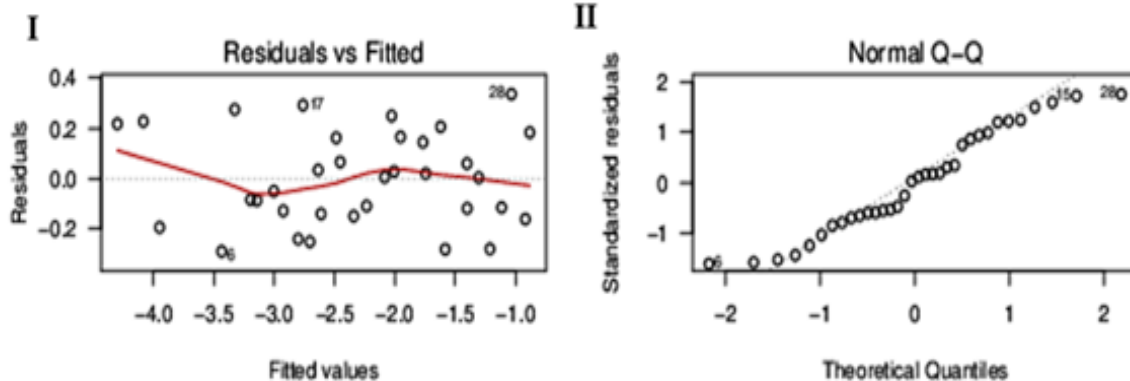


**Figure S1:** Correlation between predicted and experimental biological activity obtained by using the final structure-activity model for training (A) and test (B) set compounds. Residual histogram frequency statistics are shown for training (C) and test (D) set compounds.

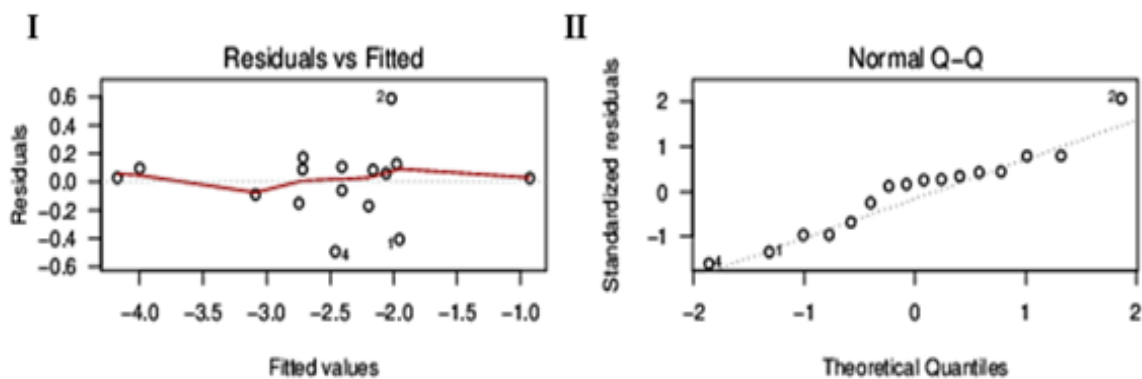
**A: Training set**

**Residual Diagnostics**



**B: Test set**

**Residual Diagnostics**



**Figure SII:** Identification of “domain of applicability” of the designed hybrid structure-activity model for (A) training set (B) test set. **I:** Residual vs Fitted values plot; **II:** Q-Q plot.