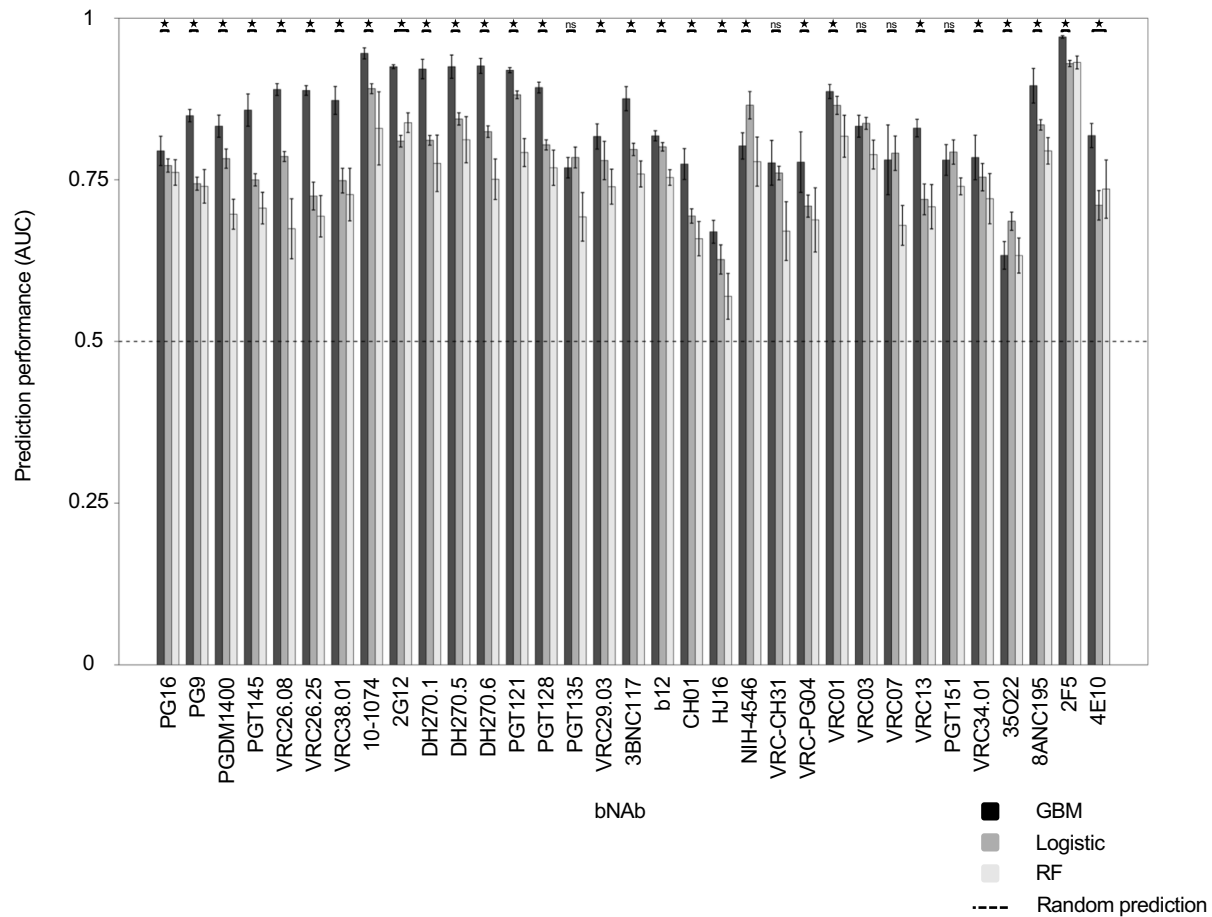


Figure S1. Prediction performance of GBM classifiers compared to Logistic Regression and Random Forest predictors.

Prediction performance (AUC) comparison of GBM (black bars), logistic regression (dark gray), and random forest (light gray) of 33 bNAb prediction models determined by ten runs of ten-fold cross-validation. For the sake of clarity, results from statistical significance testing are shown only for the top 2 models (*P-value < 0.05, ns = not significant).

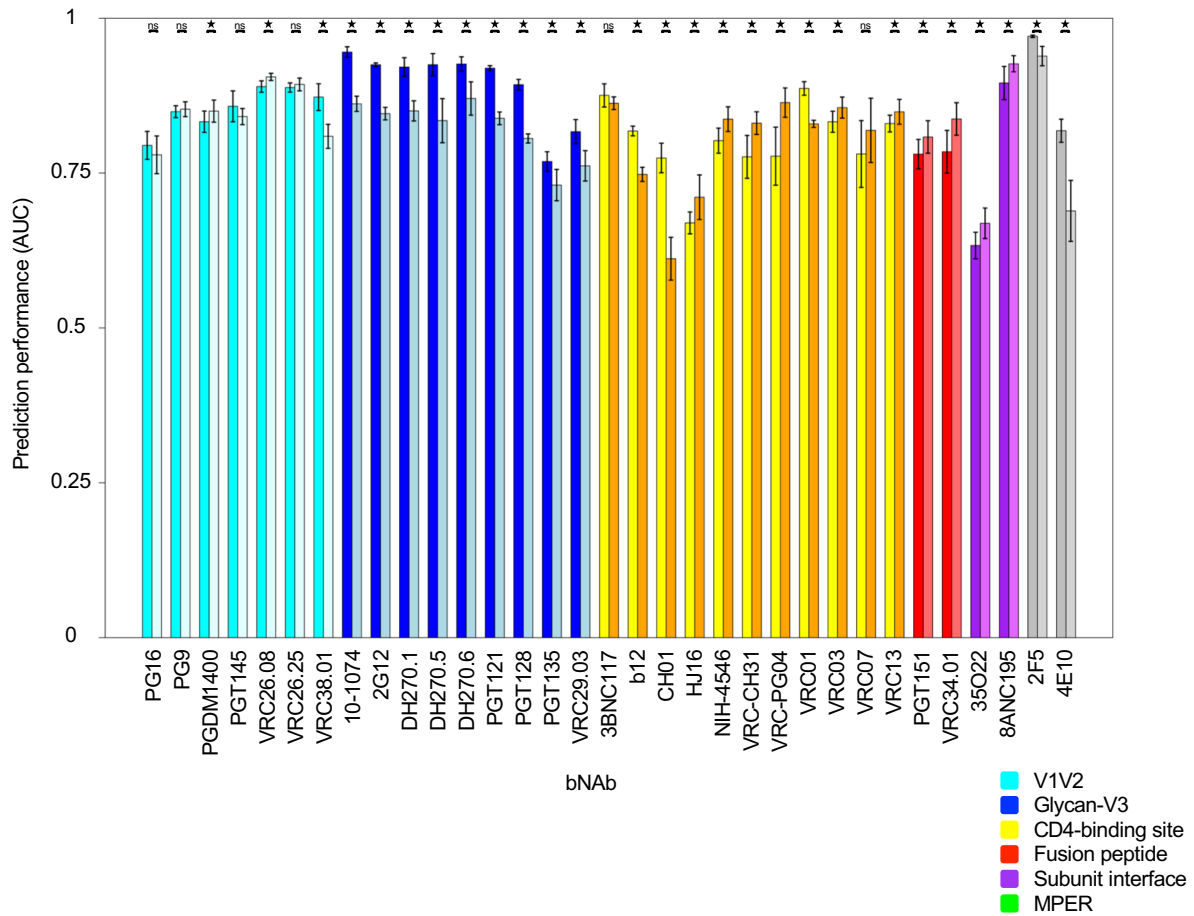


Figure S2. Prediction performance of bNAb classifiers using sequences comprising the full Env sequences or the epitope region only.

The prediction performance of the bNAb classifiers using full Env sequences or sequence subsets comprising epitope region only were determined by ten runs of ten-fold cross-validation and are shown as bar plots. The 33 different classifiers are shown on the x-axis, named according to the antibody they are trained on. The colors of the bars refer to the epitope category of the corresponding antibody. The left bar of each pair of bars refers to classifiers trained using full Env sequences, while the right bar refers to classifiers trained using epitope sequence subsets only.

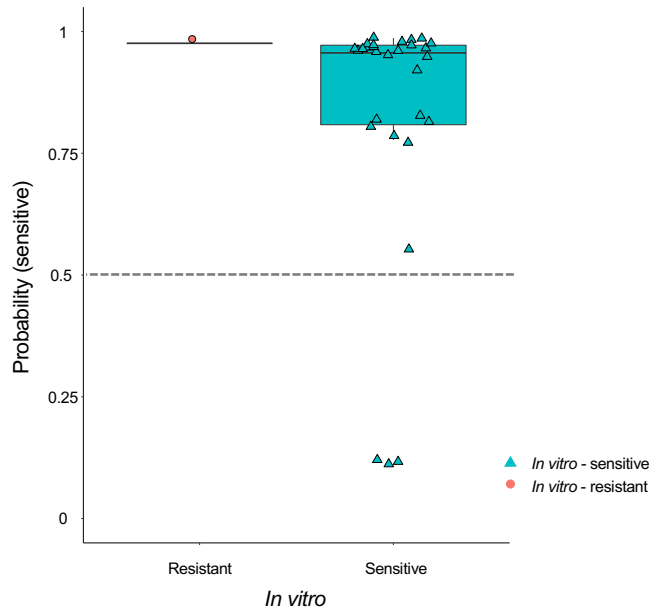


Figure S3. Prediction performance of bNAb-ReP on Env strains from bNAb 3BNC117 treatment study.

Prediction performance on bNAb 3BNC117 neutralization and sequence data shown as boxplot. *In vitro* assay neutralization classification is shown on the x-axis, with the *in silico* predicted probability for a sequence to be sensitive to 3BNC117 shown on the y-axis. The classification cutoff of 0.5 is depicted with a grey dashed line.

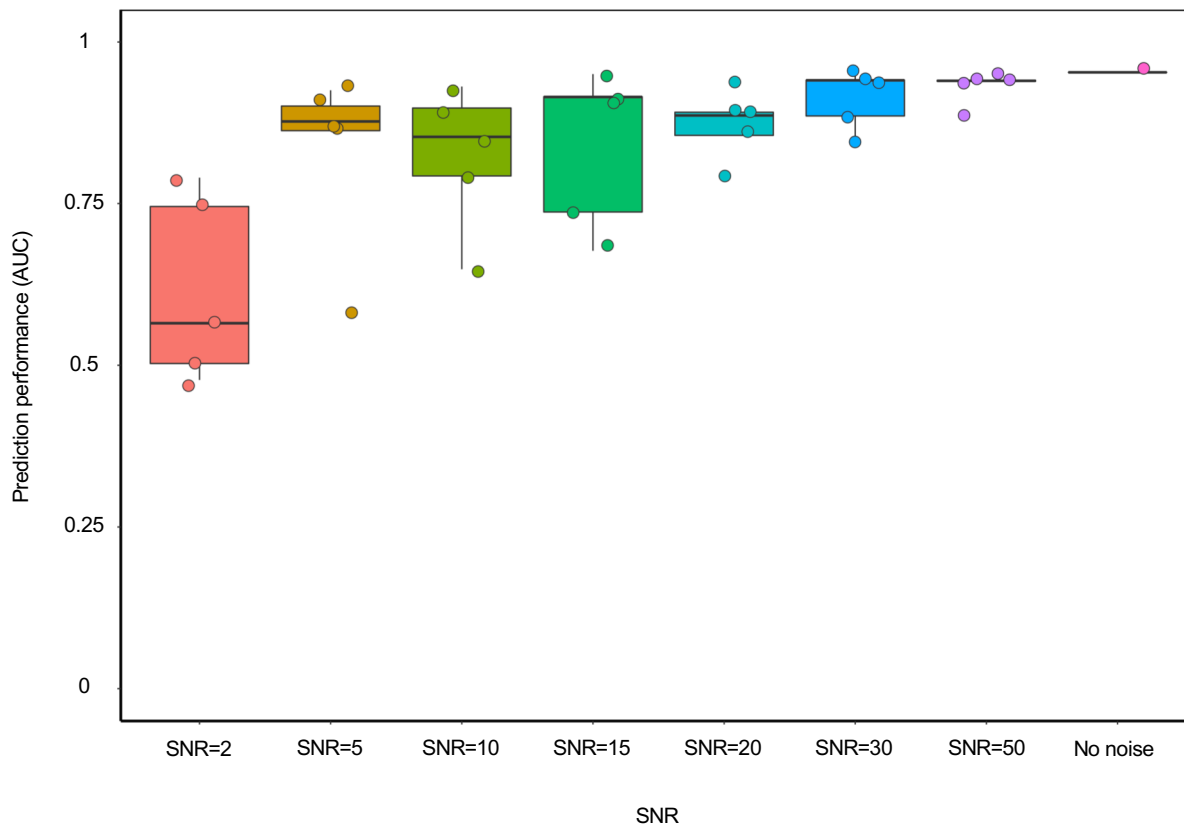


Figure S4. Prediction performance of VRC01 bNAb-ReP with noise added to training set. The prediction performance (AUC) of VRC01 bNAb-ReP with signal to noise ratio (SNR) = 2, 5, 10, 15, 20, 30, 50 on the Lynch et al. VRC01 test set is shown. Each SNR experiment was repeated five times.

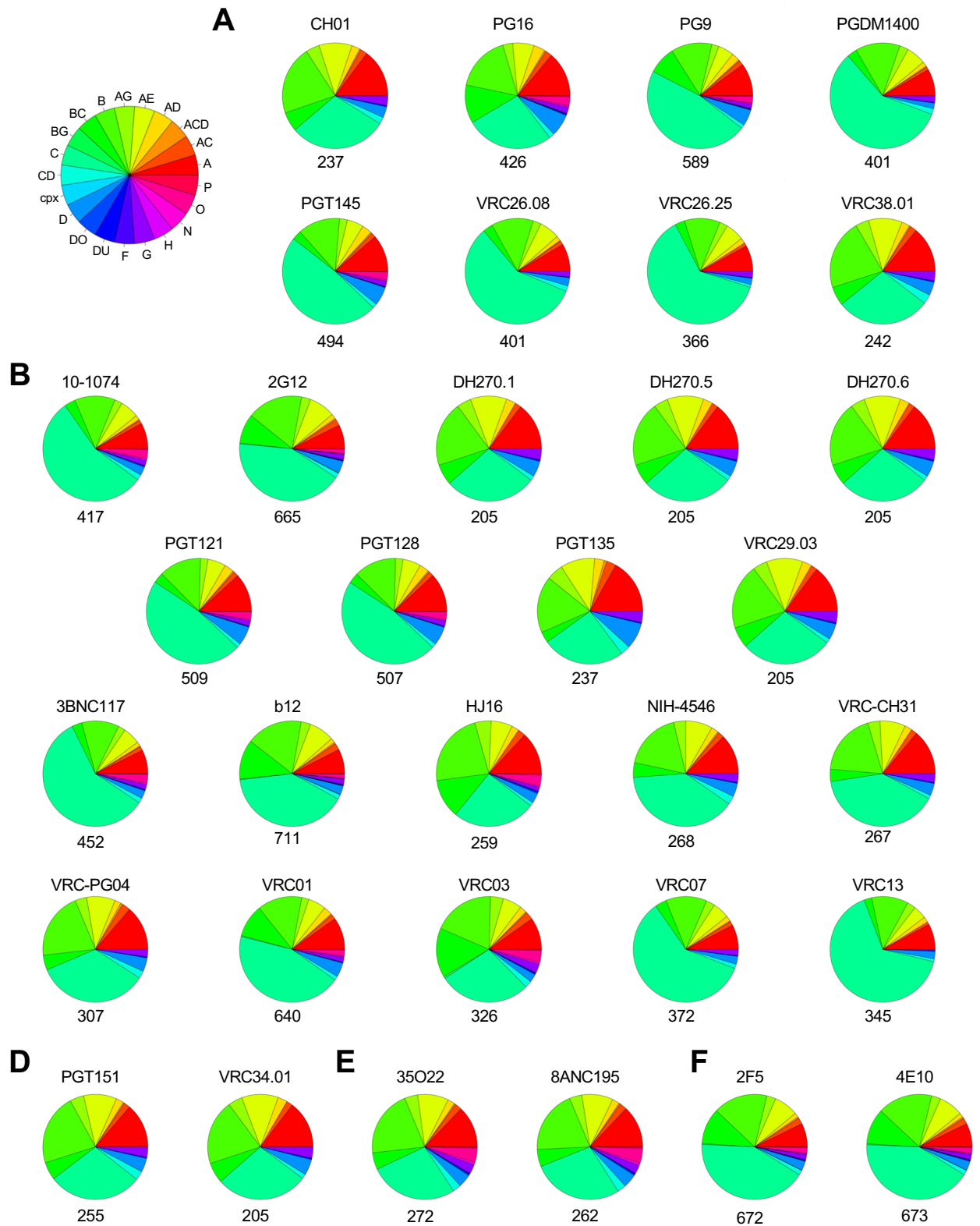


Figure S5. Training sets clade distributions

Clade distributions for each bNAb training set are illustrated as pie charts, with distinct epitope categories shown in (A) V1V2, (B) Glycan-V3, (C) CD4-binding site, (D) fusion peptide, (E) subunit interface, and (F) MPER. The number of strains within each training sets is depicted below the corresponding pie chart.

Supplementary Data S1. HIV-1 Env sequences of VRC01-ATI study

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V H L N E S V V I N C T R P N N N T R K S I N M -- G P G R A F Y A T - G I I G D I R Q A H C N I S R T A W N N T L K K
I V E K L R E Q F G K N K T I V F N Q S S G D P E I V T H S F N C G G E F F Y C N T T K L F N S T W N T S I --- E
H G S K D Q E G N I T L P C K I R Q I I N M W Q E V G K A M Y A P P I A G V I R C S S D I T G L L L T R D G G -- N E S
E S E G K E I F R P G G G D M R D N W R S E L Y K Y K V V K I E P L G I A P T K A K R R V V Q R E K R A V G - I G A L F
L G F L G A A G S T M G A A S I M L T G Q T R Q L L S G I V Q Q N N L L R A I E A Q Q H L L Q L T V W G I K Q L Q A R
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IVTKLREQFG-NKTIIFNKSSGGDPEITMHTFNCGGEFFYCDTGLFNSTWGFNDT---S
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>V09F_PRAp-2F9.2

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>V03NP_POVIp-2D5.10.2

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