Supplementary Figure 2

The figure illustrates the RMSE on the test set for different numbers of trees in Random Forest for various datasets and fingerprint types. Each subplot shows the RMSE as a function of the number of trees, with different colors indicating different fingerprint types: red for 'rv-QAFFP 440', green for 'rv-QAFFP 440 & Morgan', and black for 'rv-QAFFP 440 & Physchem'. The datasets include A2780, CCRF-CEM, DU-145, HCT-116, HCT-15, HeLa, HepG2, HL-60, and HT-29.
Supplementary Figure 8