



Supplementary Material

In the figures, which show the intermolecular interactions between investigated compounds and cyclooxygenases, hydrophobic interactions are marked in blue and hydrogen bonds are marked in red.

In the figures, which show the binding mode of analyzed compounds, some ribbons were removed to expose the interactions.

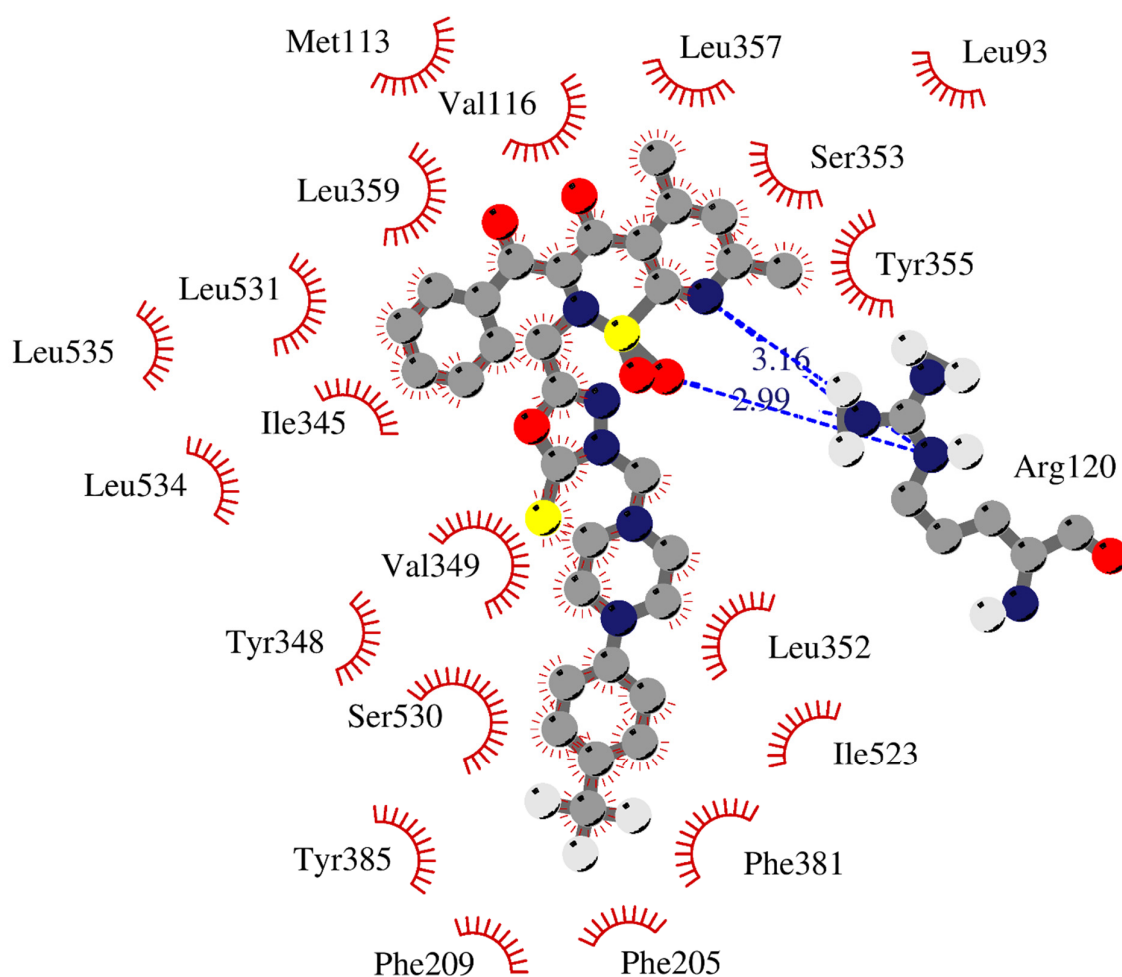


Figure S1. The intermolecular interactions of the investigated compound TG4 and cyclooxygenase (COX)-1.

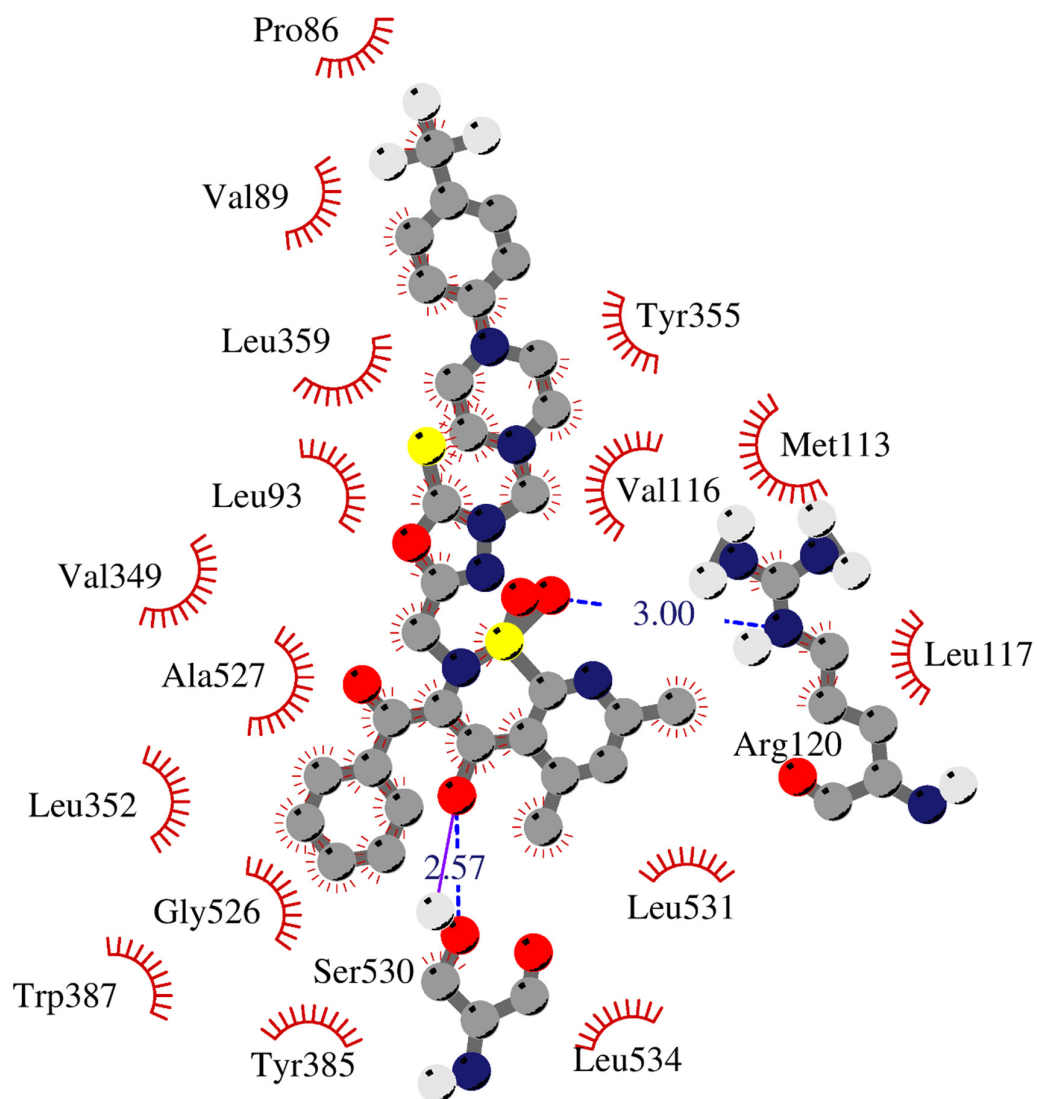


Figure S2. The intermolecular interactions between the investigated compound **TG4** and cyclooxygenase COX-2.

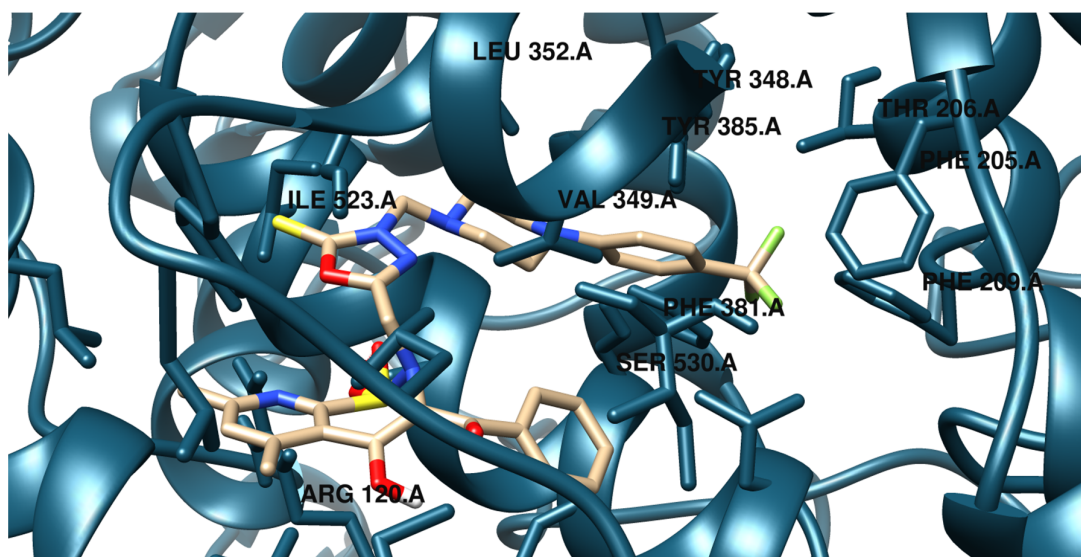


Figure S3. The binding mode of the analyzed compound TG4–COX-1 complex.

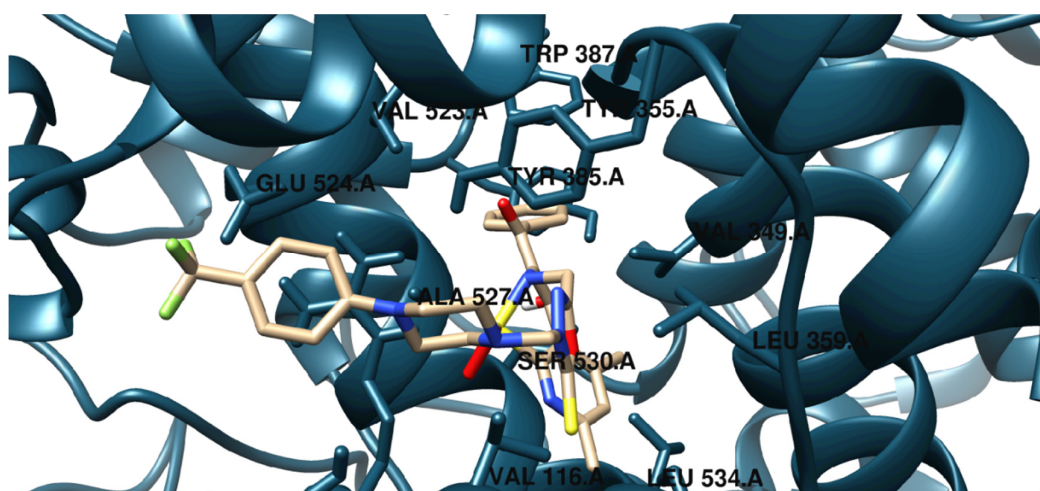


Figure S4. The binding mode of the analyzed compound TG4–COX-2 complex.

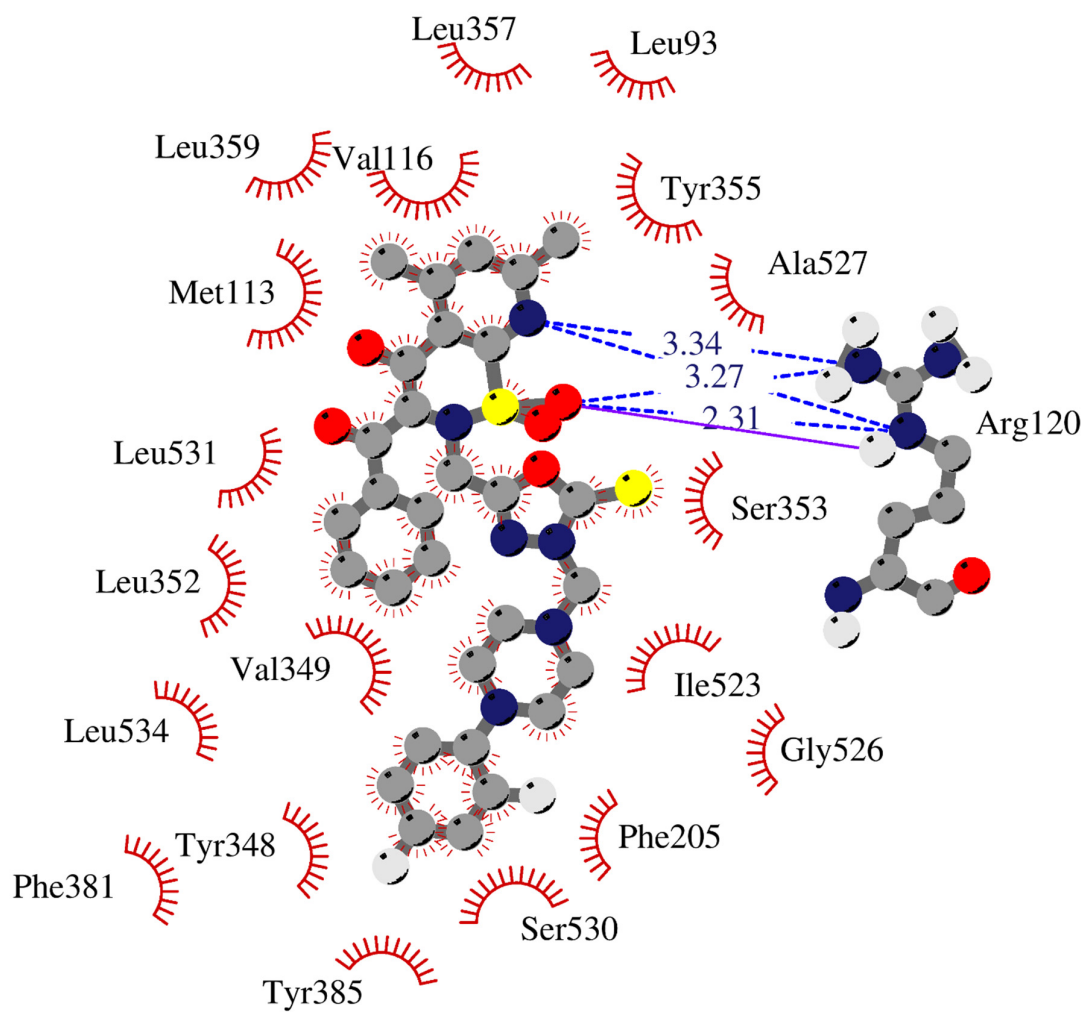


Figure S5. The intermolecular interactions between the investigated compound **TG6** and cyclooxygenase COX-1.

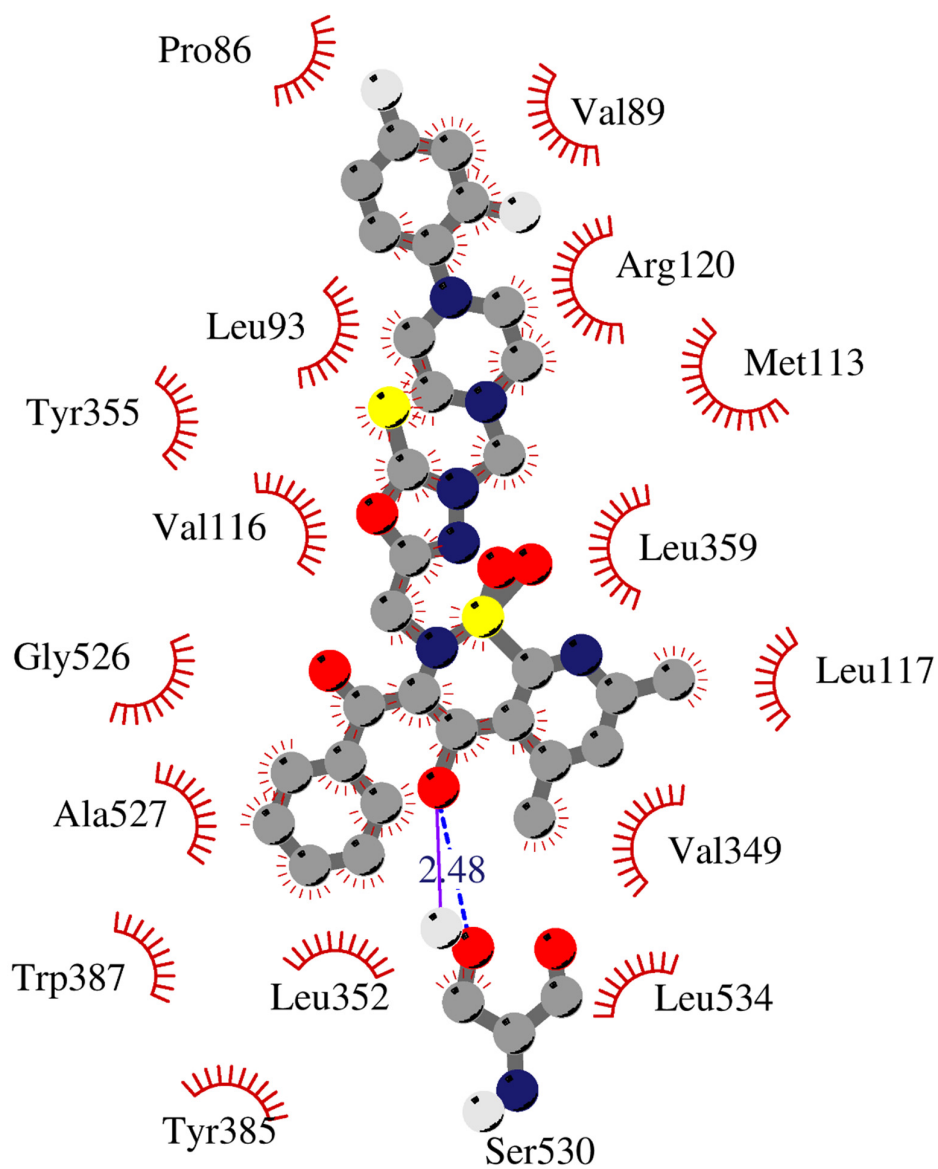


Figure S6. The intermolecular interactions between the investigated compound TG6 and cyclooxygenase COX-2.

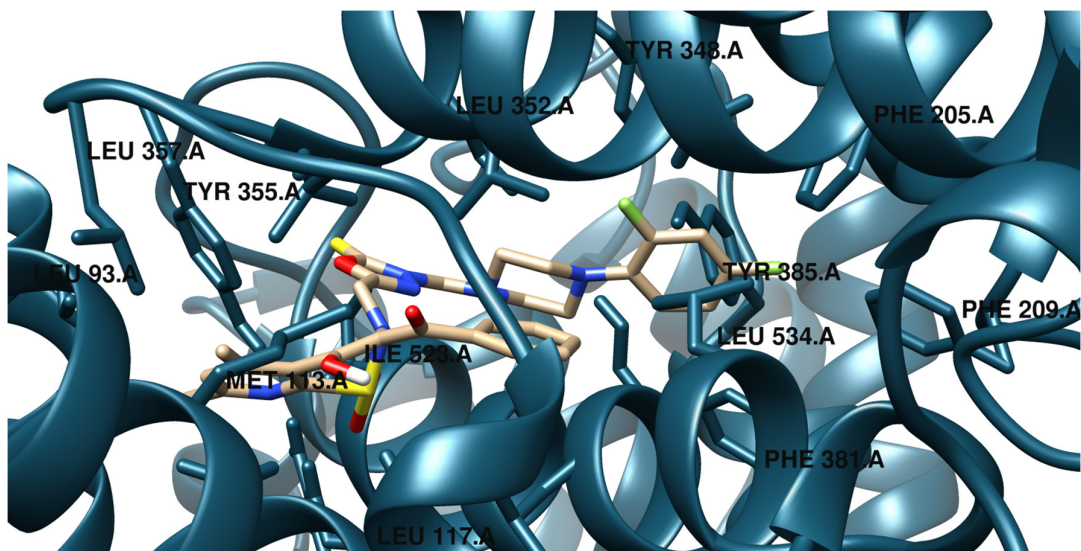


Figure S7. The binding mode of the analyzed compound TG6–COX-1 complex.

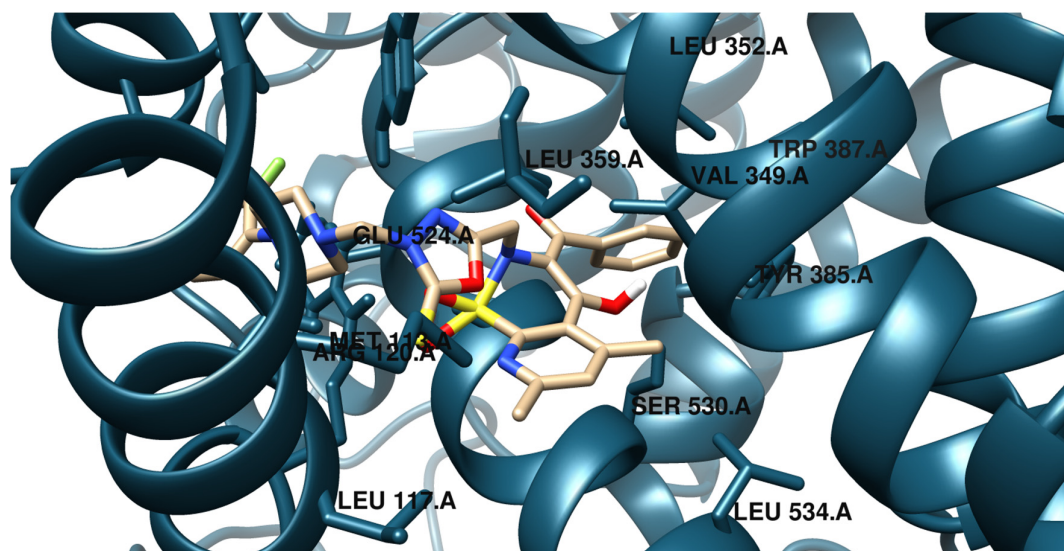


Figure S8. The binding mode of the analyzed compound TG6–COX-2 complex.

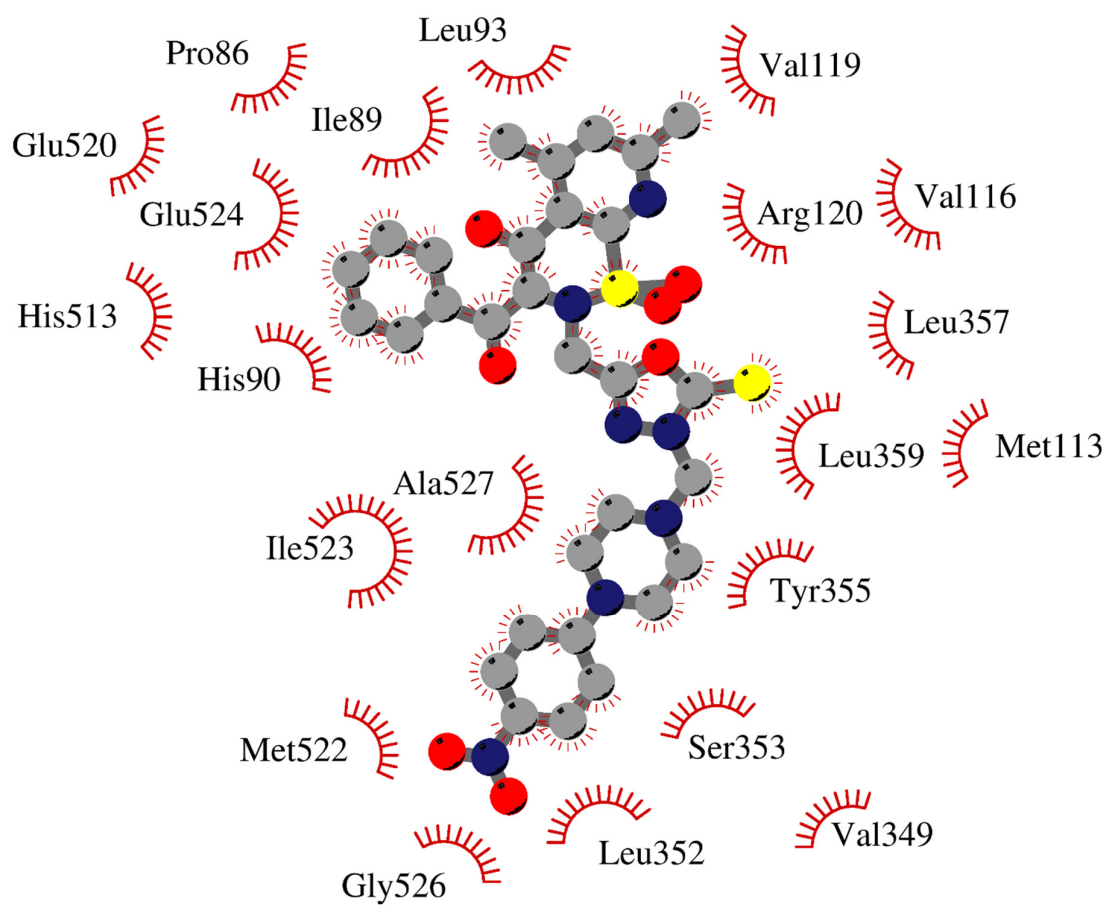


Figure S9. The intermolecular interactions between the investigated compound TG10 and cyclooxygenase COX-1.

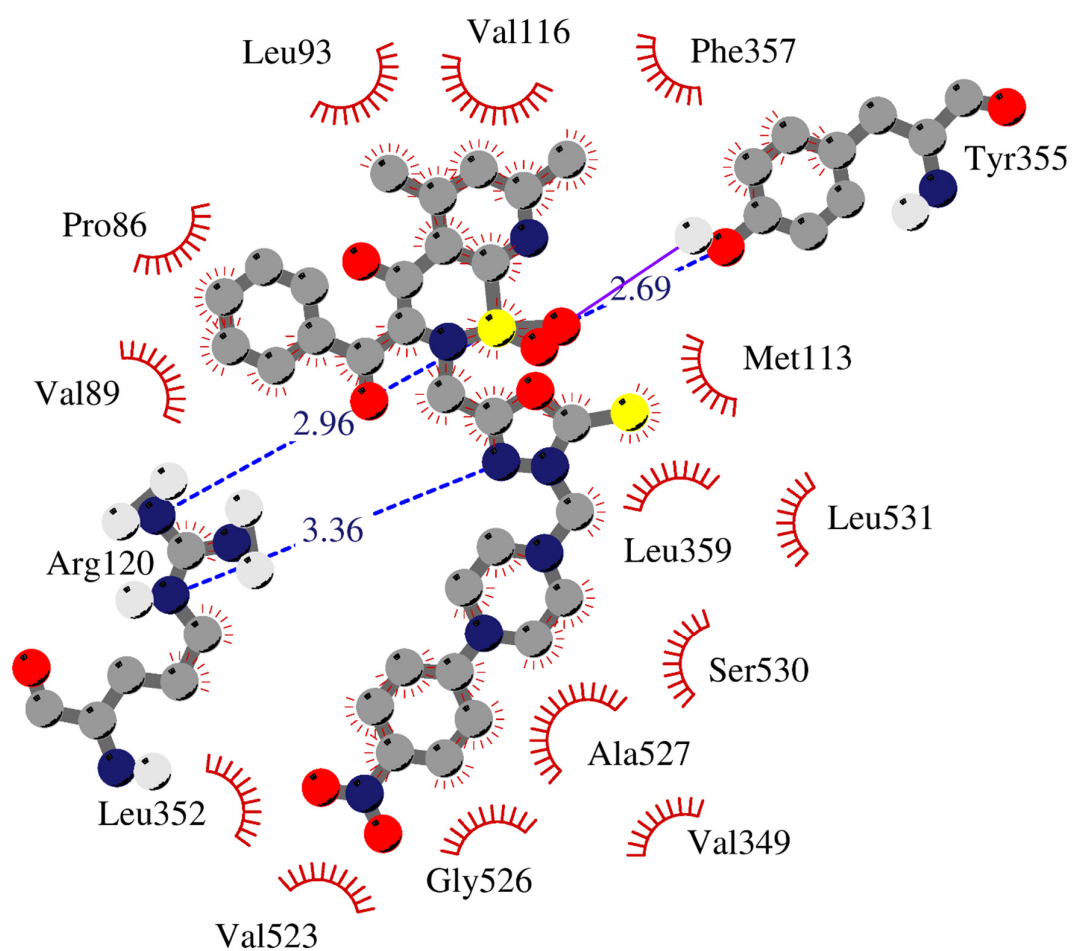


Figure S10. The intermolecular interactions between the investigated compound **TG10** and cyclooxygenase COX-2.

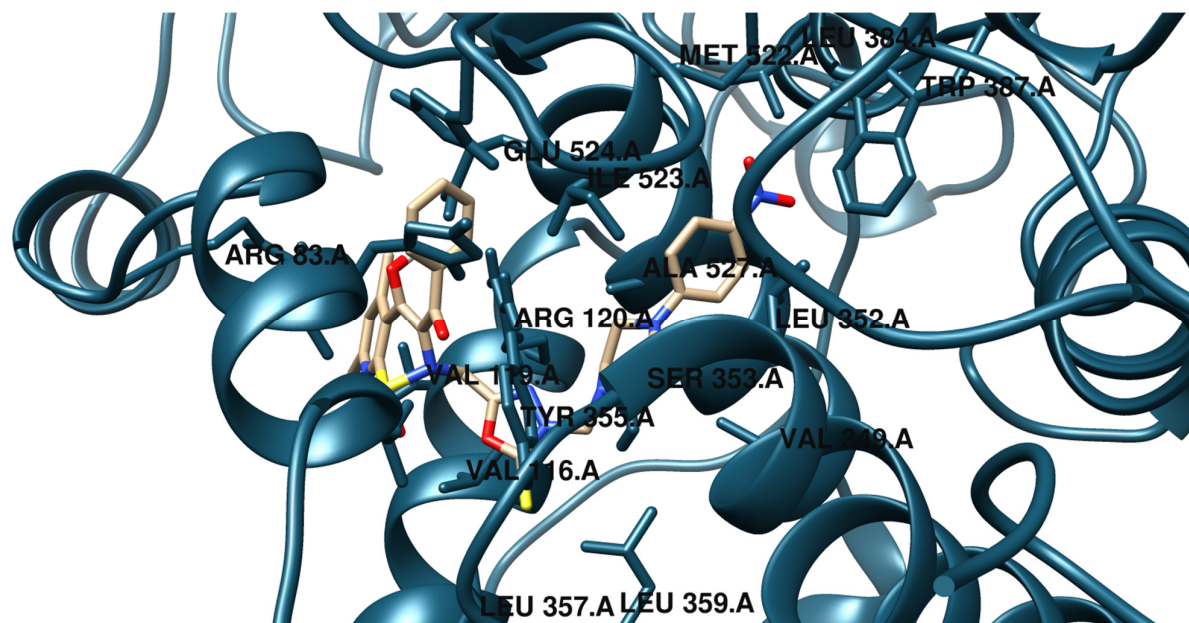


Figure S11. The binding mode of the analyzed compound TG10–COX-1 complex.

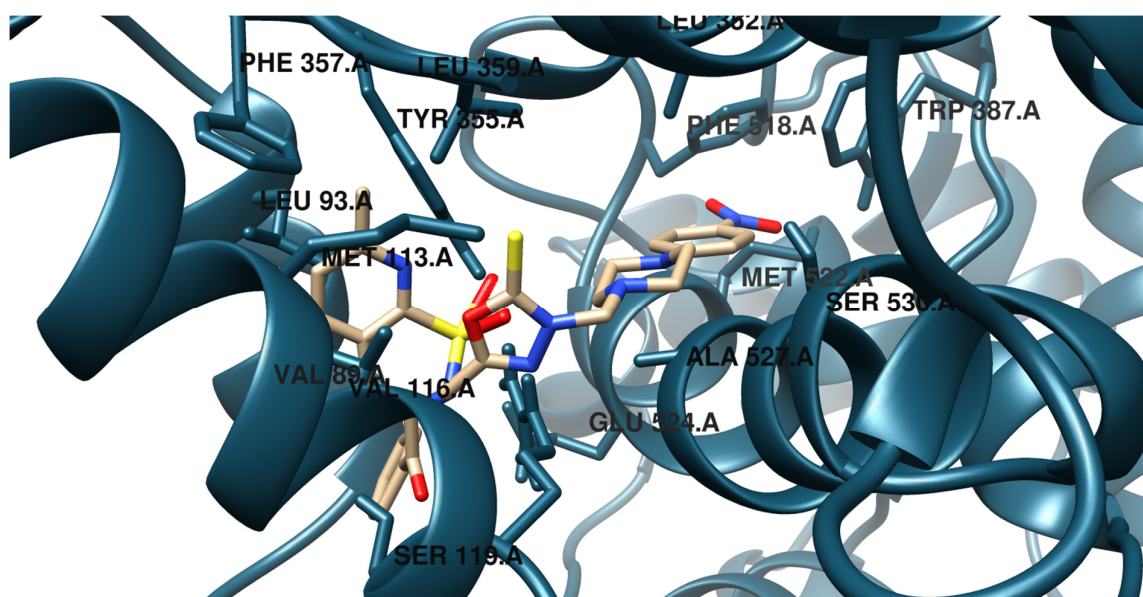


Figure S12. The binding mode of the analyzed compound TG10–COX-2 complex.

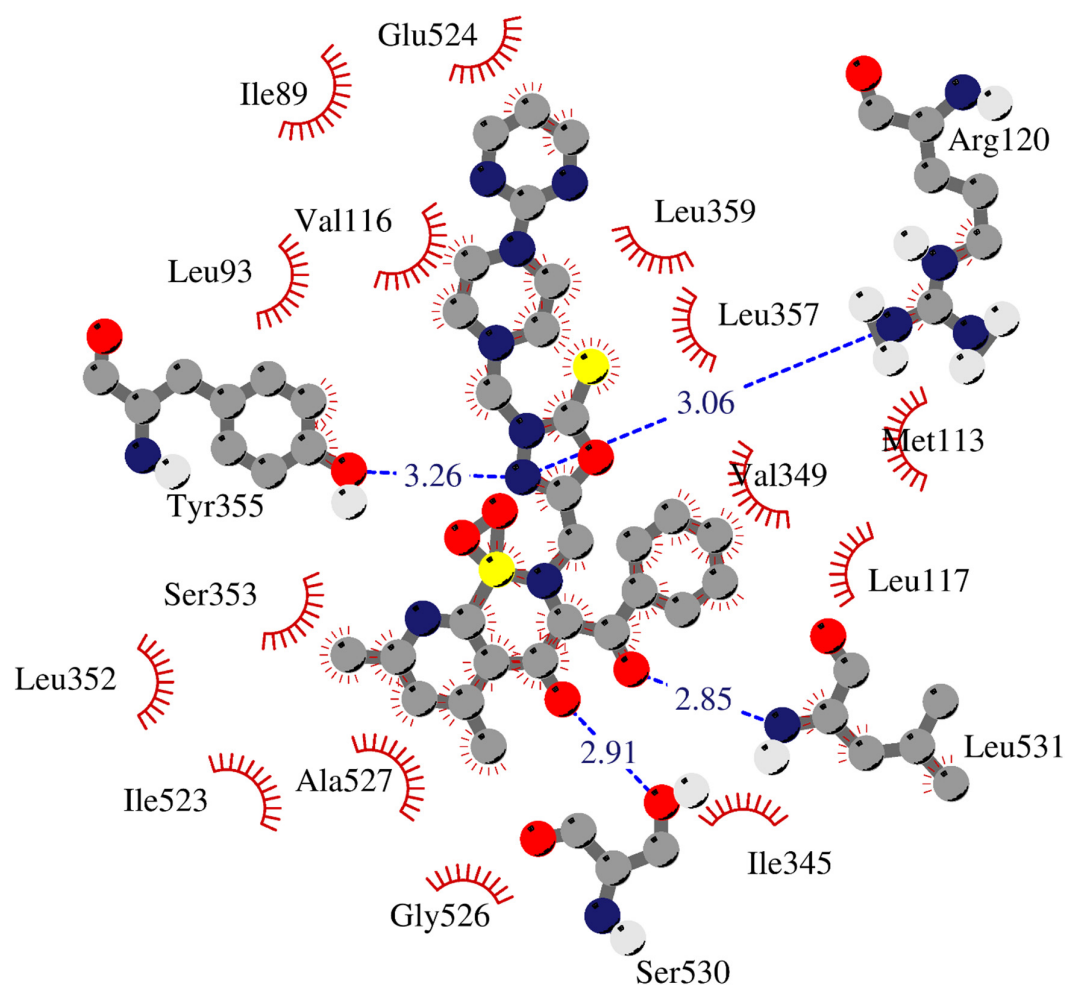


Figure S13. The intermolecular interactions between the investigated compound TG12 and cyclooxygenase COX-1.

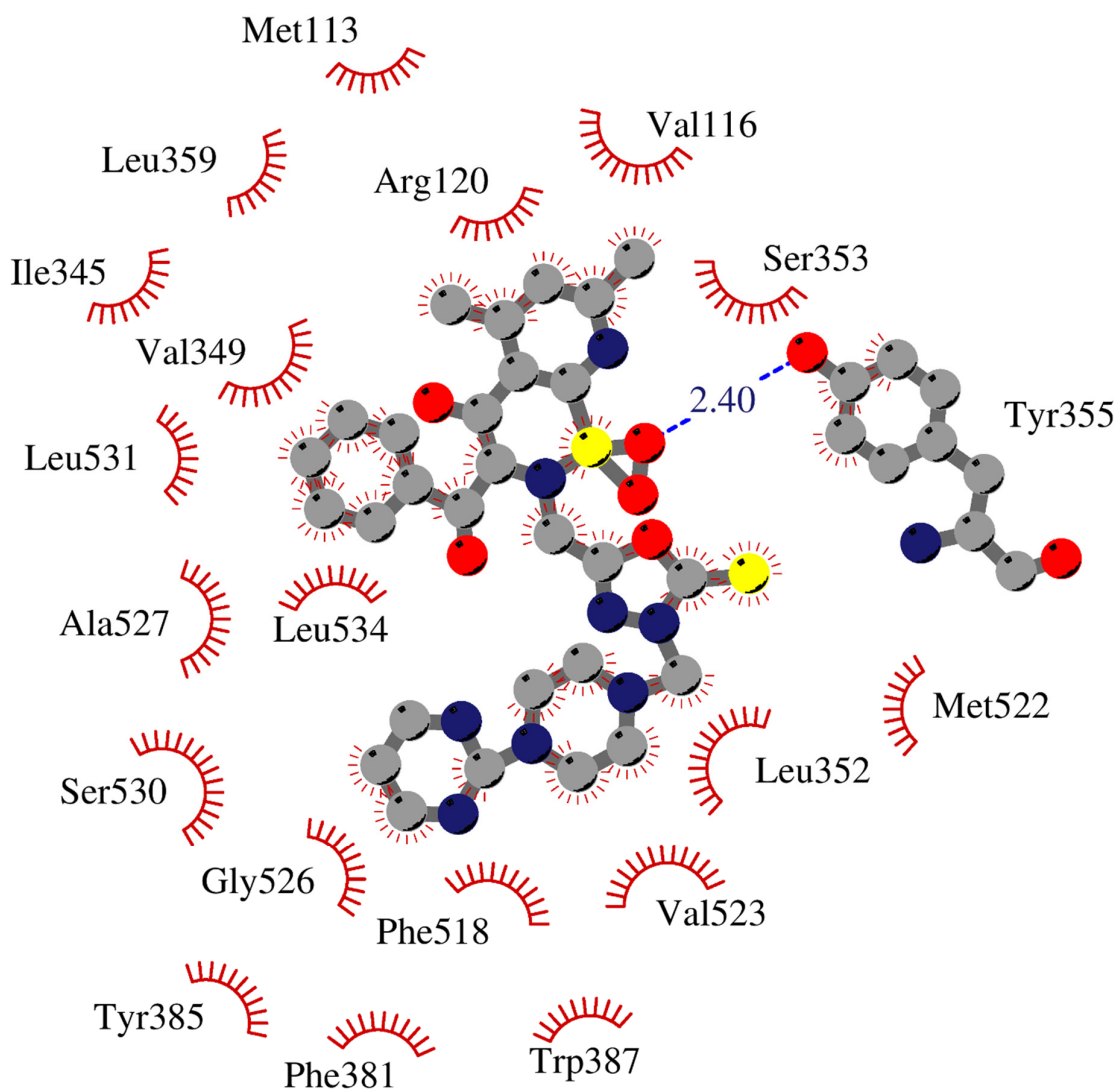


Figure S14. The intermolecular interactions between the investigated compound **TG12** and cyclooxygenase COX-2.

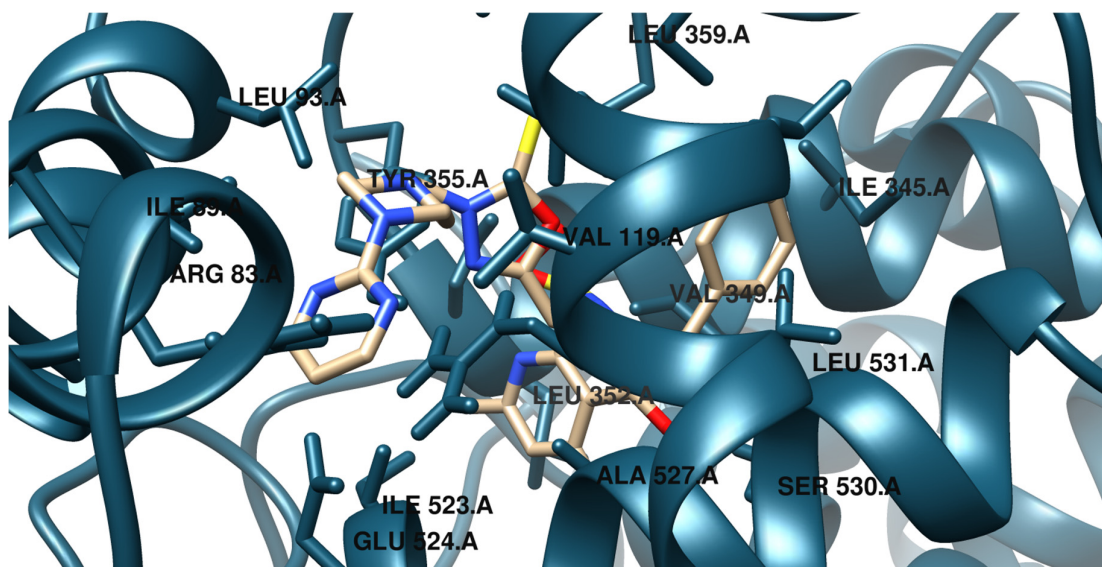


Figure S15. The binding mode of the analyzed compound TG12–COX-1 complex.

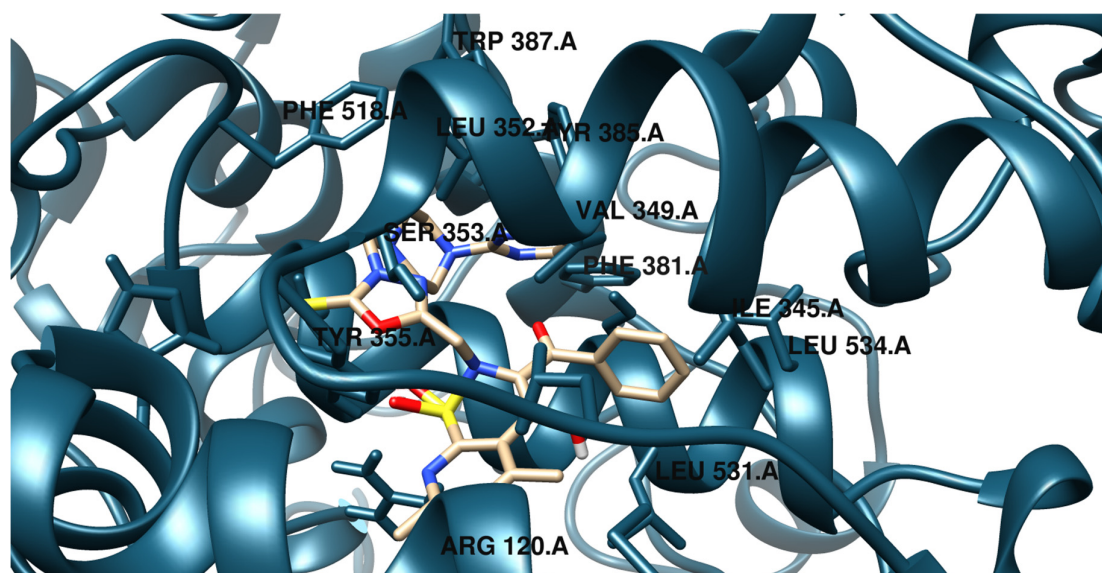


Figure S16. The binding mode of the analyzed compound TG12–COX-2 complex.