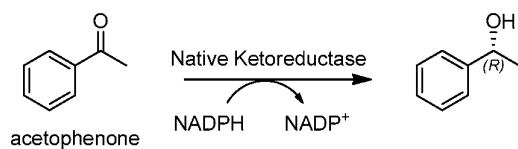
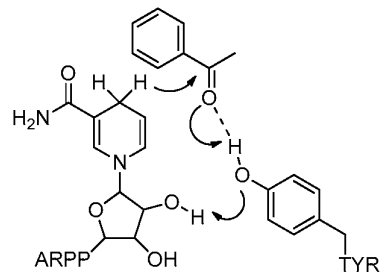
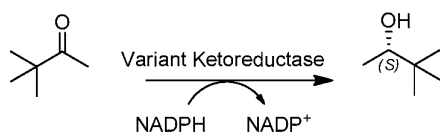
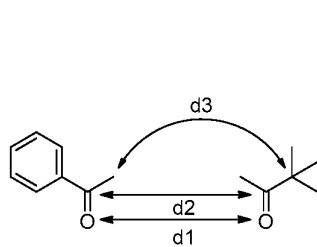
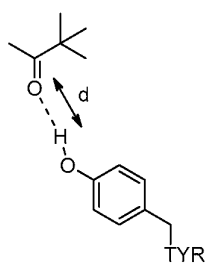
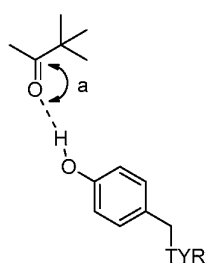


Native Reaction and Selectivity**Mechanism of catalysis and selectivity****Desired Reaction and Selectivity****Various types of Constraints**

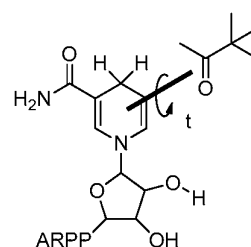
Positional Constraint



Distance Constraint



Angle Constraint



Torsion Constraint

FIG. 1

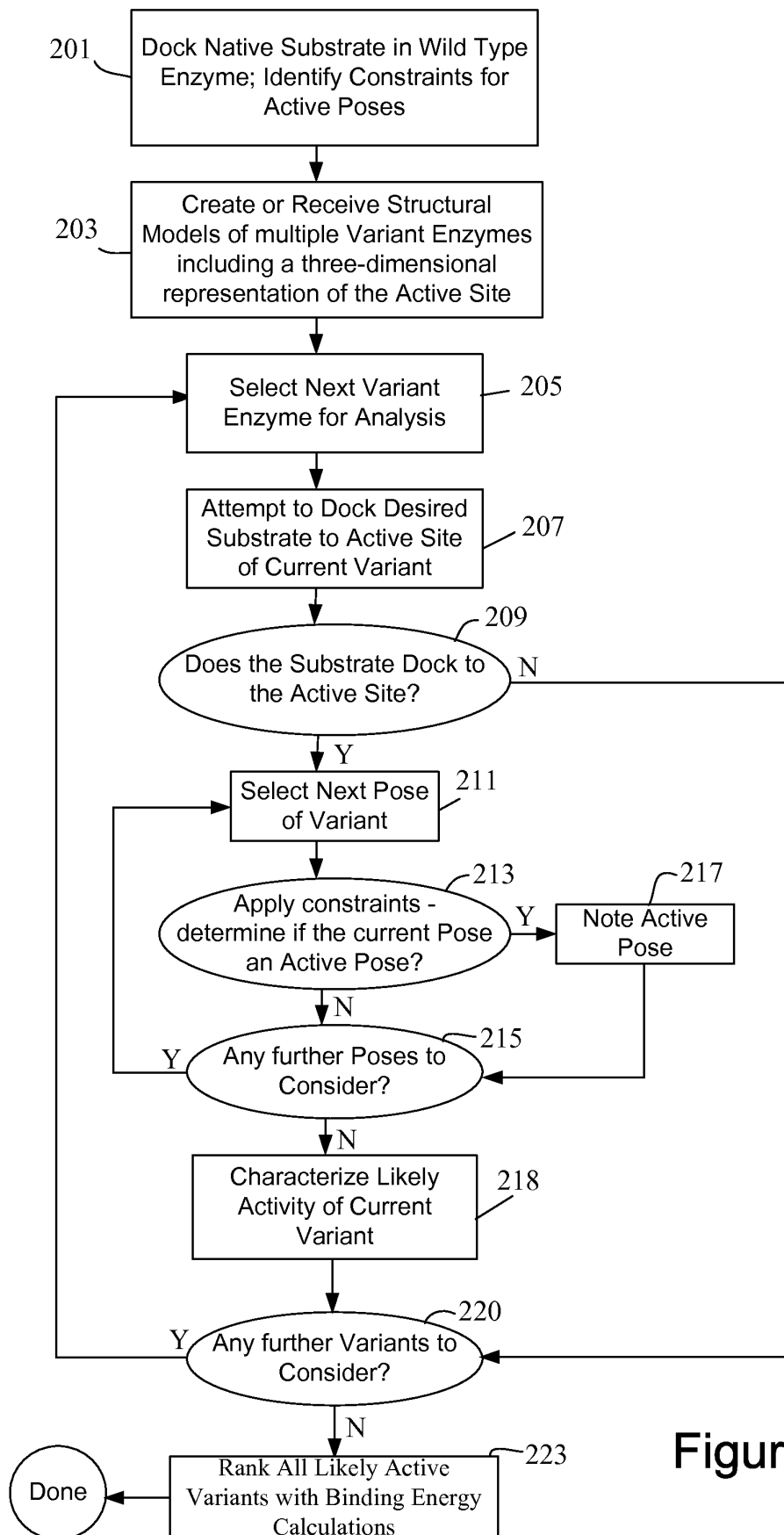
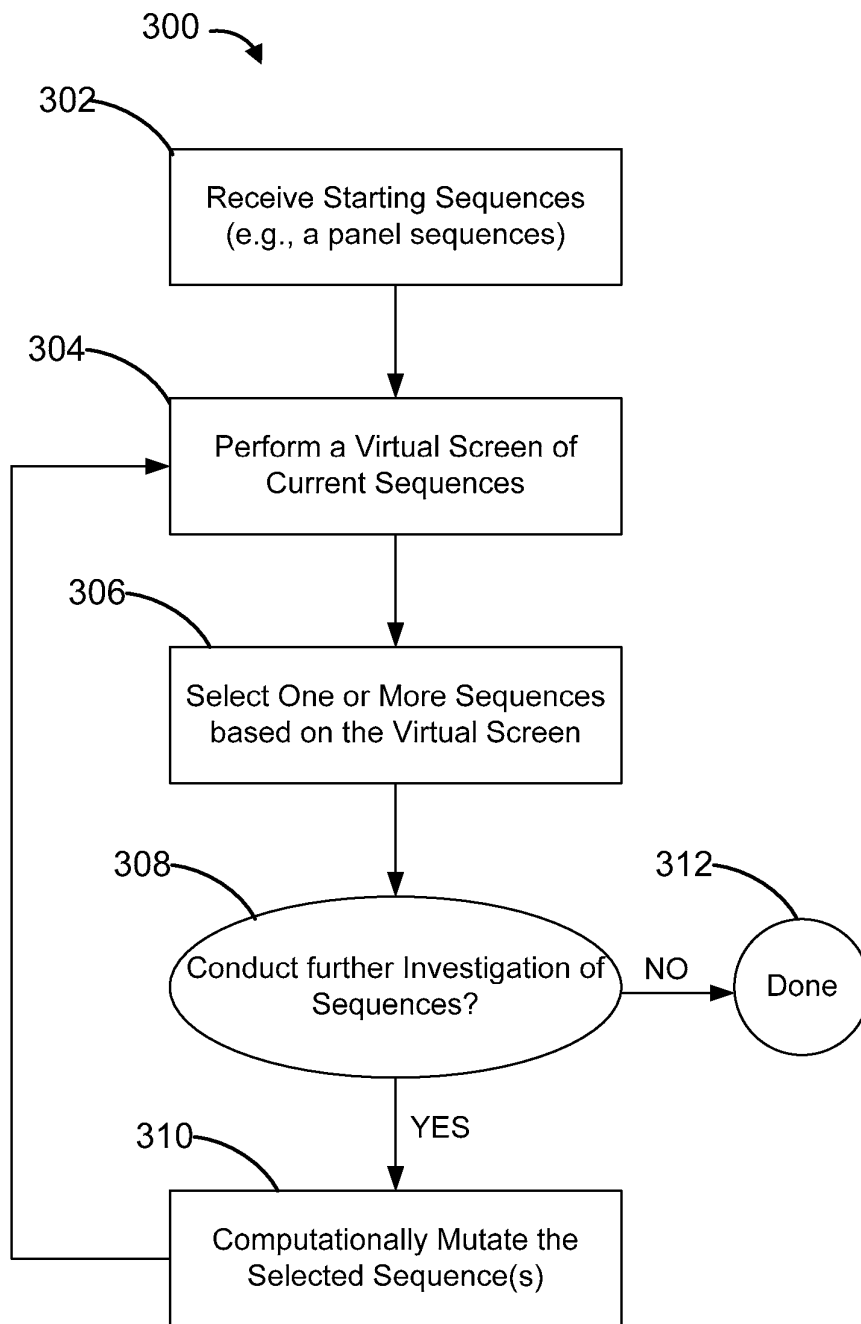
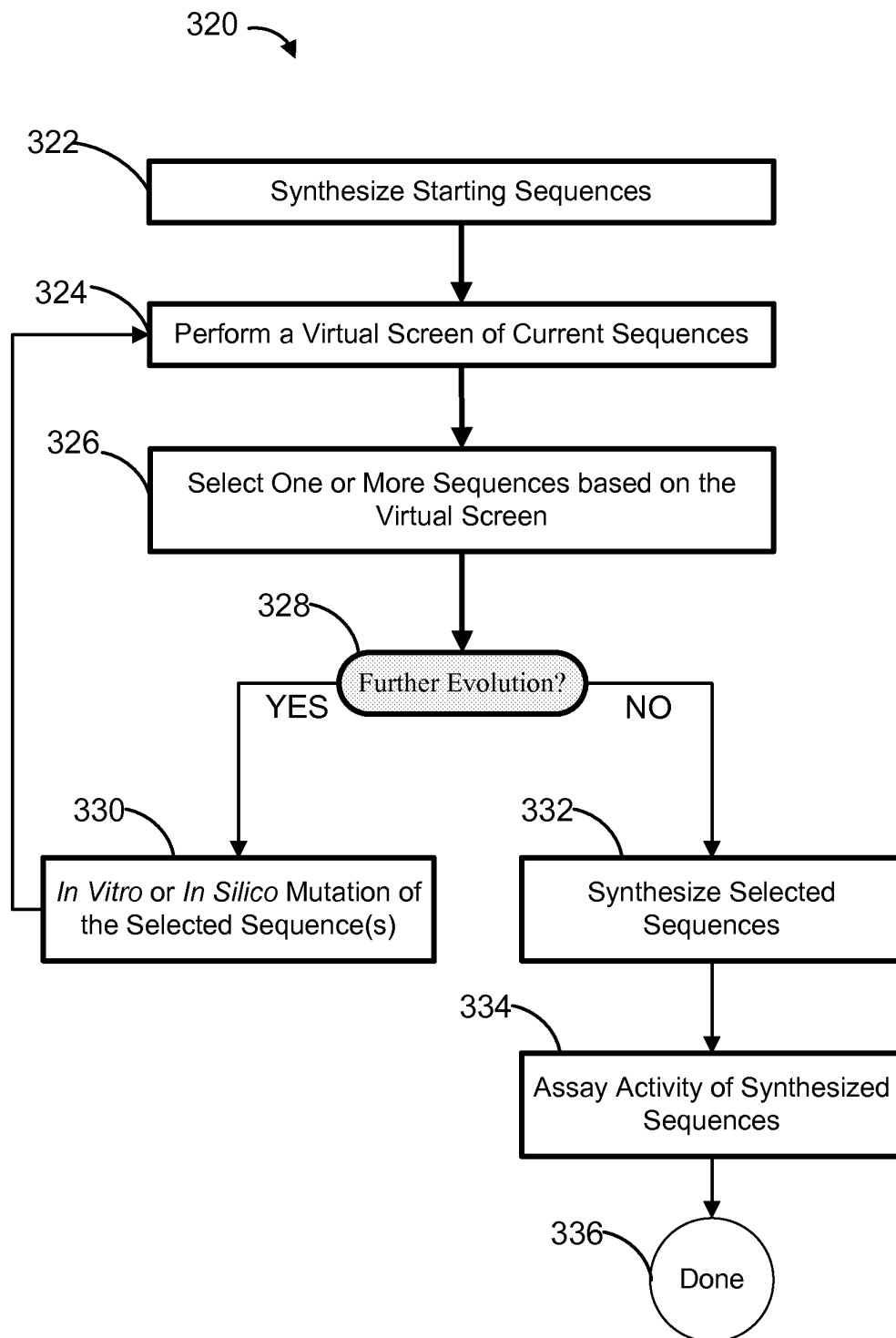
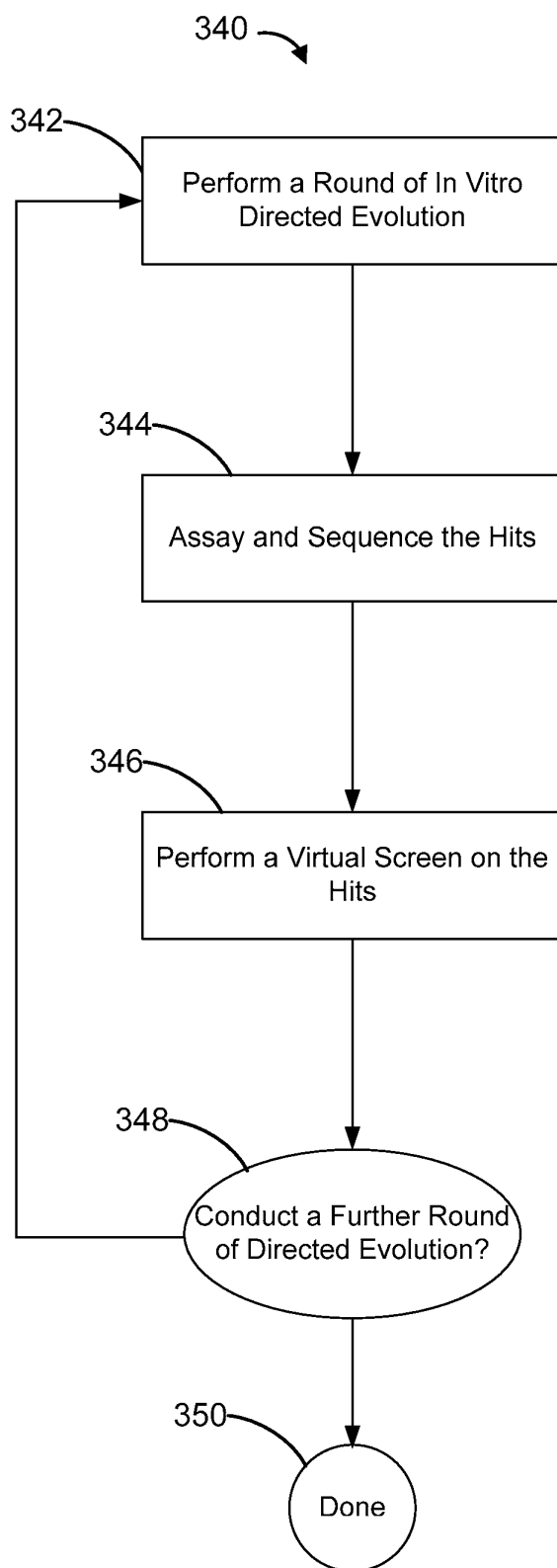
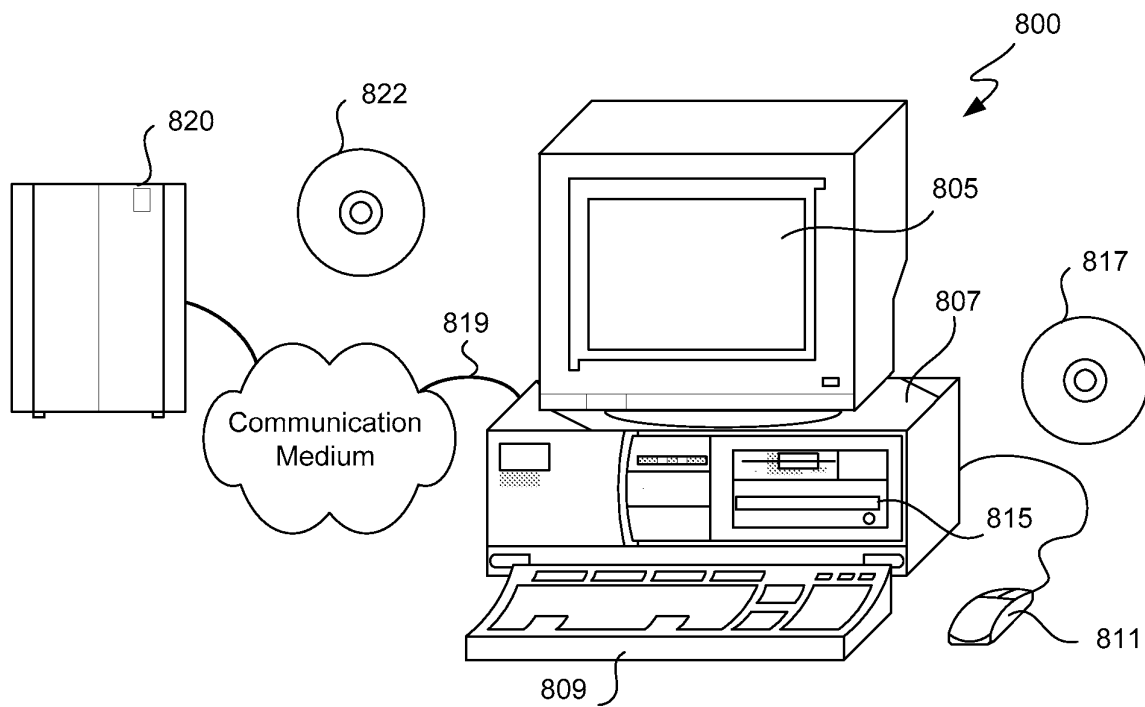


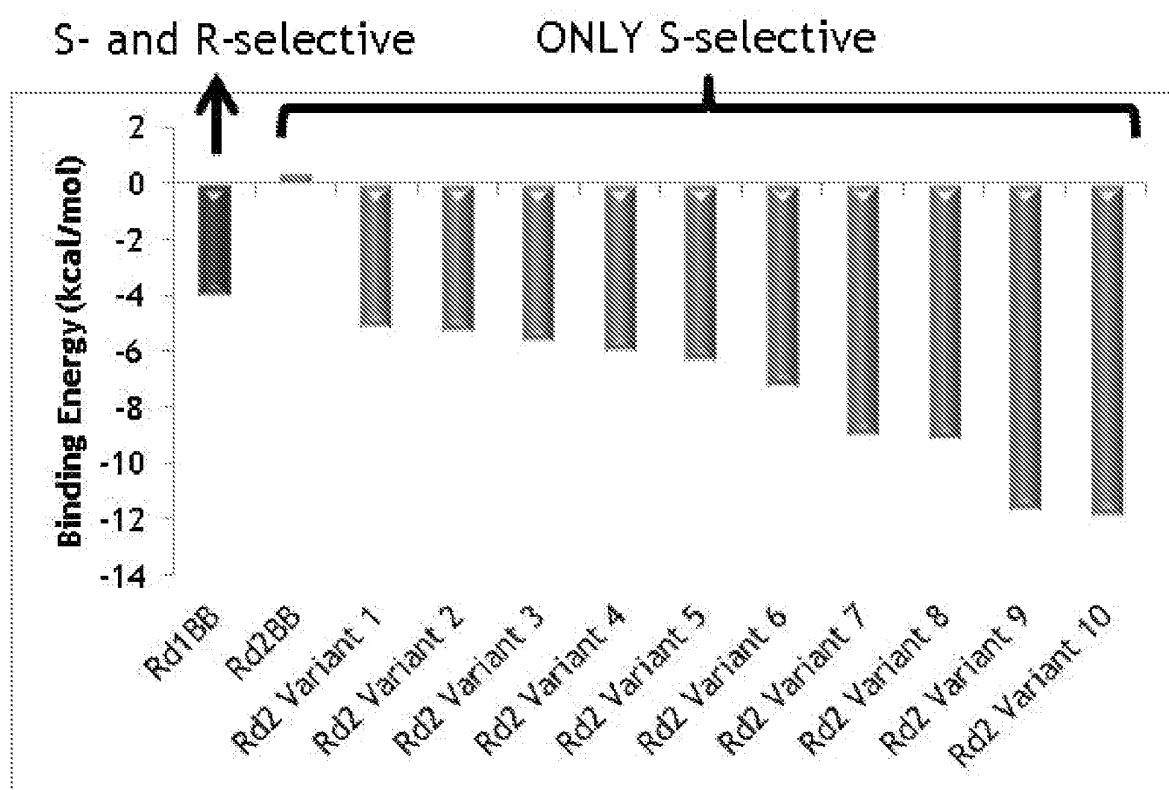
Figure 2

**FIG. 3A**

**FIG. 3B**

**FIG. 3C**

**FIG. 4**

**FIG. 5**

Model Fit

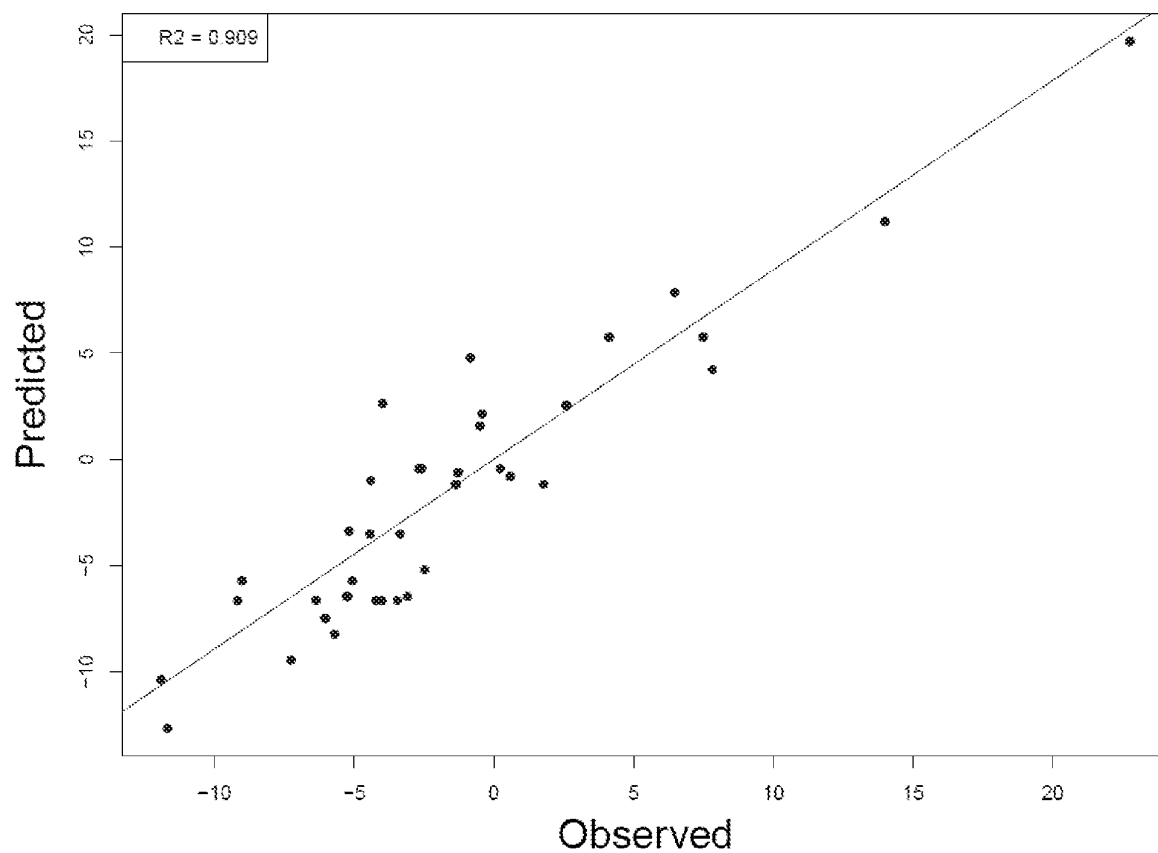
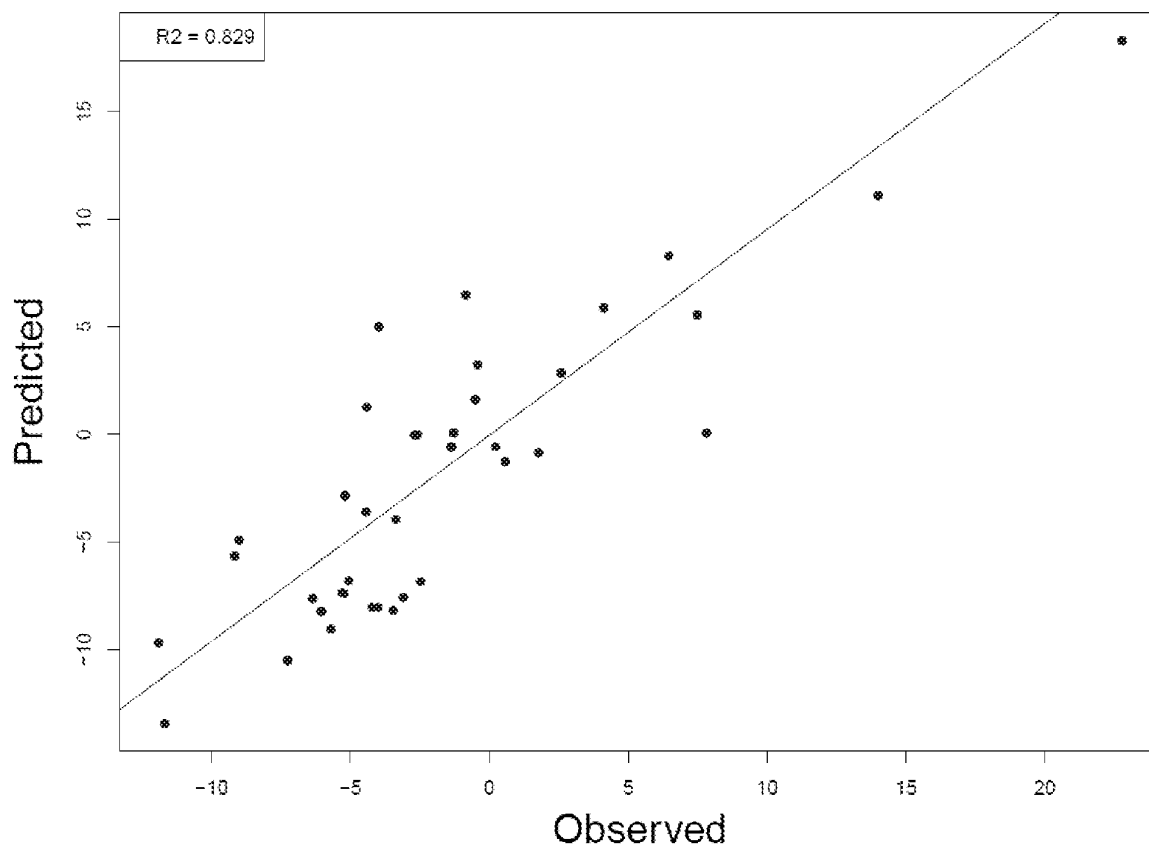
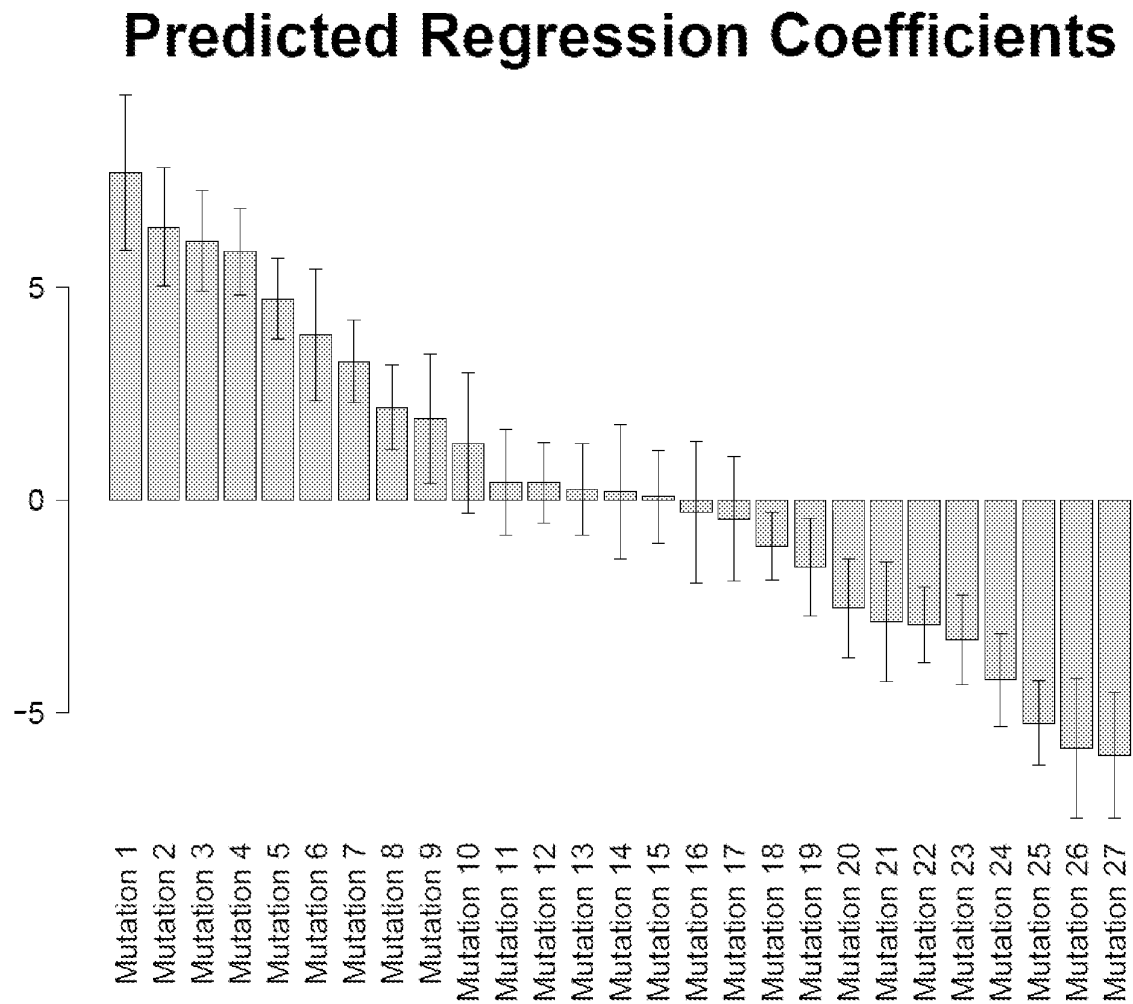
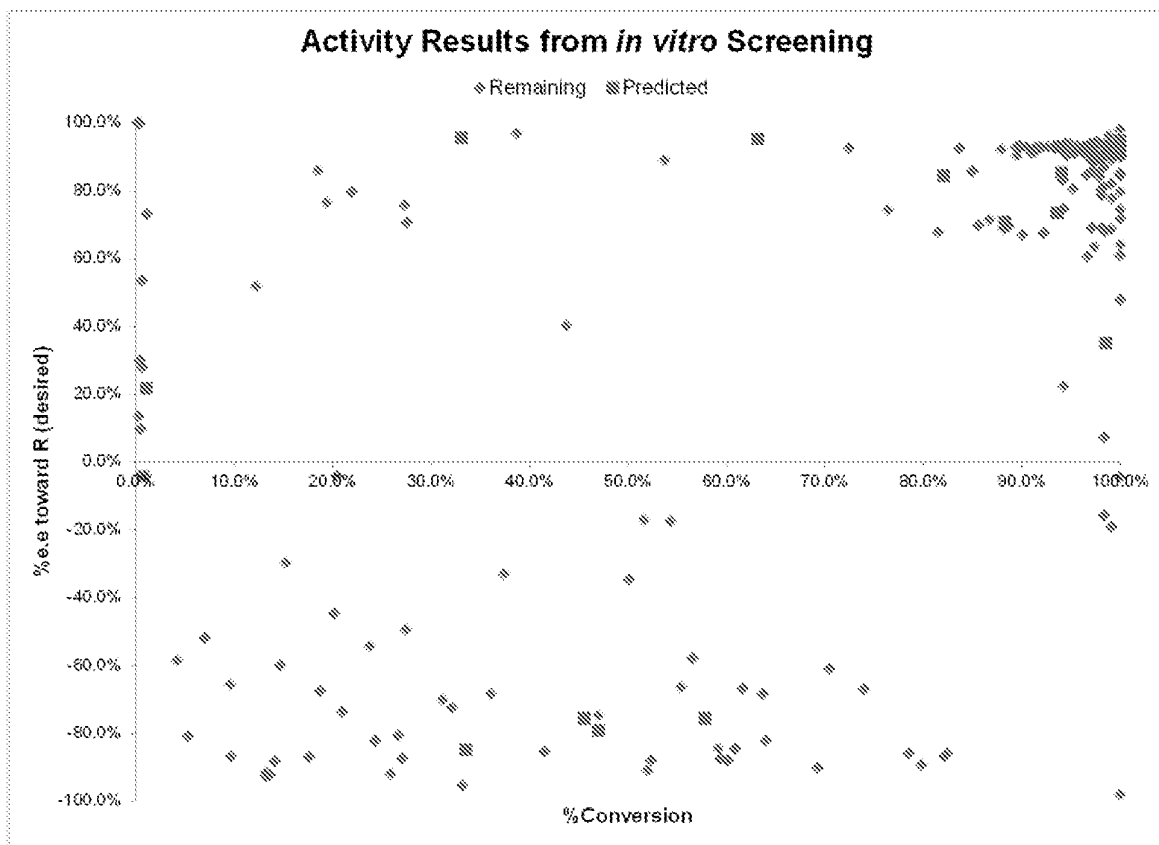
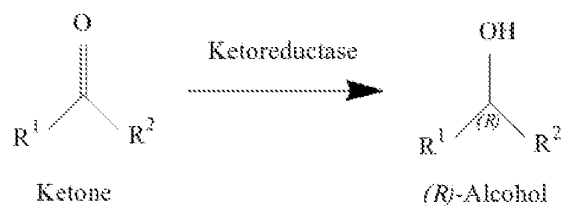


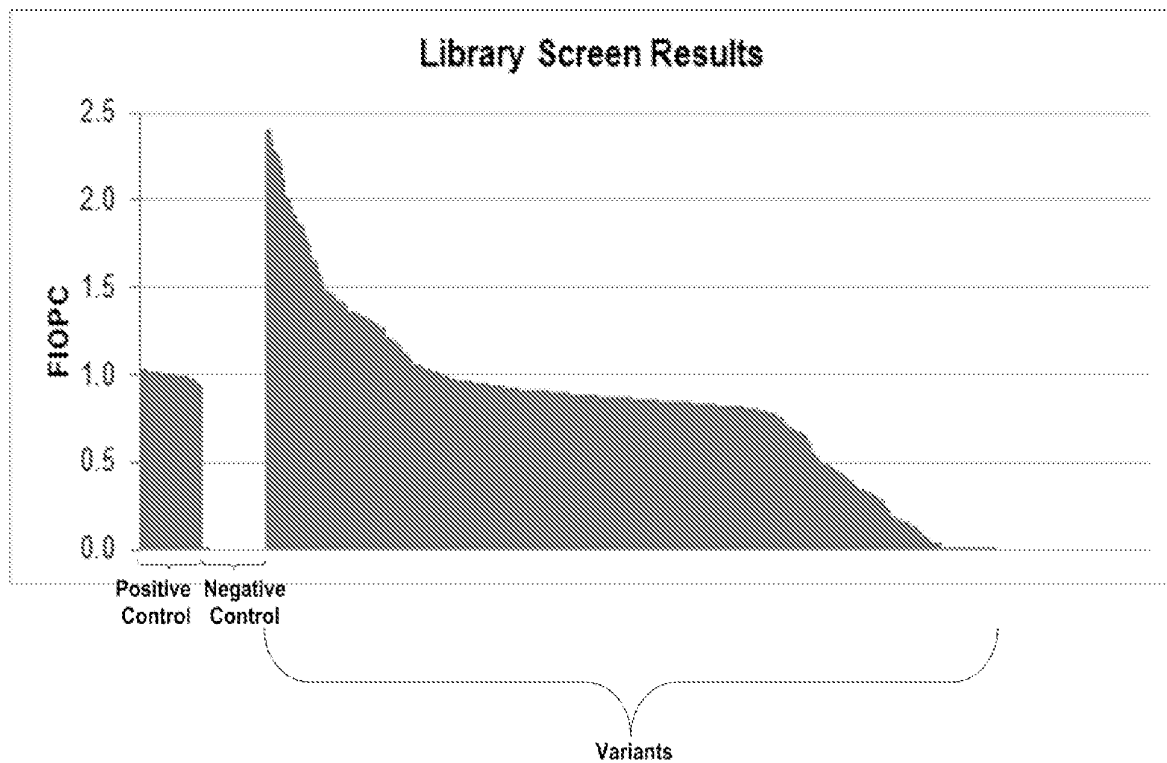
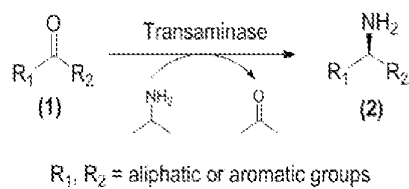
FIG. 6A

Crossvalidation



**FIG. 6C**

**FIG. 7**

**FIG. 8**