**Table S1.** Accuracy, sensitivity, specificity, and MCC values of the IF-based ANN modelsa and DIF-based ANN modelsb in classifying the resistant and susceptible patterns for each ARVsc,d.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Metric | Model | ATV | DRV | FPV | IDV | LPV | NFV | SQV | TPV |
| Accuracy | IF | 0.912 | 0.953 | 0.907 | 0.888 | 0.919 | 0.893 | 0.890 | 0.958 |
| DIF | 0.917 | 0.941 | 0.927 | 0.898 | 0.924 | 0.912 | 0.925 | 0.943 |
| Sensitivity | IF | 0.857 | 0.876 | 0.823 | 0.783 | 0.869 | 0.845 | 0.829 | 0.755 |
| DIF | 0.872 | 0.817 | 0.850 | 0.816 | 0.894 | 0.894 | 0.865 | 0.762 |
| Specificity | IF | 0.946 | 0.964 | 0.928 | 0.944 | 0.956 | 0.933 | 0.913 | 0.970 |
| DIF | 0.944 | 0.961 | 0.948 | 0.940 | 0.944 | 0.925 | 0.949 | 0.947 |
| MCC | IF | 0.812 | 0.804 | 0.724 | 0.750 | 0.834 | 0.785 | 0.728 | 0.645 |
| DIF | 0.821 | 0.758 | 0.788 | 0.768 | 0.841 | 0.820 | 0.817 | 0.419 |

a IF (isolate-fold-change)-based models are trained for each inhibitor to predict fold-change values from the given isolate information.

bDIF (drug-isolate-fold-change)-based model is trained using all the data of the inhibitors to predict fold-change values from the descriptors of both isolates and molecules.

cAccuracy, sensitivity, and specificity values represent the rate of true predictions, true positive rate, and true negative rate, respectively.

d The threshold fold change value of 3 is chosen for classifying resistant and susceptible patterns.