**Table S1.** Mean square error (MSE), linear correlation coefficient (R) and area under the curve (AUC) metric values for linear regression (LR) and artificial neural network (ANN) models for predicting fold-change values in $IC\_{50}$ values of the six NRTIs.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Metric/Drug | 3TC | ABC | AZT | D4T | DDI | TDF | Mean |
| LR | ANN | LR | ANN | LR | ANN | LR | ANN | LR | ANN | LR | ANN | LR | ANN |
| MSE | 2.02 | **0.06** | 0.38 | **0.02** | 1.11 | **0.12** | 0.14 | **0.01** | 0.09 | **0.01** | 0.11 | **0.03** | 0.64 | **0.04** |
| R | 0.93 | **0.95** | 0.92 | 0.92 | 0.88 | **0.91** | 0.90 | **0.92** | 0.88 | 0.88 | 0.78 | **0.84** | 0.88 | **0.90** |
| AUC | 0.97 | **0.98** | **0.97** | 0.96 | 0.97 | **0.98** | 0.96 | **0.97** | **0.96** | 0.92 | 0.93 | **0.96** | 0.96 | 0.96 |