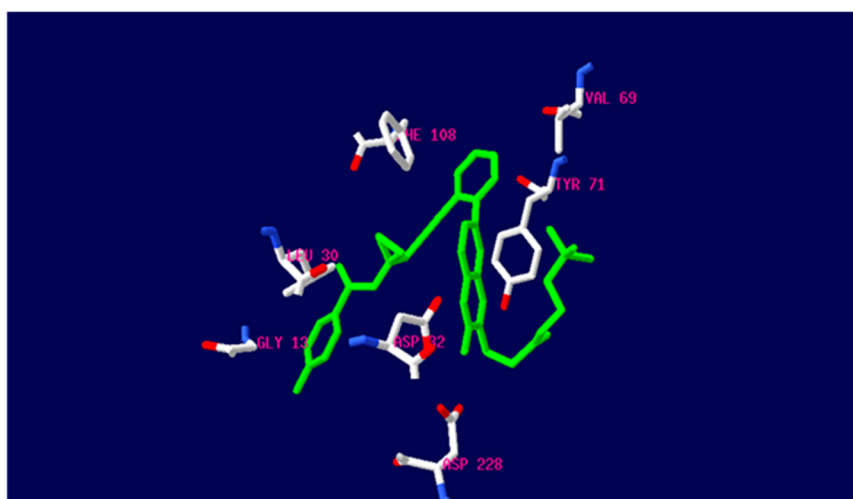


FigureS2: : 5i3v



FigureS2: : Different views of binding of inhibitor 4 in 5i3v

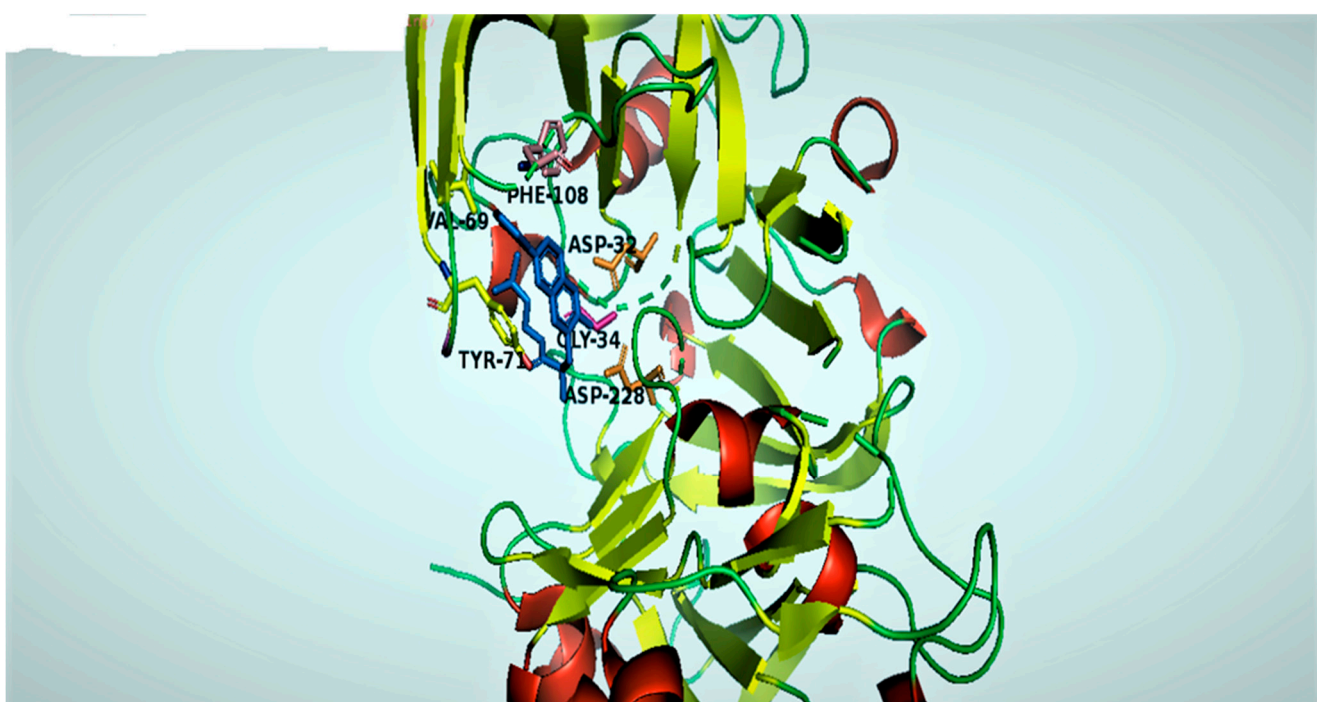
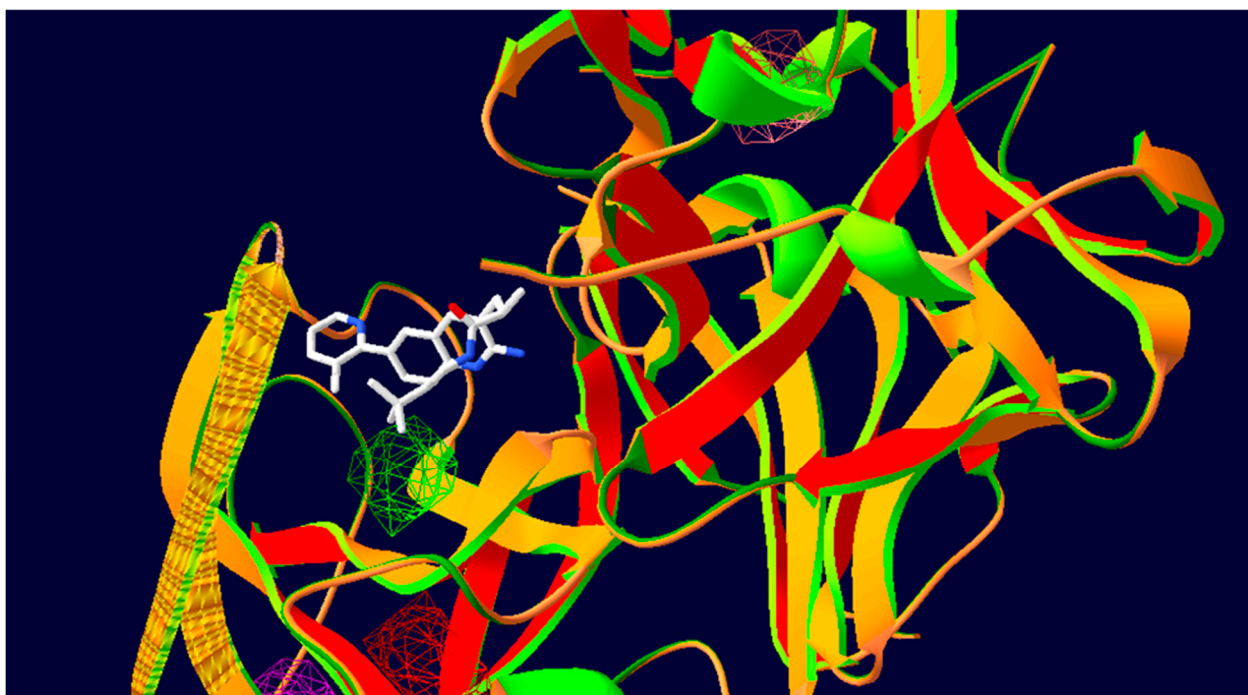
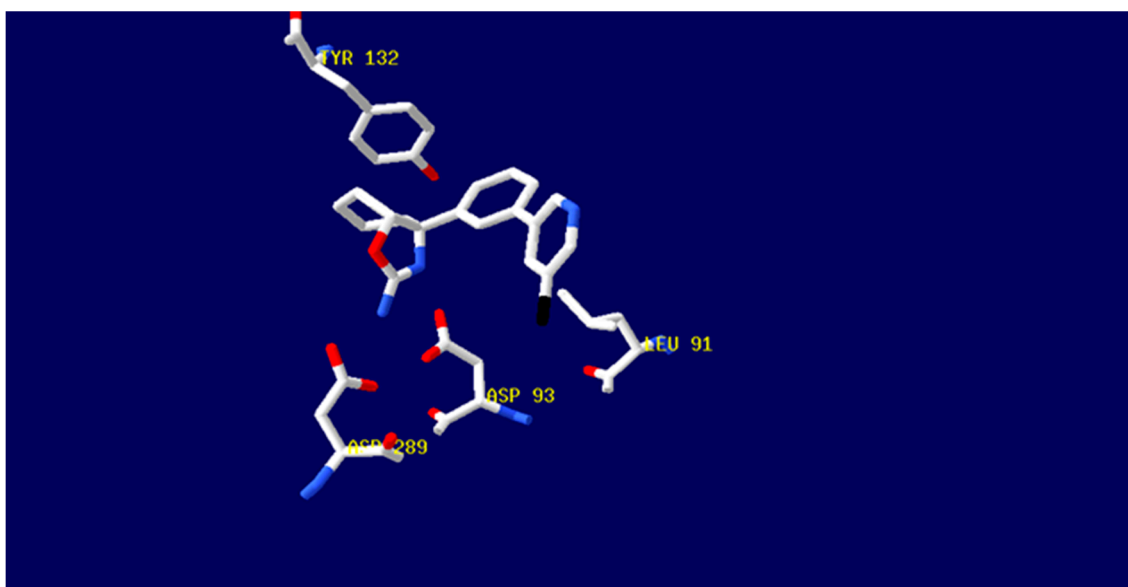
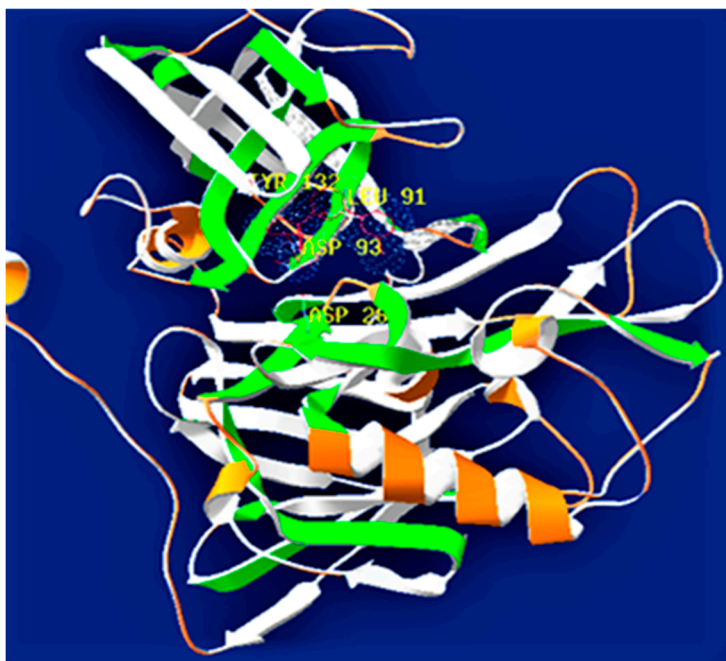
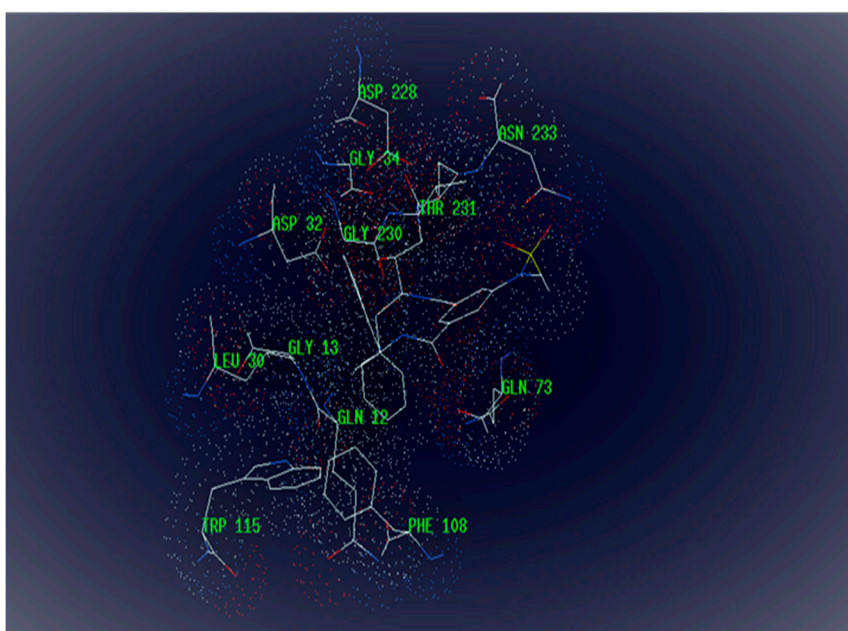
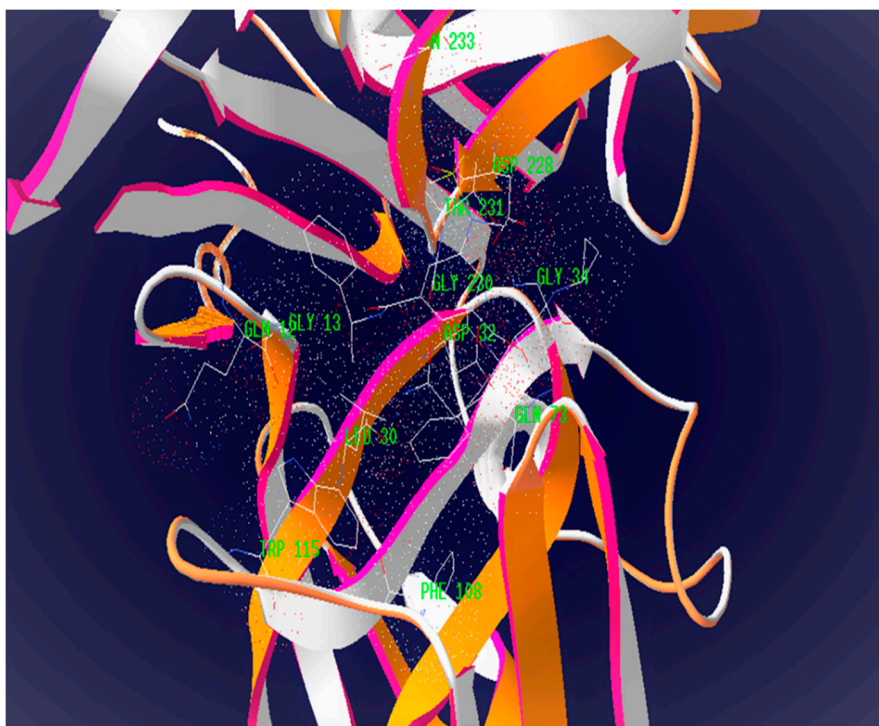
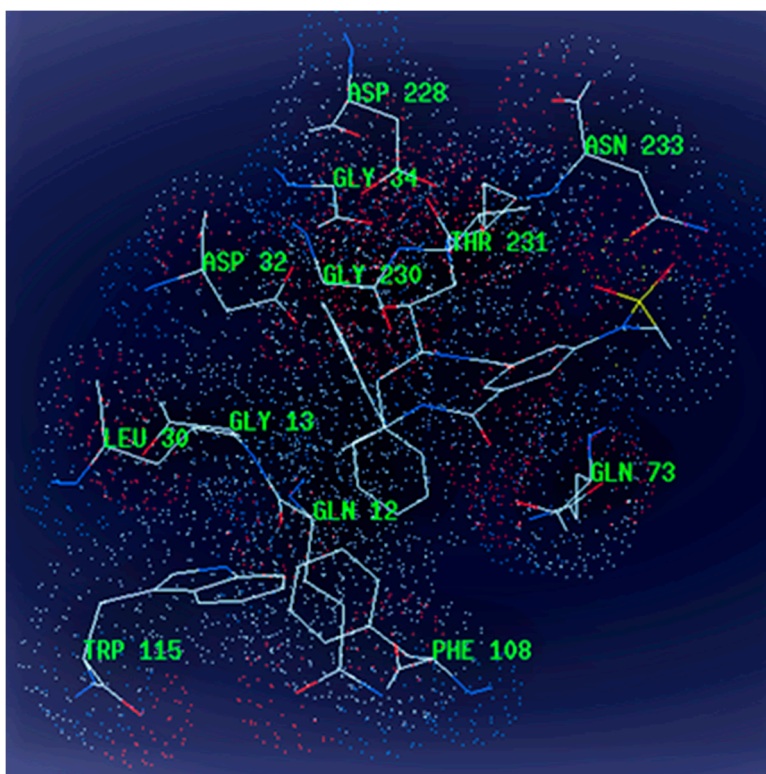


Figure S3: Binding mode of Inhibitor 6 in 4LC7 Different views

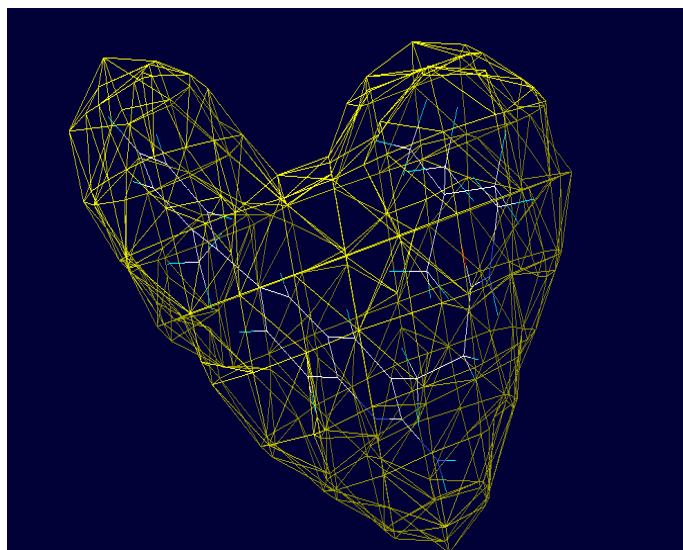


FigureS4: protein view of inhibitor 7 in 3TPP



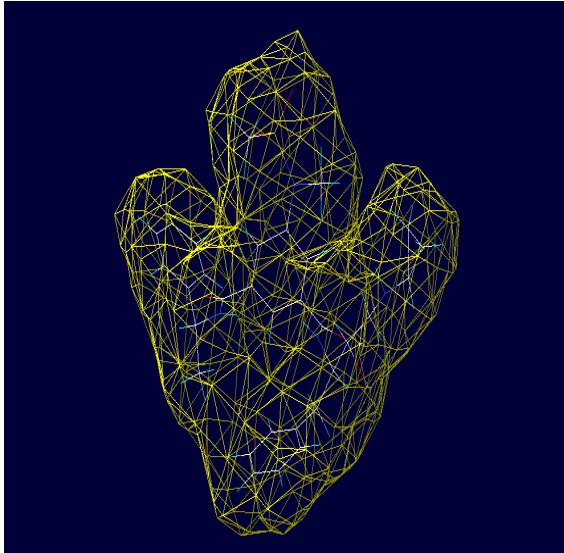


FigureS5 surface areas of inhibitors and the BACE1 surface

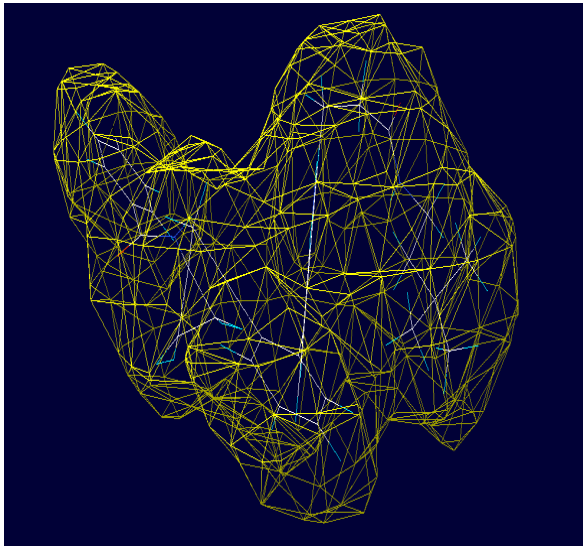


6BS -30.5

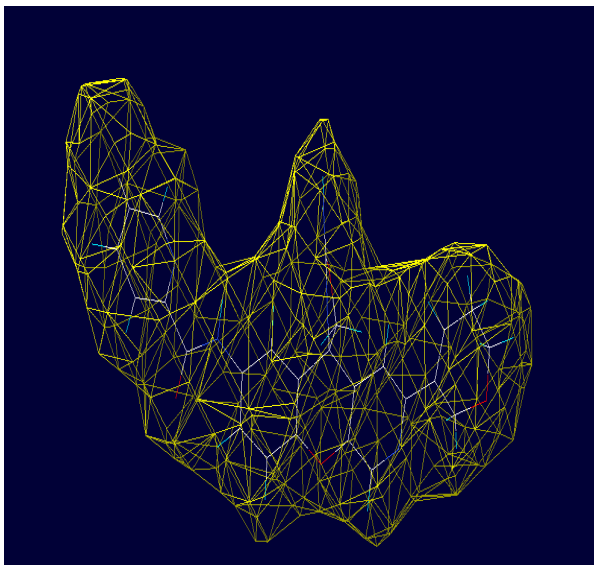




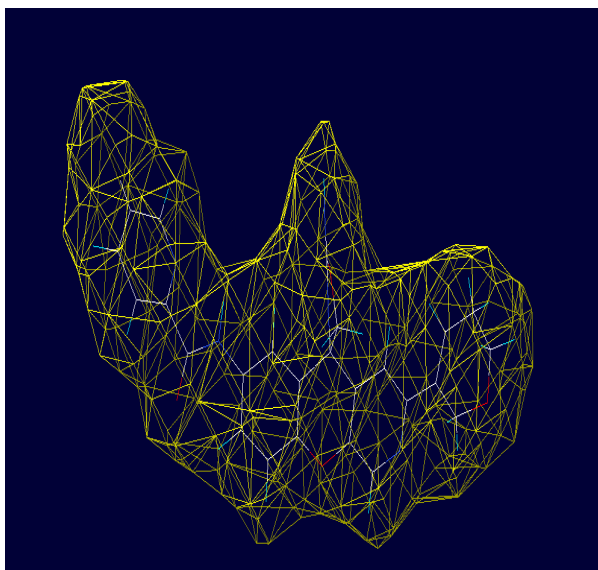
5HA -35.6



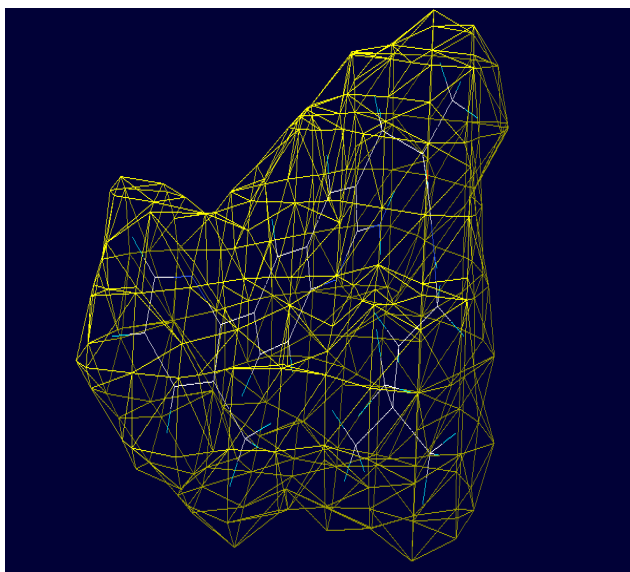
68j



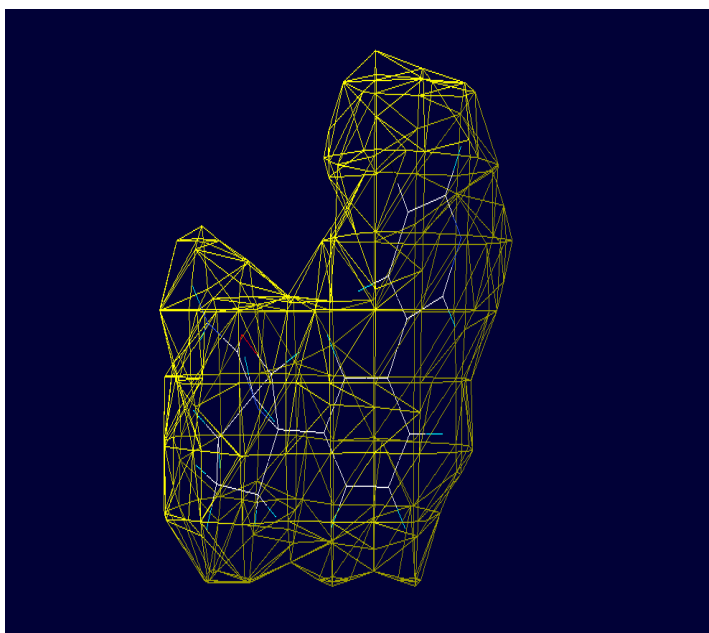
68K



68L



68M



1WP

Figure S6: Views of Inhibitor 3 binding protein view (5ie1)

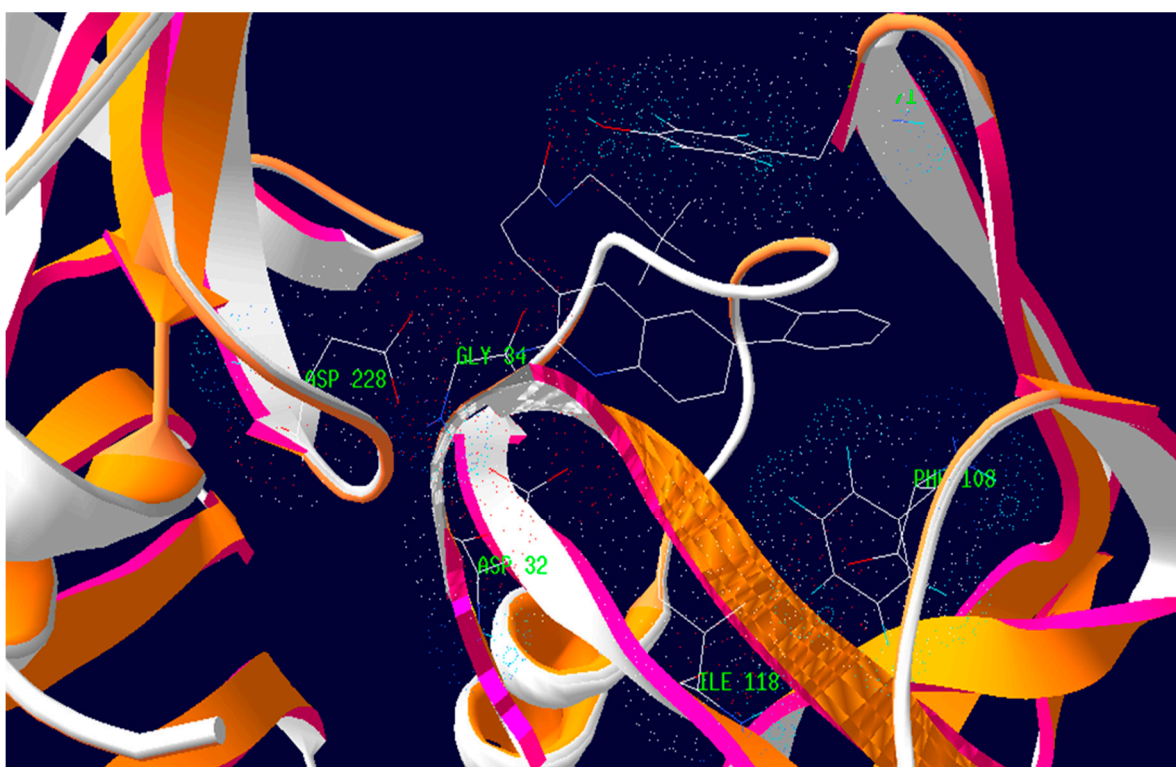


Figure S7: views of inhibitor 2 to BACE1 (5i3Y)



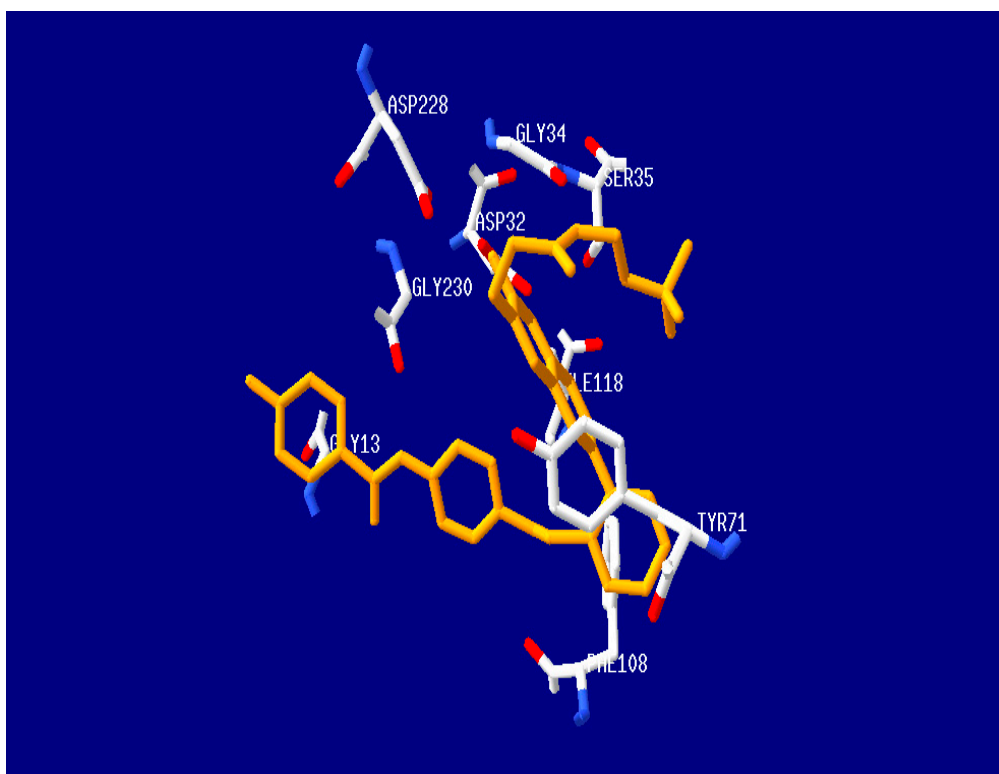
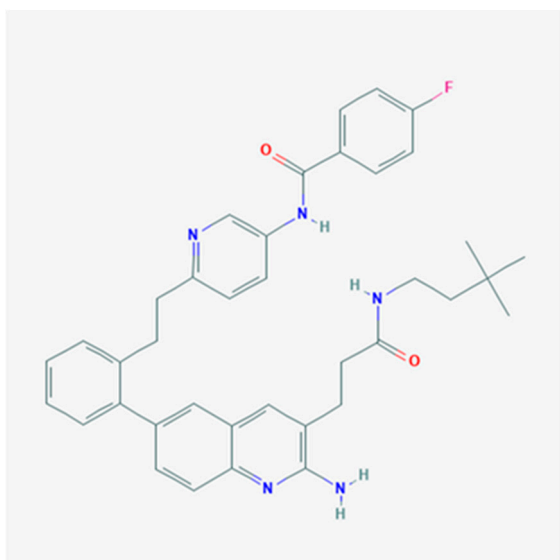


Figure S8: 5i3W binding of inhibitor 5 to BACE1

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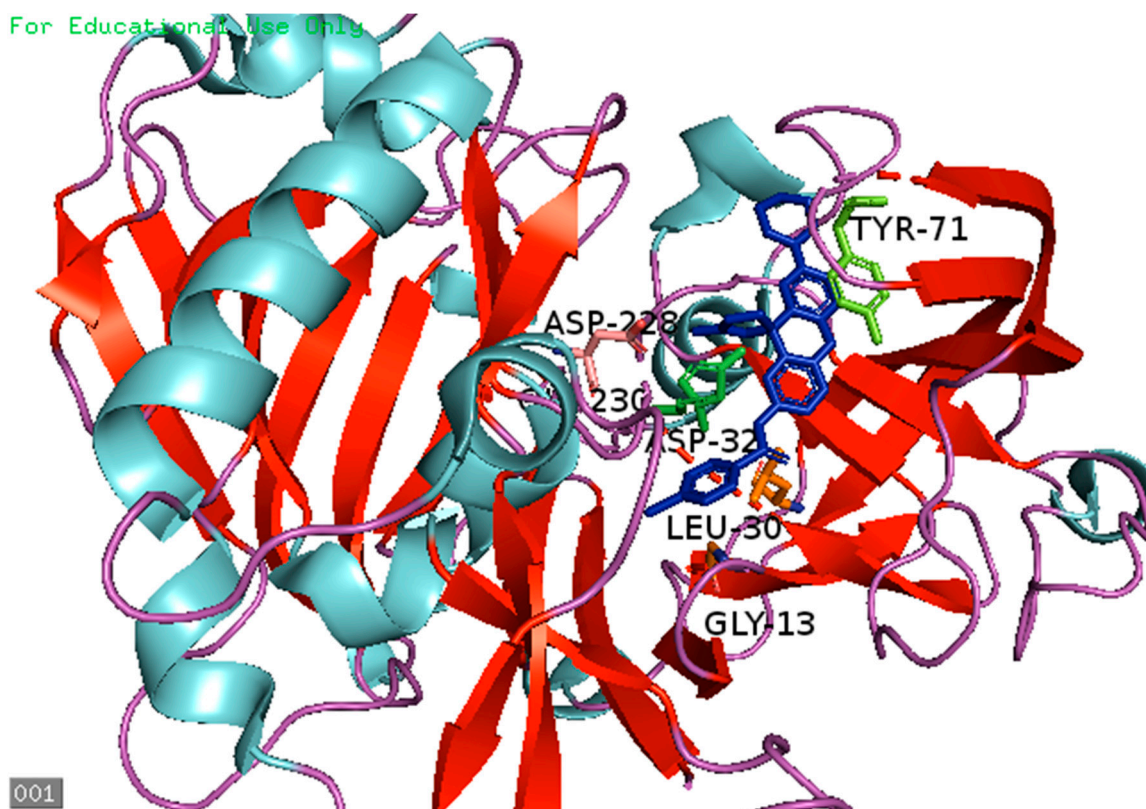


Figure S9: The dendrogram (cluster trees) of the BACE1-Inhibitor in 5i3X

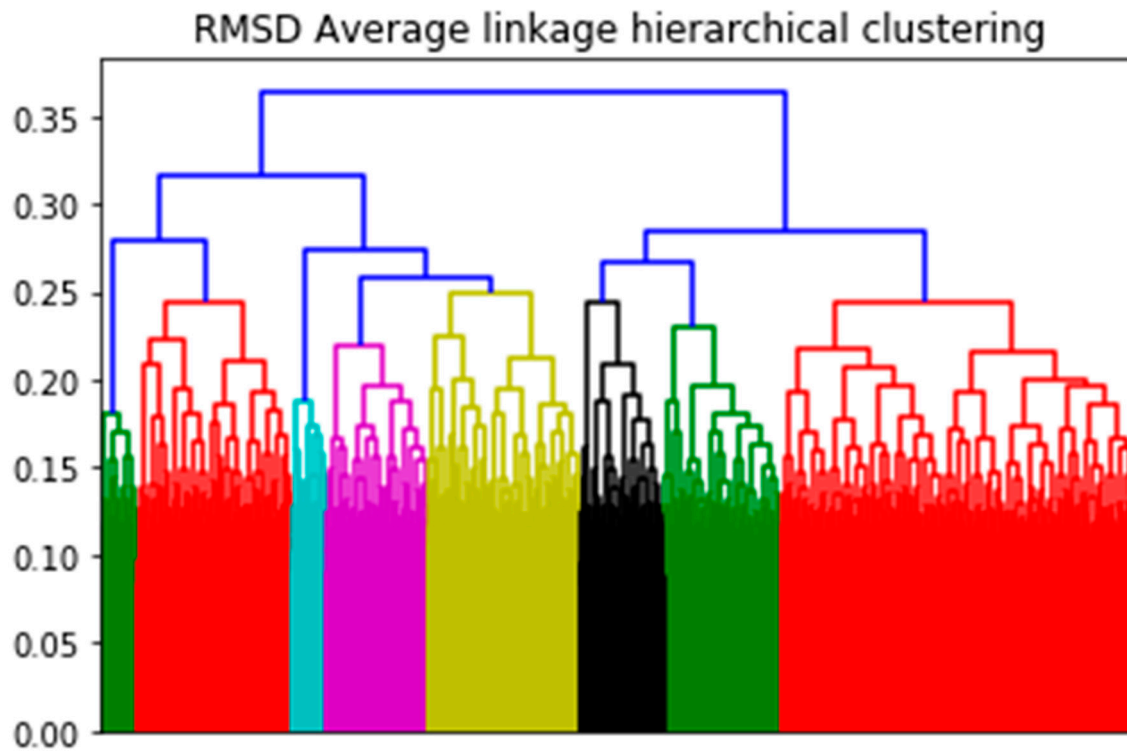


Figure S10: The dendrogram (cluster trees) of the BACE1-Inhibitor in 5i3X complex employing RMSD.