

Although Am6 obtained a very good score in the COX-2 active site, Am4 seems to have the best affinity towards the enzyme active site. Figure 4.2.B shows how Am4 nicely fits in the COX-2 pocket, making many van der Waal contacts with the surrounding hydrophobic residues. In terms of electrostatics, interestingly, two unusual and strong hydrogen bonding interactions are made between the protonated nitrogen and the backbone amide of Leu352 and Ser353, and another weak hydrogen bond are made between the cyclic carbonyl and the Ser530 hydroxyl group in the top of the catalytic pocket.