

Supplementary Material

Investigation into the Molecular Properties of 3-(4-Hydroxyphenyl) Prop-2-en-1-one 4-Phenyl Schiff Base and Some of Its Derivatives-DFT and Molecular Docking Studies

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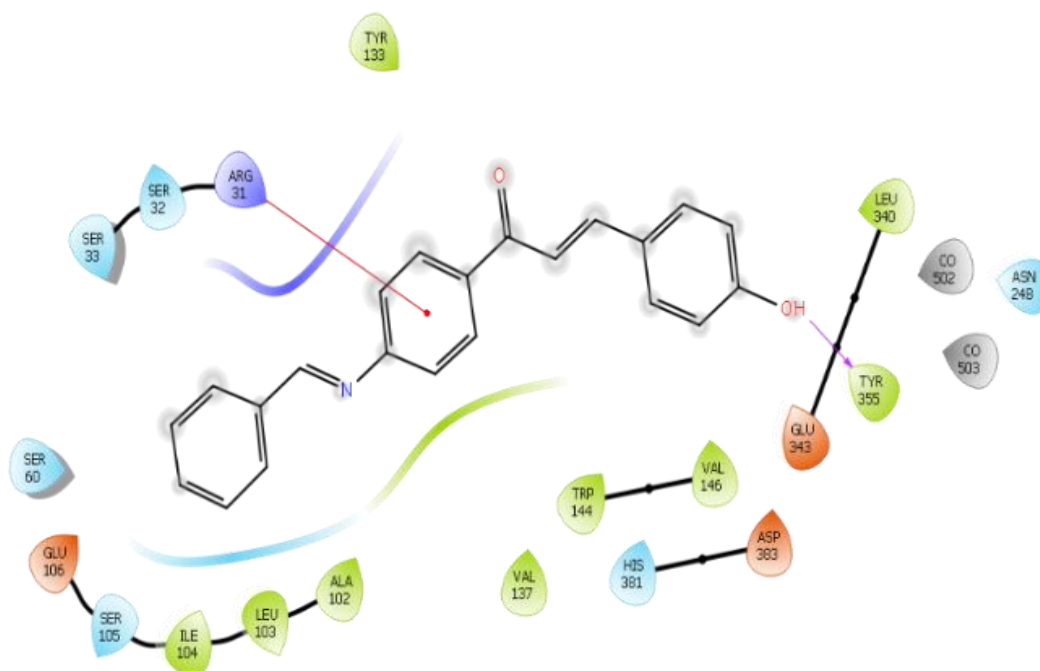


Fig. S1 R= -H within 4Å of *AmpS* active site with the hydrogen bond network (purple) and pi-cation (red) communication.

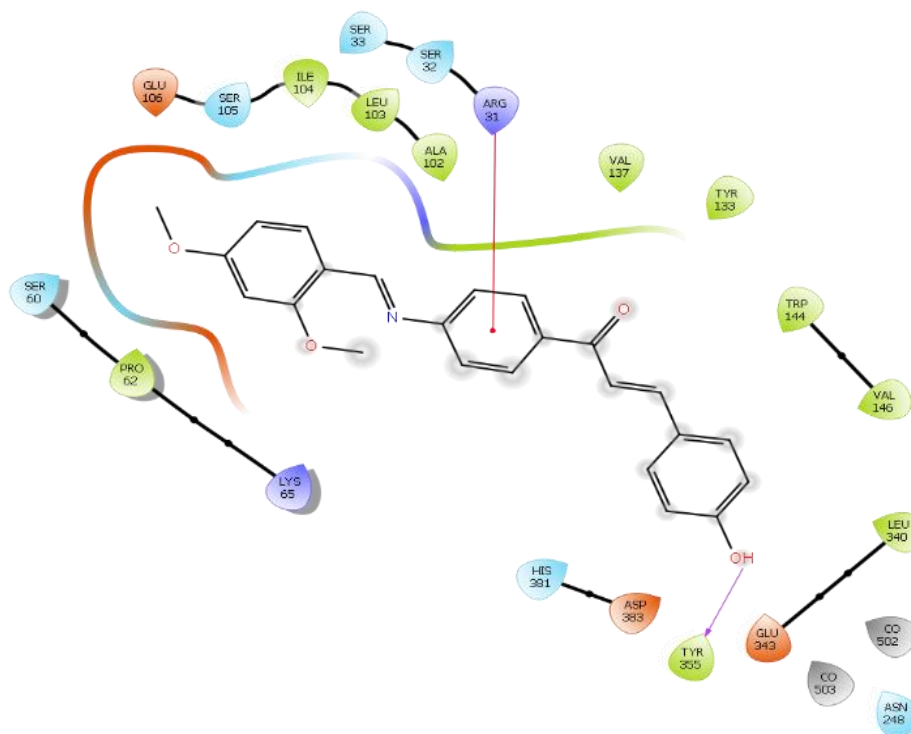


Fig. S2 R= 4-OCH₃ within 4Å of *AmpS* active site with the hydrogen bond network (purple) and pi-cation (red) and pi-pi stacking (green) communications.

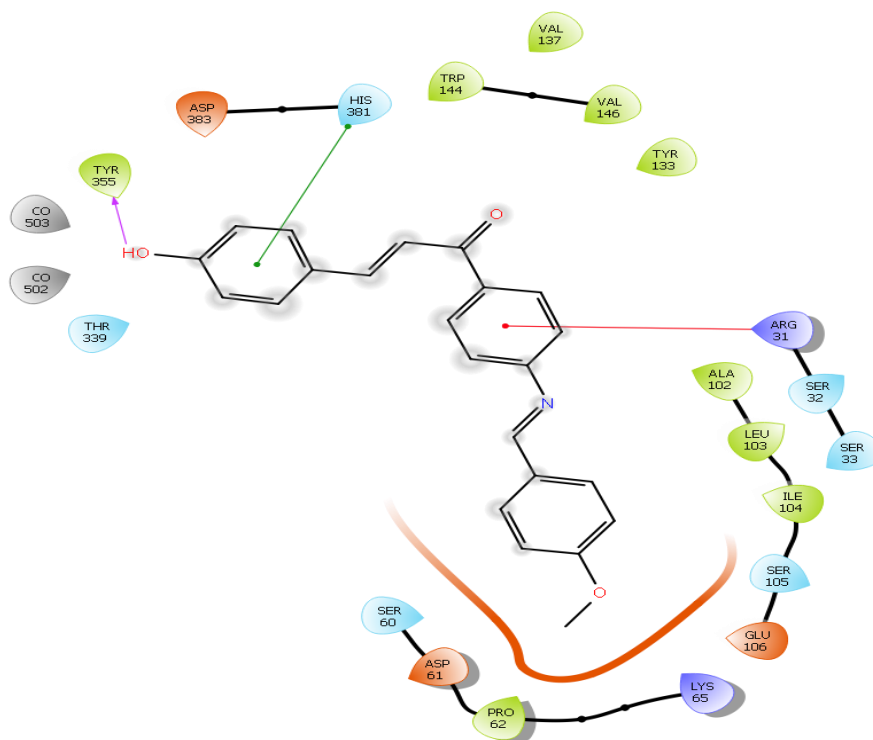


Fig. S3 R= 2-OCH₃, 4- OCH₃ within 4Å of *AmpS* active site with the hydrogen bond network (purple), pi-cation (red).

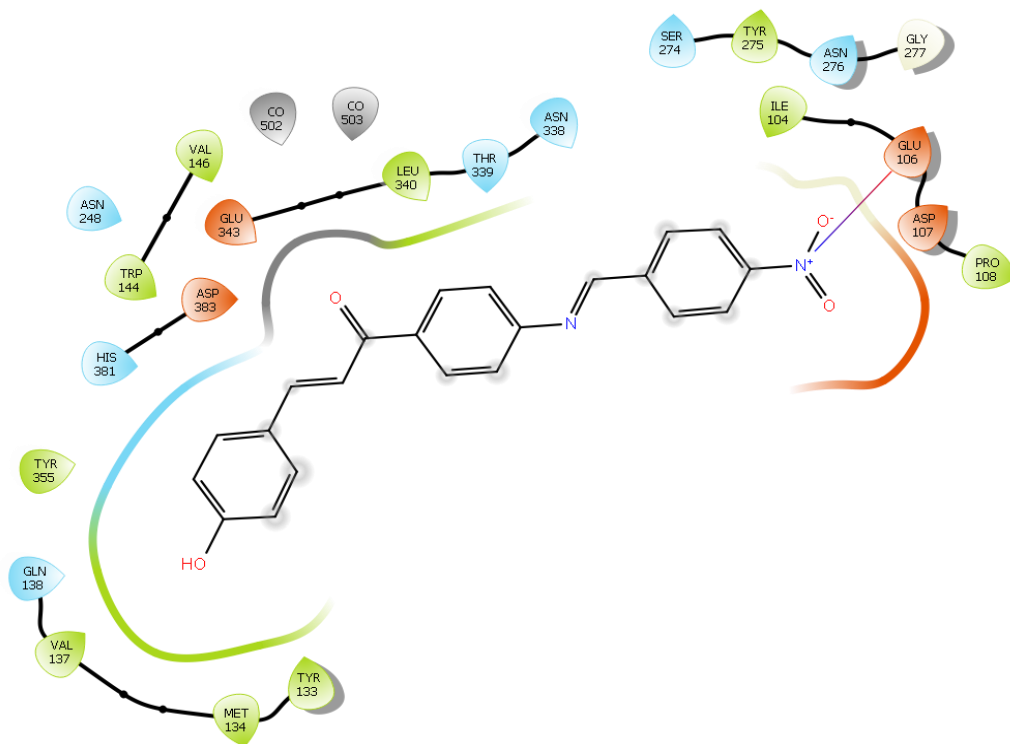


Fig. S4 R = 4-NO₂ within 4Å of *AmpS* active site with salt-bridge communication.

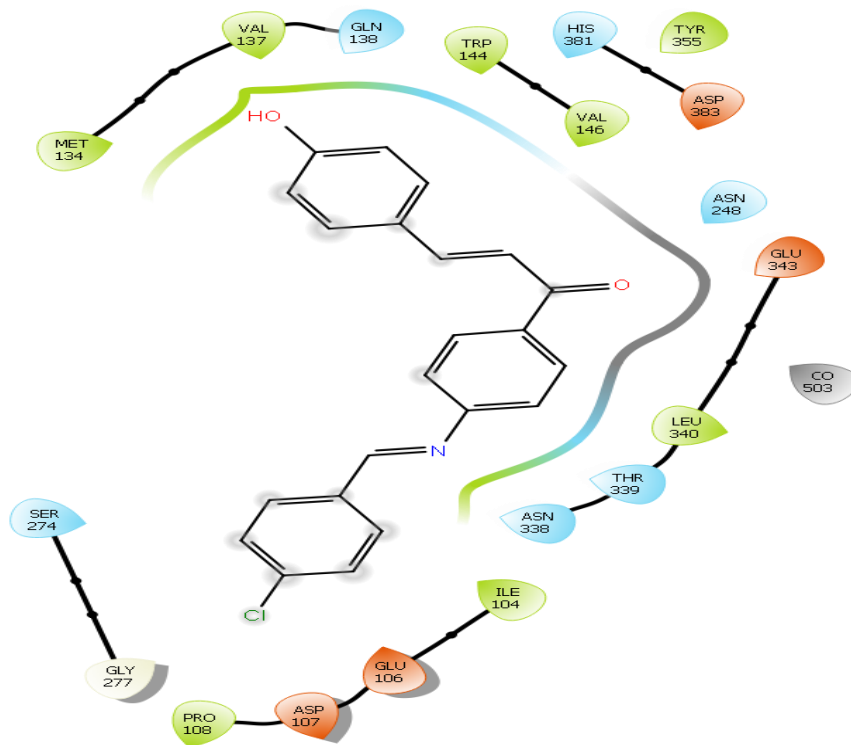


Fig. S5 R = 4-Cl within 4Å of *AmpS* active site with no bond communication.

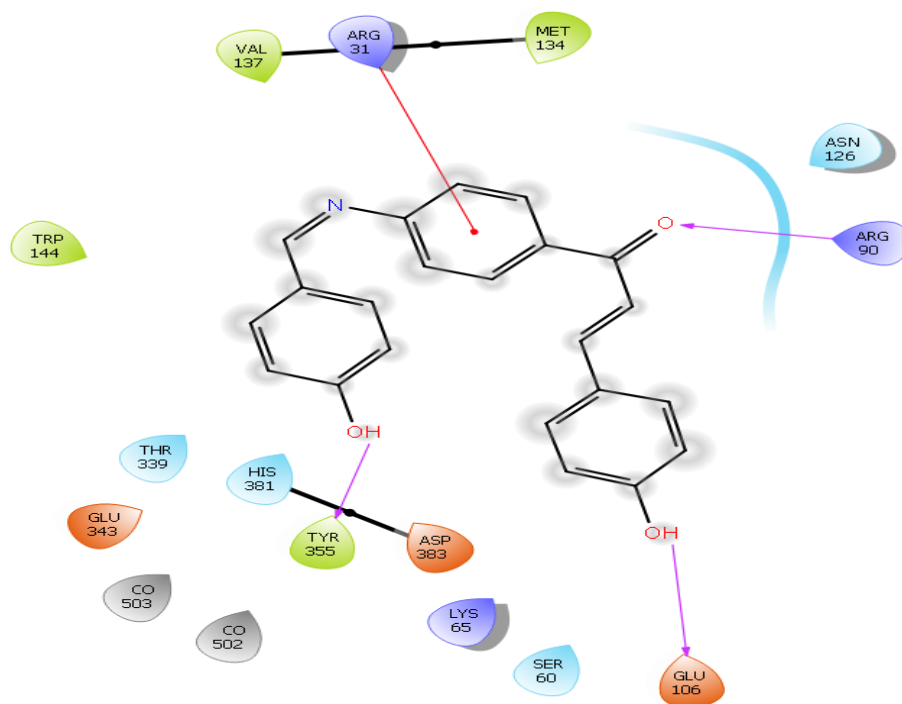


Fig. S6 R = 4-OH within 4Å of *AmpS* active site with hydrogen bond (purple) and pi-cation (red) communication.

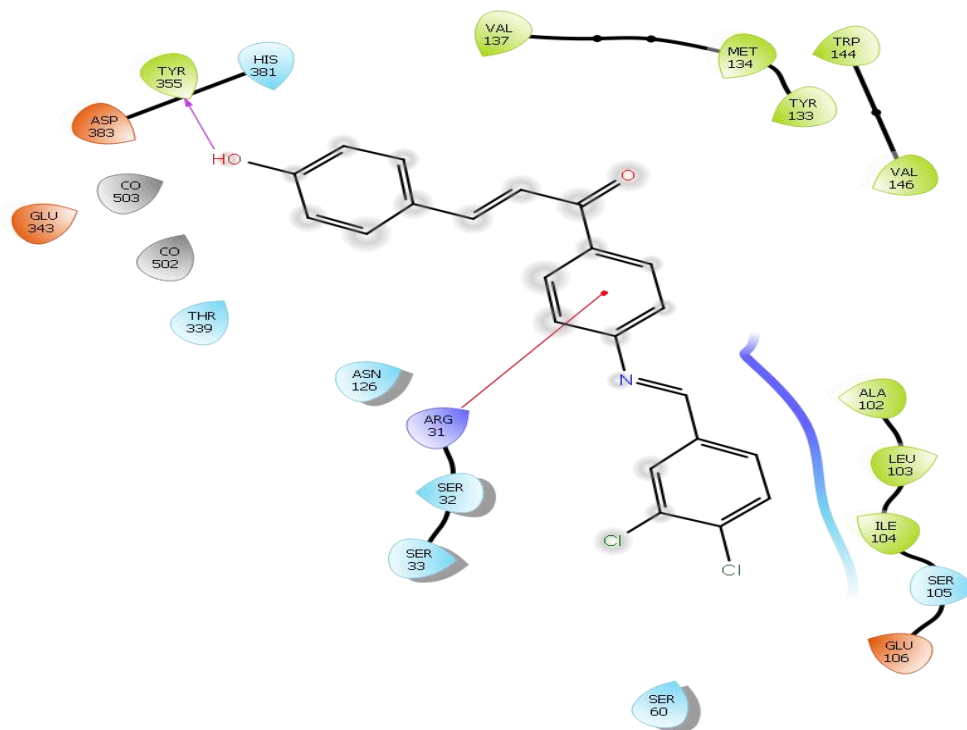


Fig. S7 R = 3-Cl, 4-Cl within 4Å of *AmpS* active site with hydrogen bond (purple) and pi-cation (red) communication.

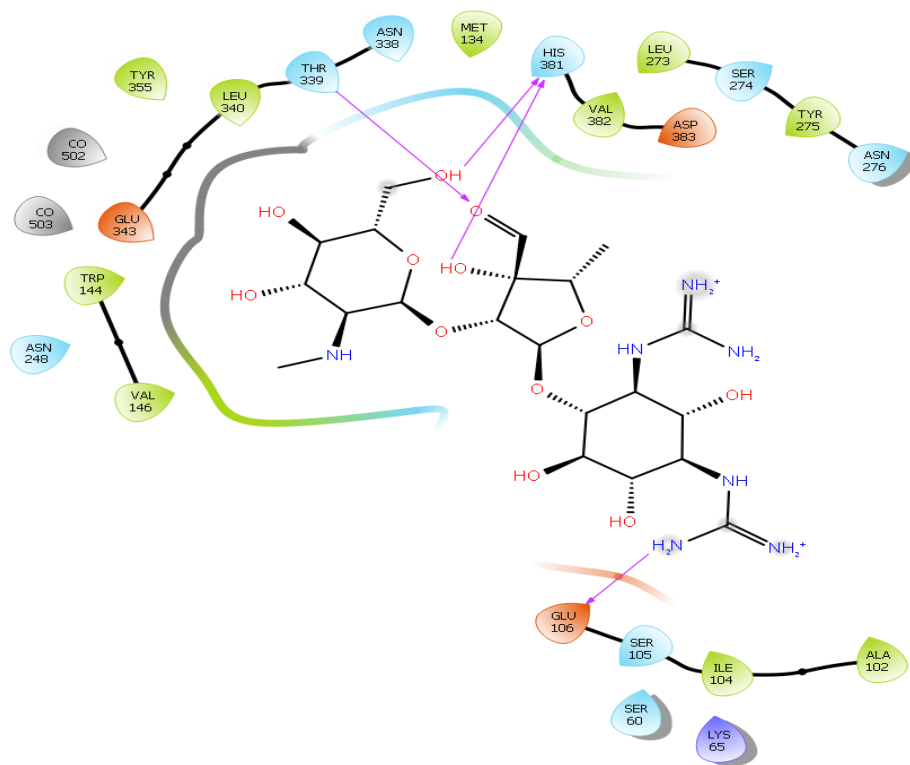


Fig. S8 Streptomycin within 4Å of *AmpS* active site with hydrogen bond (purple) communication.