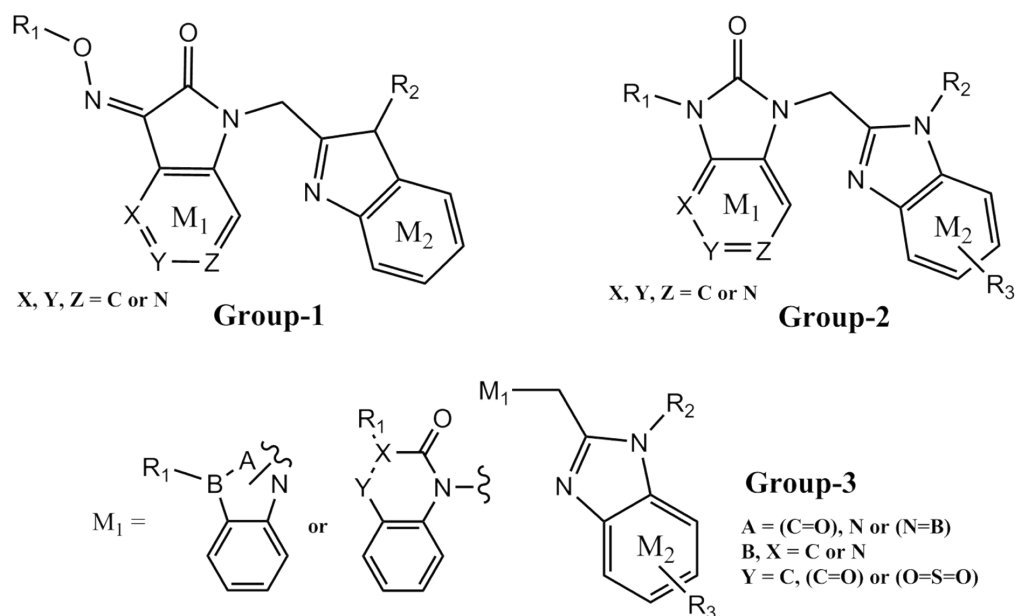


A



B

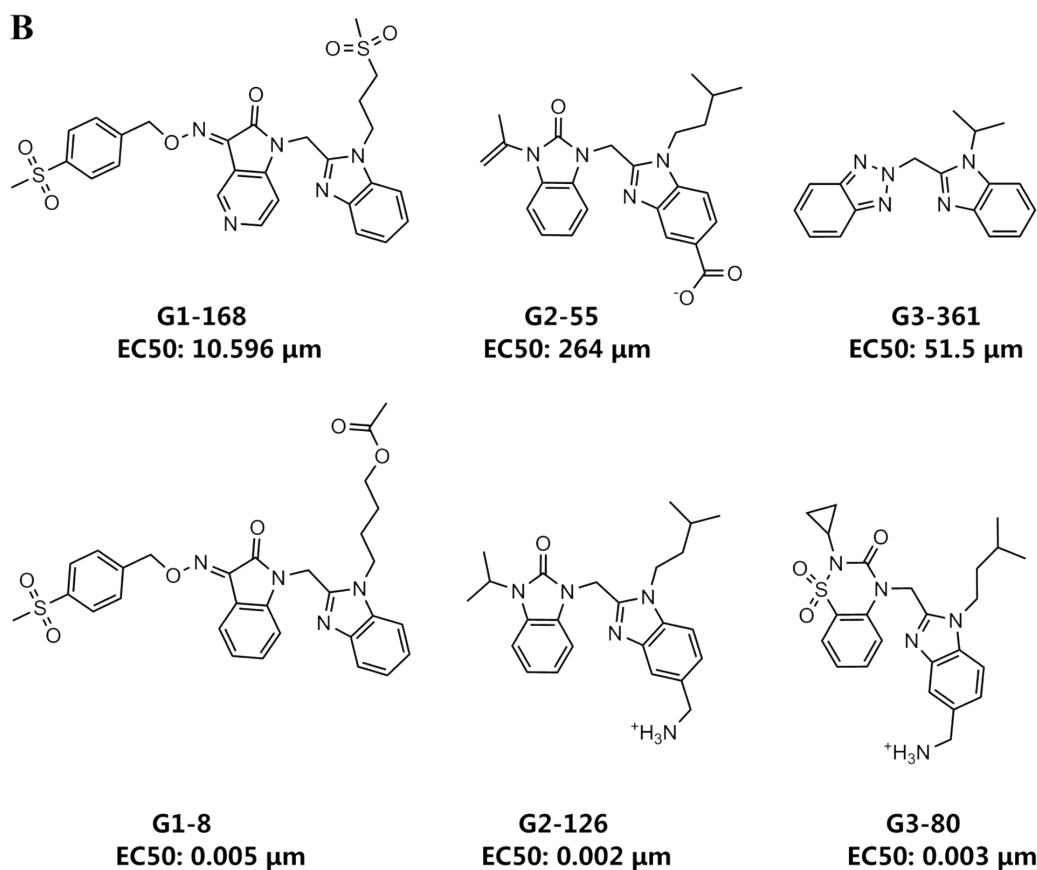


Figure S1. Skeleton and representative structures. A: Structural skeleton of 3 groups.

B: Representative molecules of three groups.

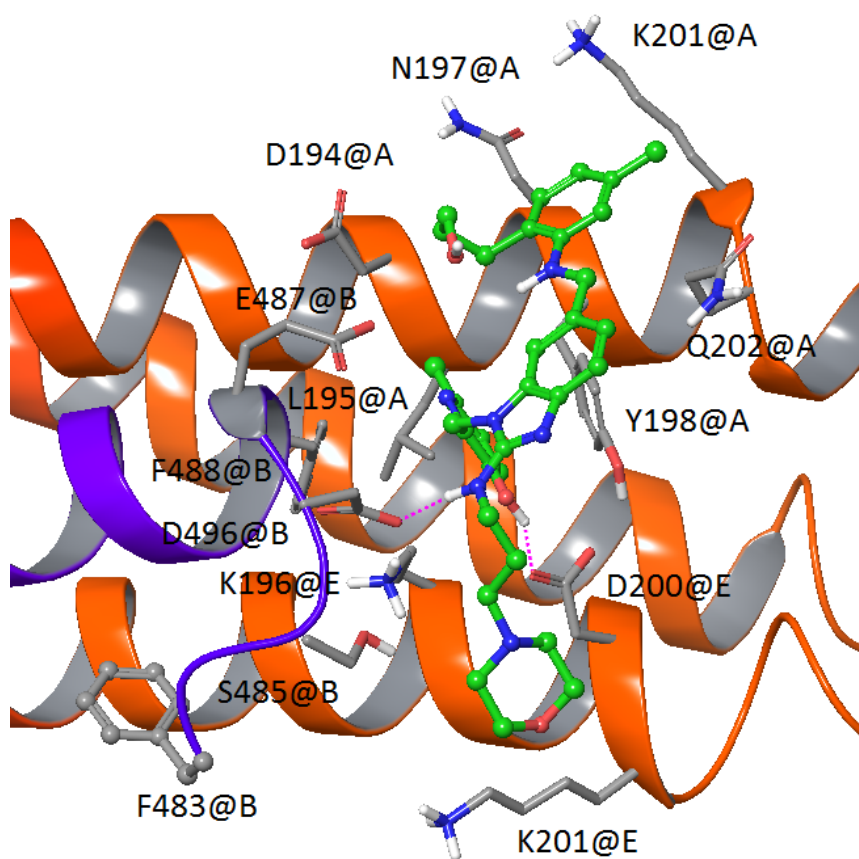


Figure S2. Binding mode of TMC TMC353121 and RSVF protein.

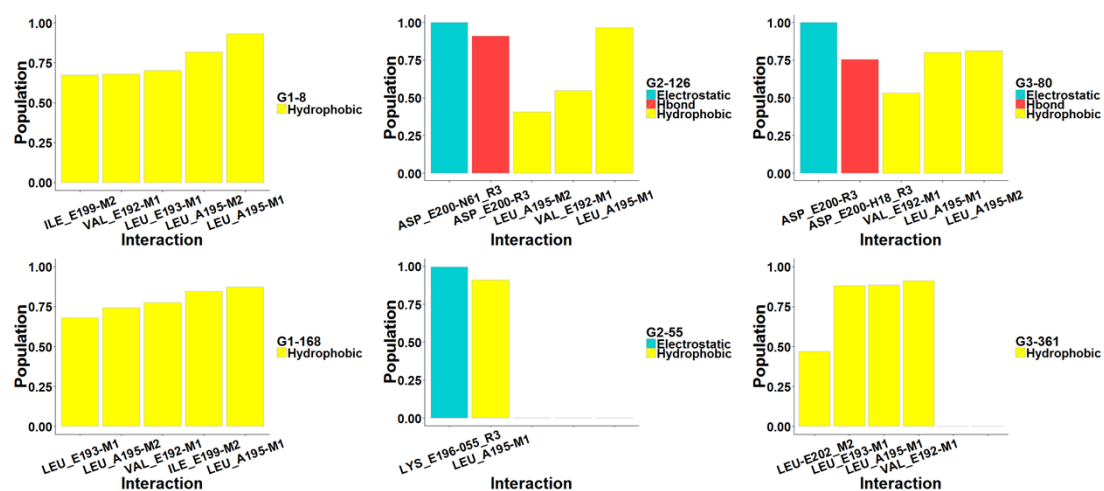


Figure S3. Interaction between ligand and RSVF receptor for 6 complexes.

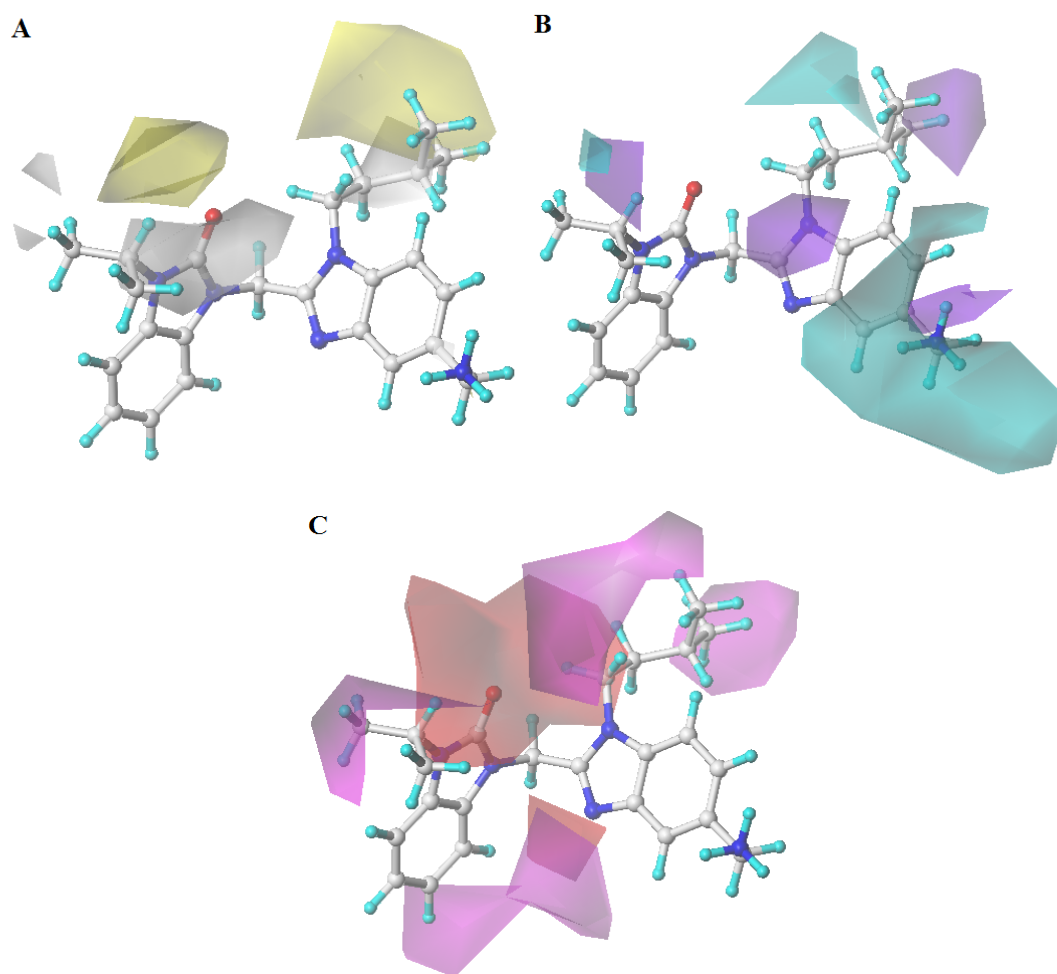


Figure S4. CoMSIA contour plot with molecule G3-80. A: Contour map of hydrophobic field in CoMSIA. B: Contour map of hydrogen bond donor field in CoMSIA. C: Contour map of hydrogen bond acceptor field in CoMSIA. Yellow contours indicate regions where hydrophobic groups are favorable for activity and white contours indicate regions where hydrophobic groups are unfavorable for activity. Cyan contours indicate regions where groups with hydrogen bond donor could increase activity whereas purple contours indicate regions where groups with hydrogen bond donor charge could decrease activity. Magenta contours indicate regions where hydrogen bond acceptor groups are favorable for activity and dark-red contours indicate regions where hydrogen bond acceptor groups are unfavorable for activity.

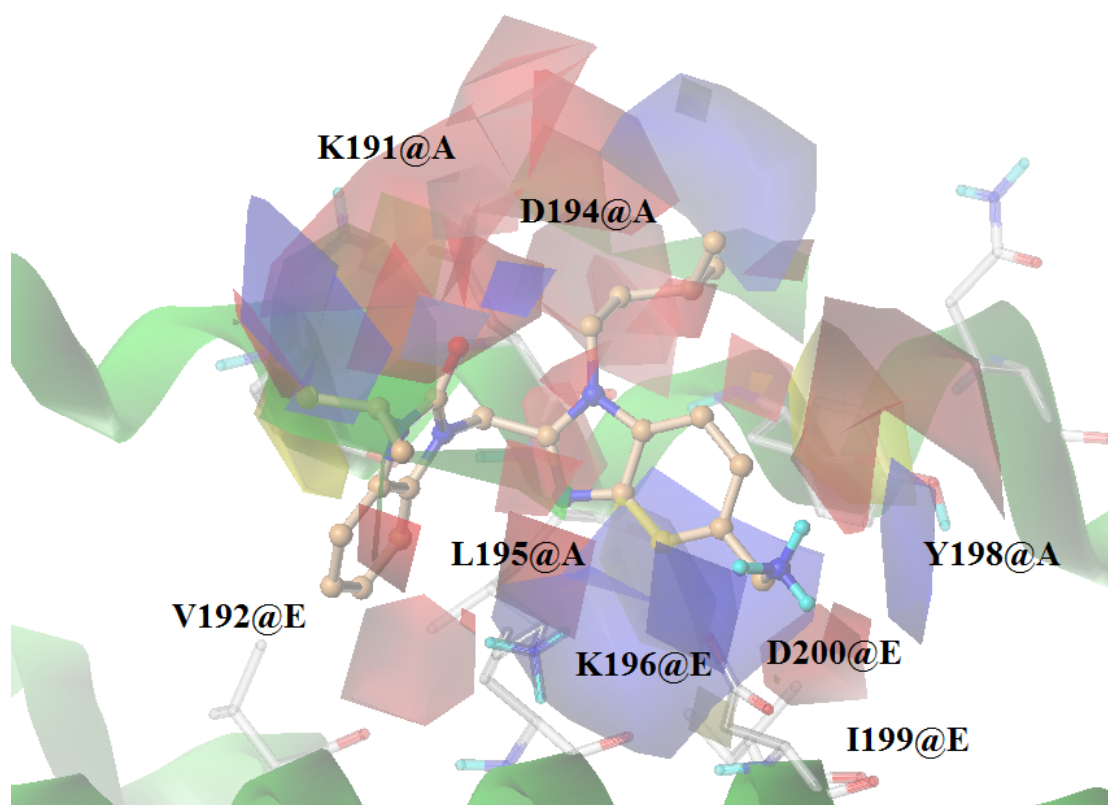


Figure S5. Superposition of CoMFA model and complex for G3-80/RSVF. G3-80 is marked in orange.