Supplementary Data

This supplementary data is a part of a paper entitled "Molecular Docking and Molecular Dynamic Investigations of Xanthone-Chalcone Derivatives against Epidermal Growth Factor Receptor for Preliminary Discovery of Novel Anticancer Agent".

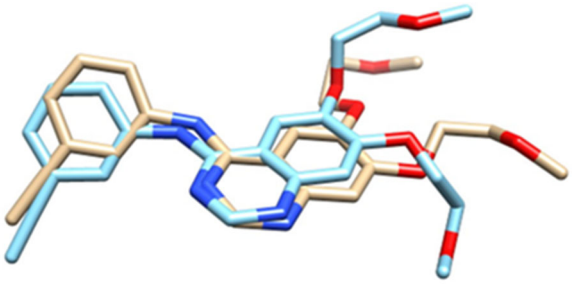

Fig S1. The superimposed structures of the native ligand before (light-brown color) and after (light-blue color) re-docking process in the active site of EGFR, in which the oxygen and nitrogen atoms are shown in red and dark blue color, respectively

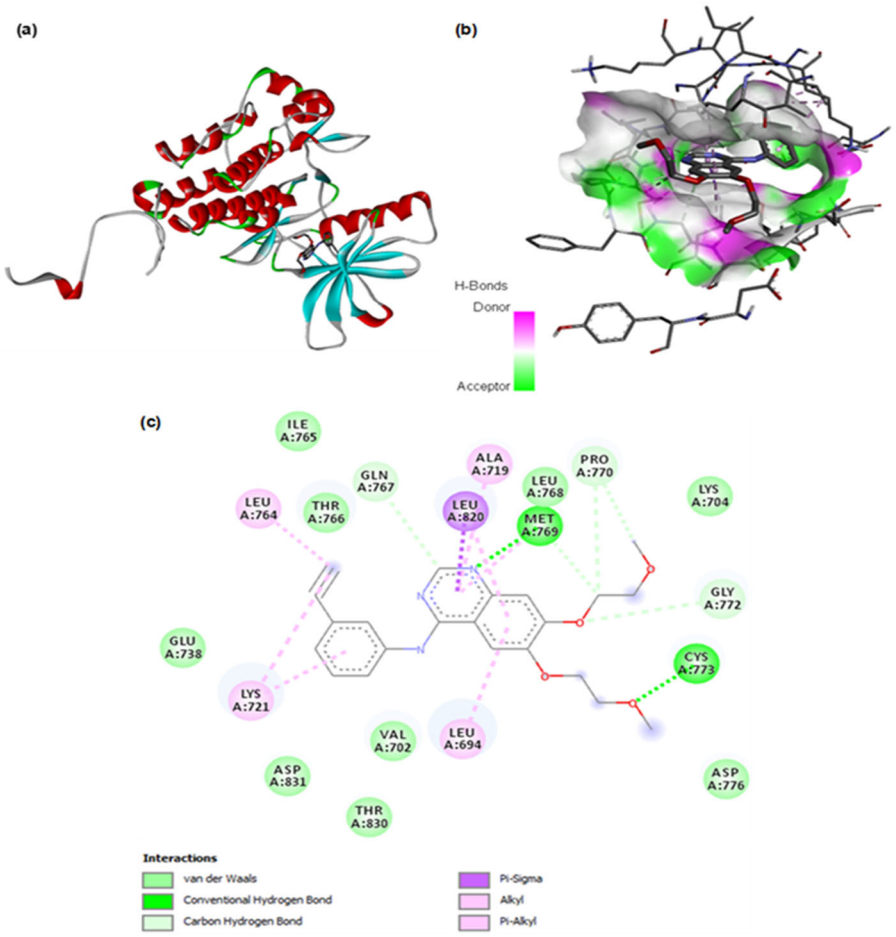

Fig S2. Re-docking of the native ligand in the (a) whole structure and (b) active site of EGFR and (c) non-covalent interactions between native ligand and the active site of EGFR

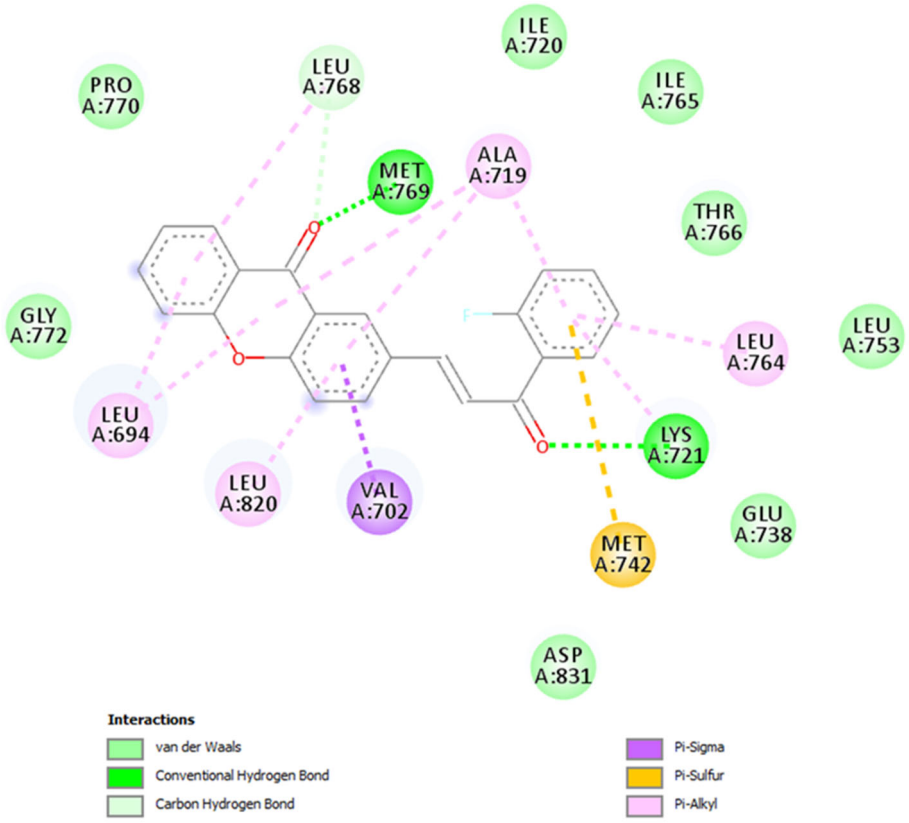

Fig S3. Non-covalent interactions between compound 2F and the active site of EGFR

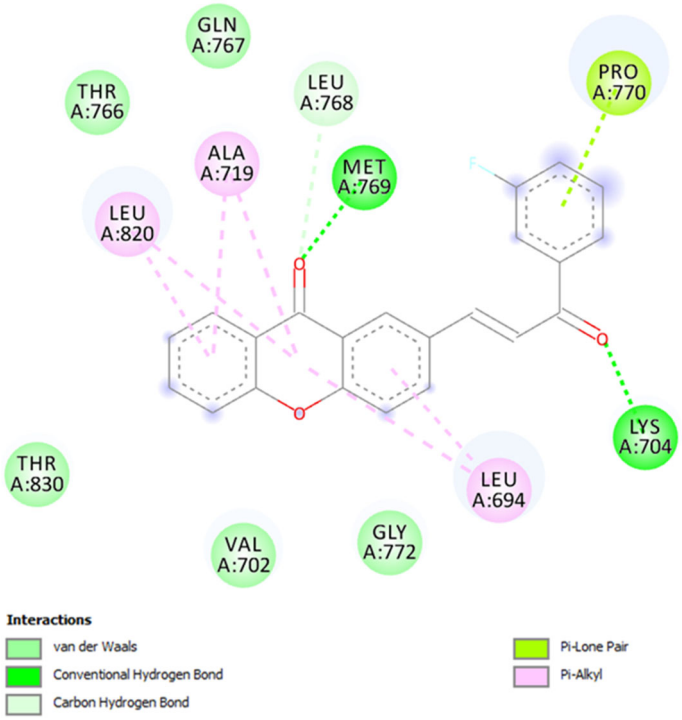

Fig S4. Non-covalent interactions between compound 3F and the active site of EGFR

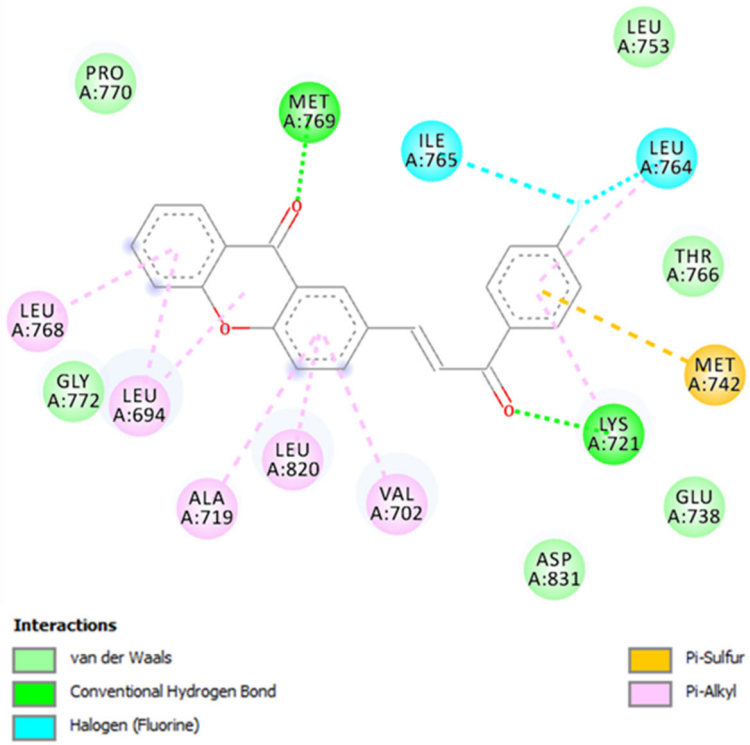

Fig S5. Non-covalent interactions between compound 4F and the active site of EGFR

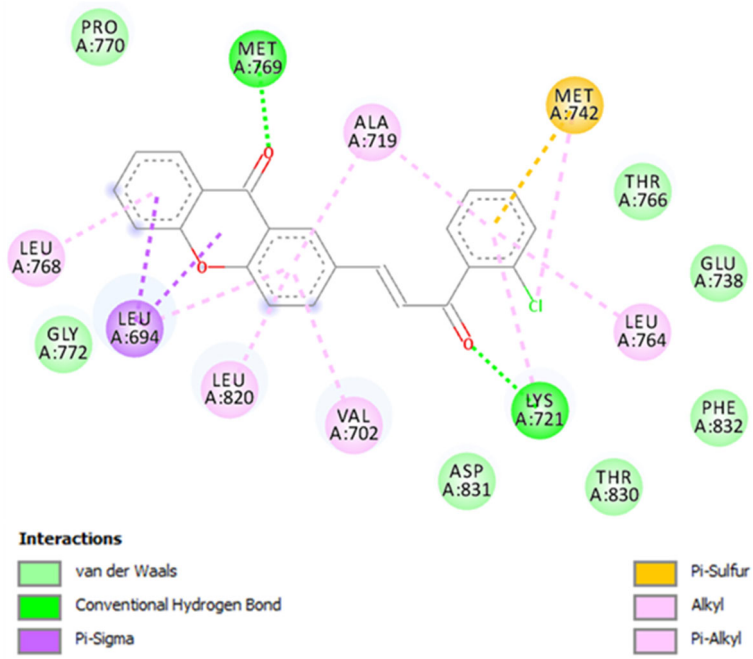

Fig S6. Non-covalent interactions between compound 2Cl and the active site of EGFR

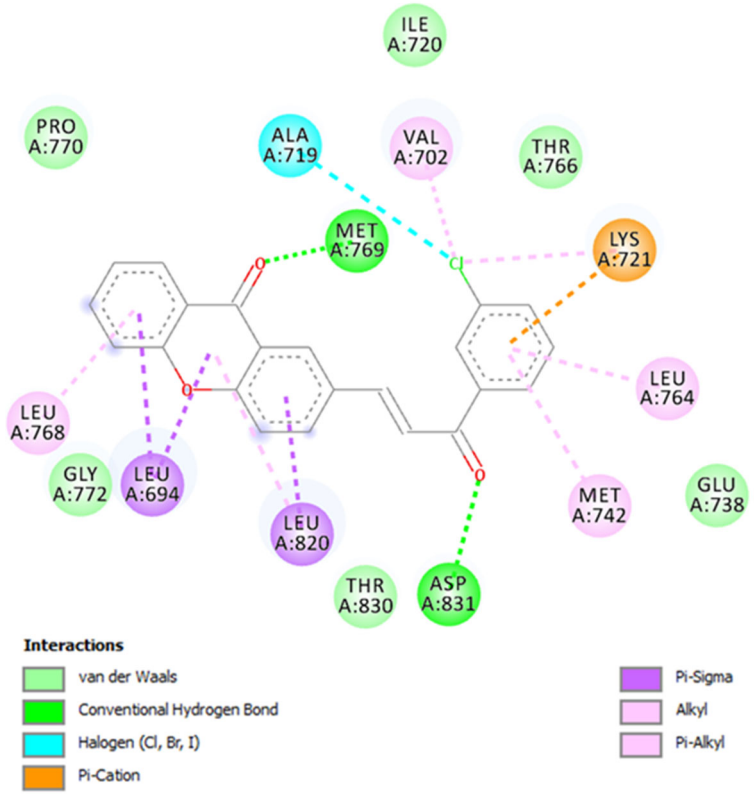

Fig S7. Non-covalent interactions between compound 3Cl and the active site of EGFR

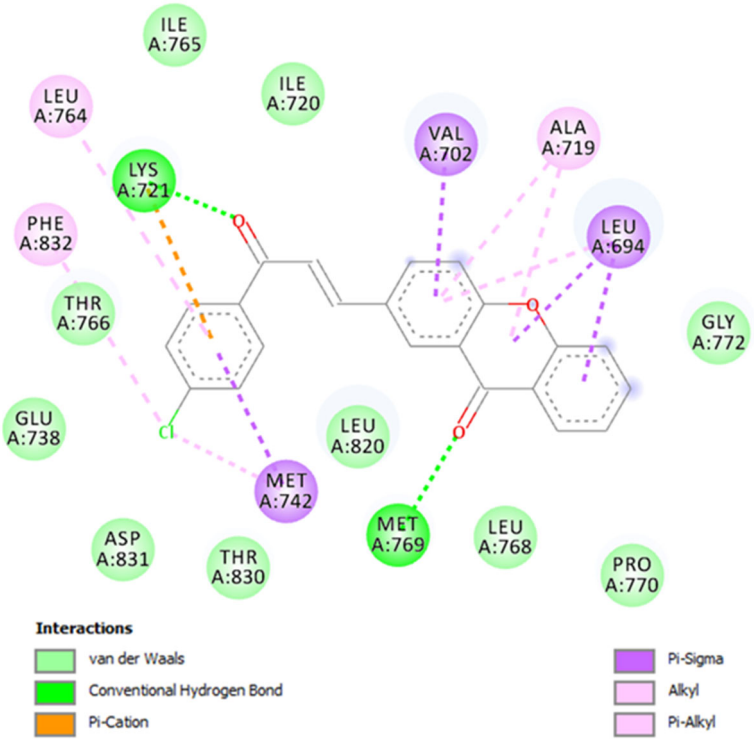

Fig S8. Non-covalent interactions between compound 4Cl and the active site of EGFR

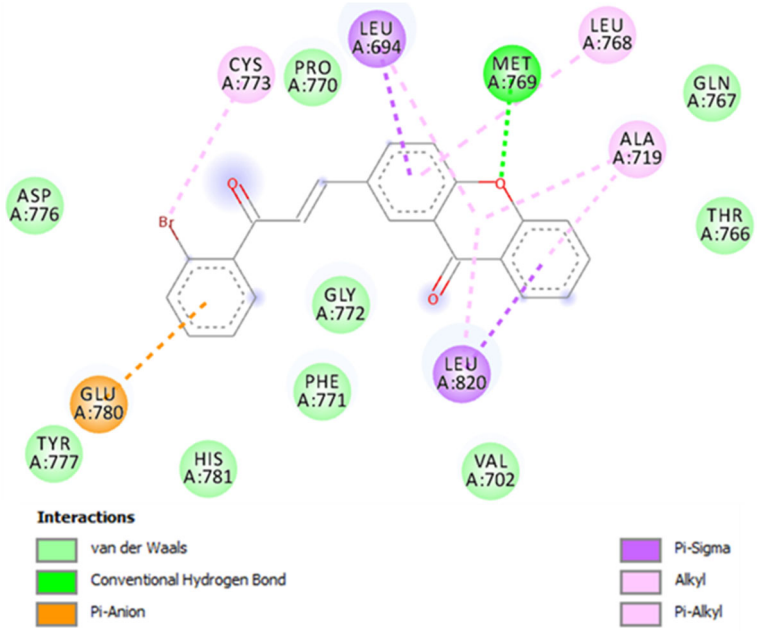

Fig S9. Non-covalent interactions between compound 2Br and the active site of EGFR

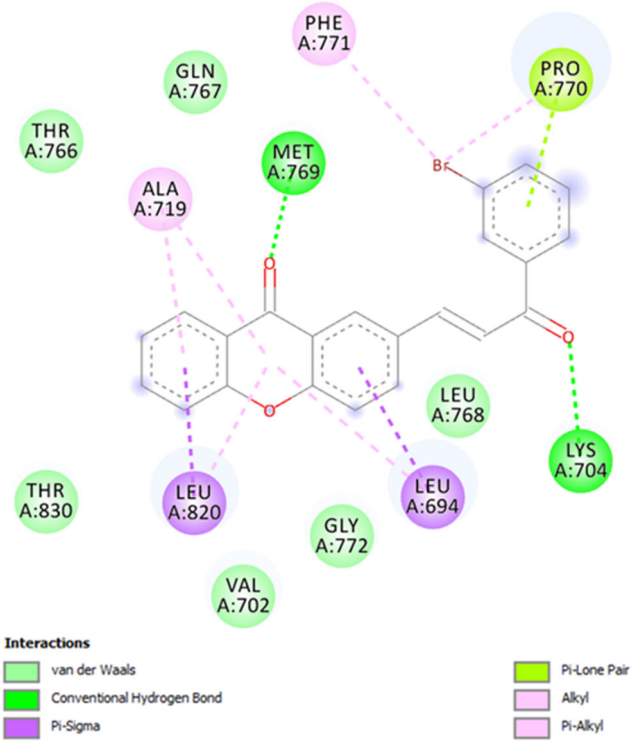

Fig S10. Non-covalent interactions between compound 3Br and the active site of EGFR

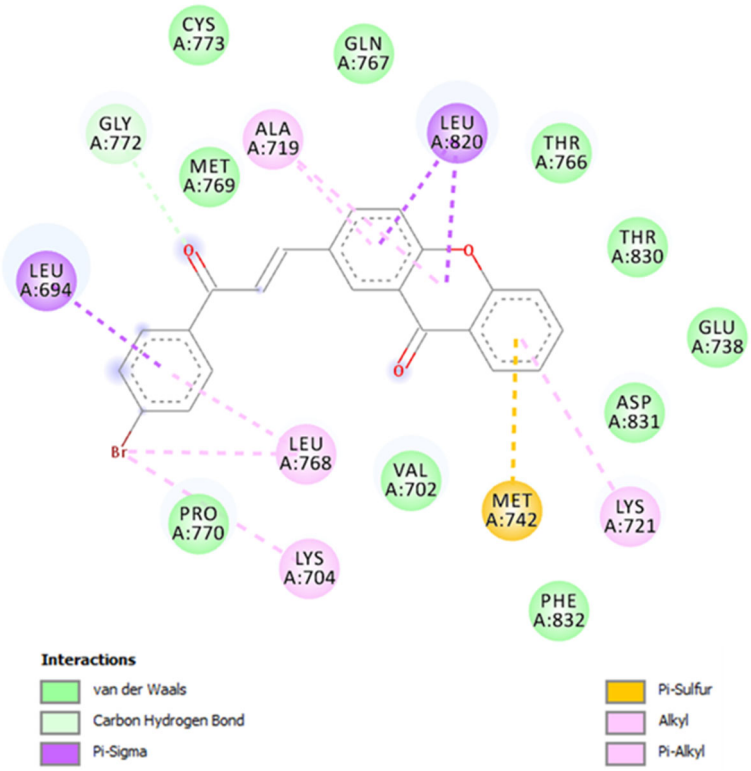

Fig S11. Non-covalent interactions between compound 4Br and the active site of EGFR

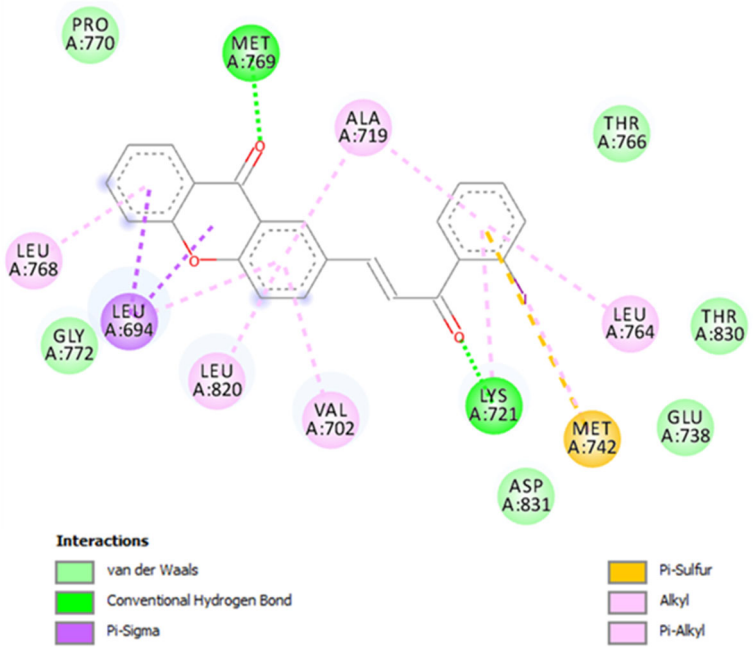

Fig S12. Non-covalent interactions between compound 2I and the active site of EGFR

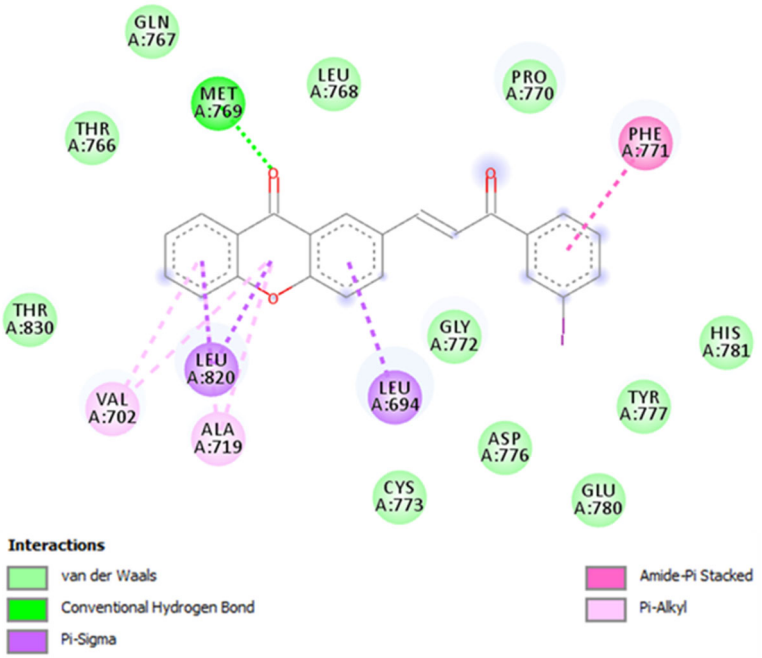

Fig S13. Non-covalent interactions between compound 3I and the active site of EGFR

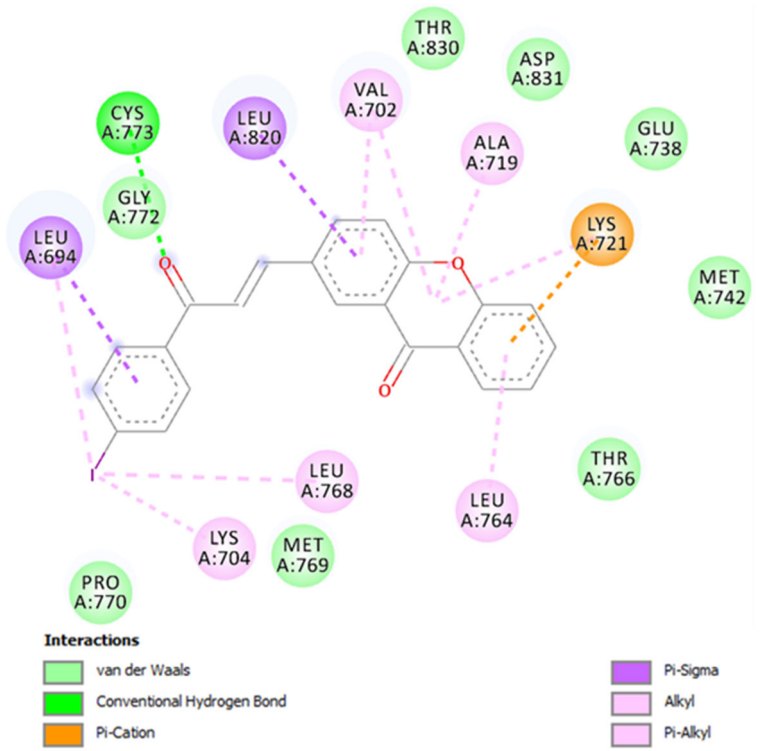

Fig S14. Non-covalent interactions between compound 4I and the active site of EGFR

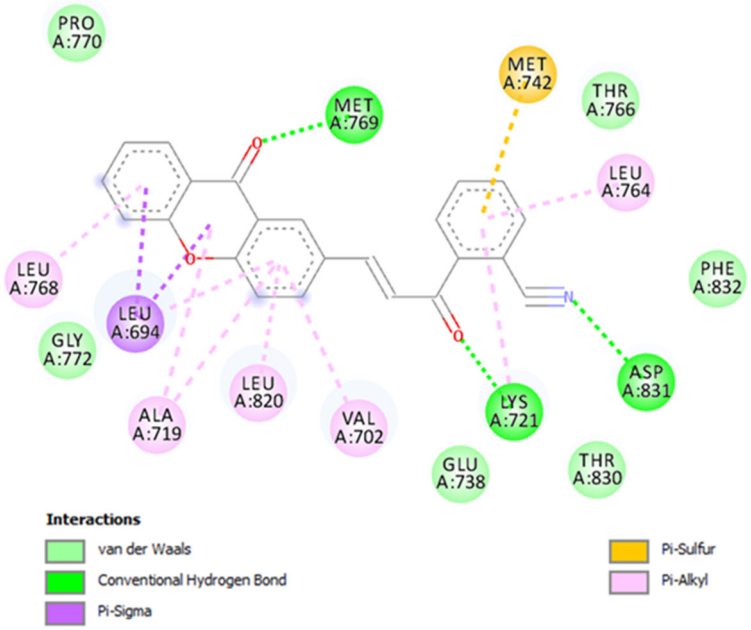

Fig S15. Non-covalent interactions between compound 2CN and the active site of EGFR

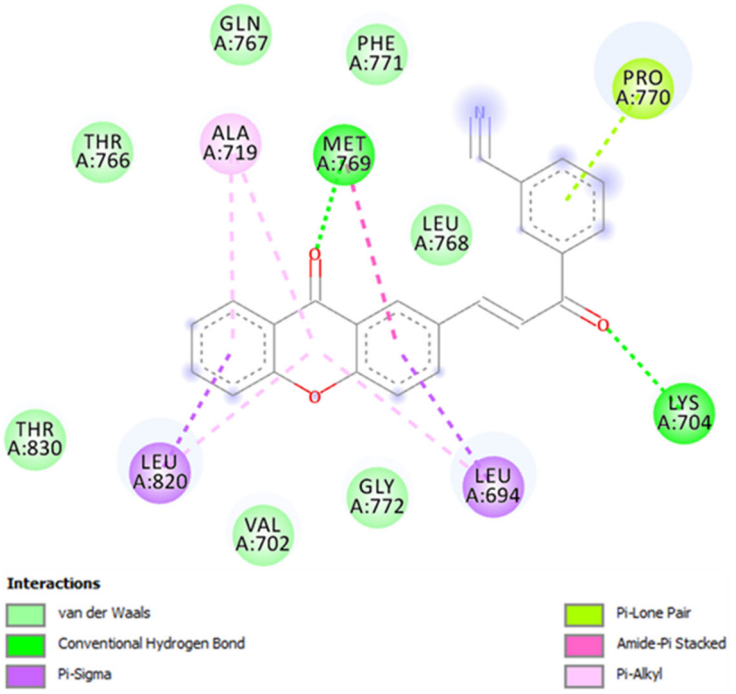

Fig S16. Non-covalent interactions between compound 3CN and the active site of EGFR

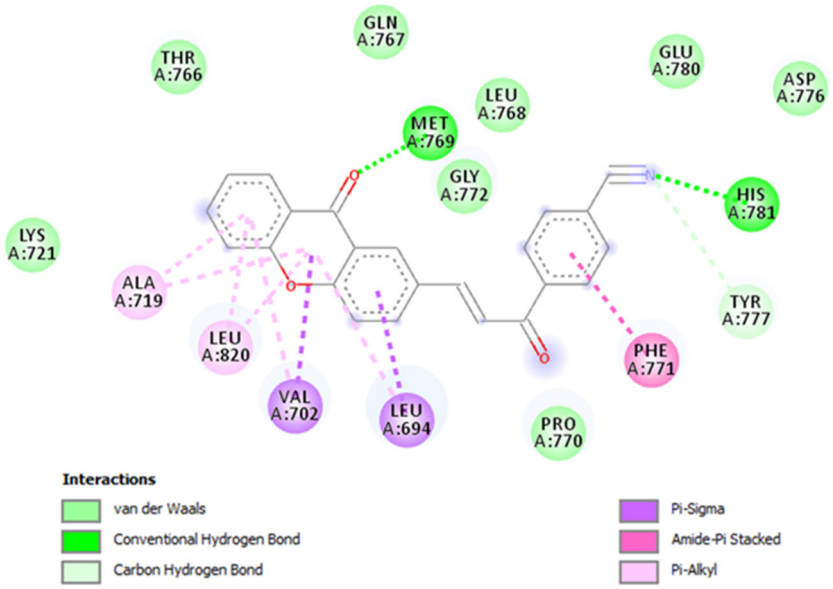

Fig S17. Non-covalent interactions between compound 4CN and the active site of EGFR

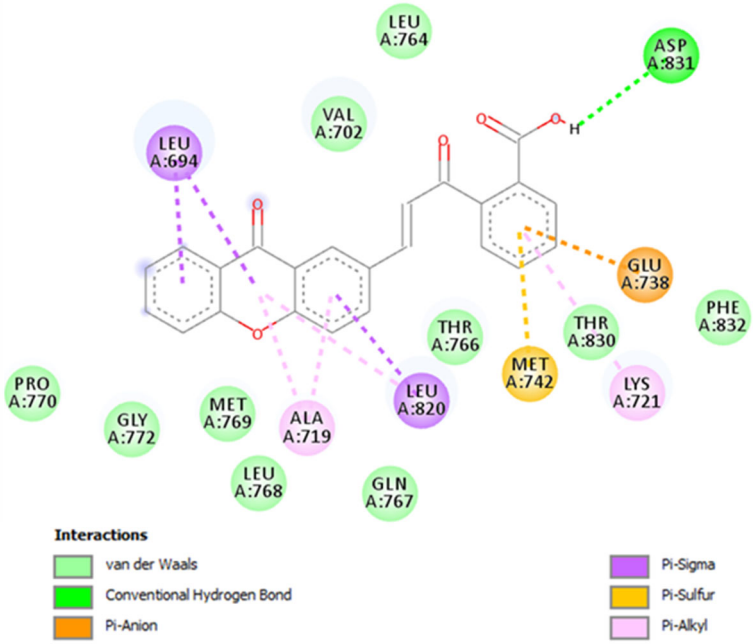

Fig S18. Non-covalent interactions between compound $2CO_2H$ and the active site of EGFR

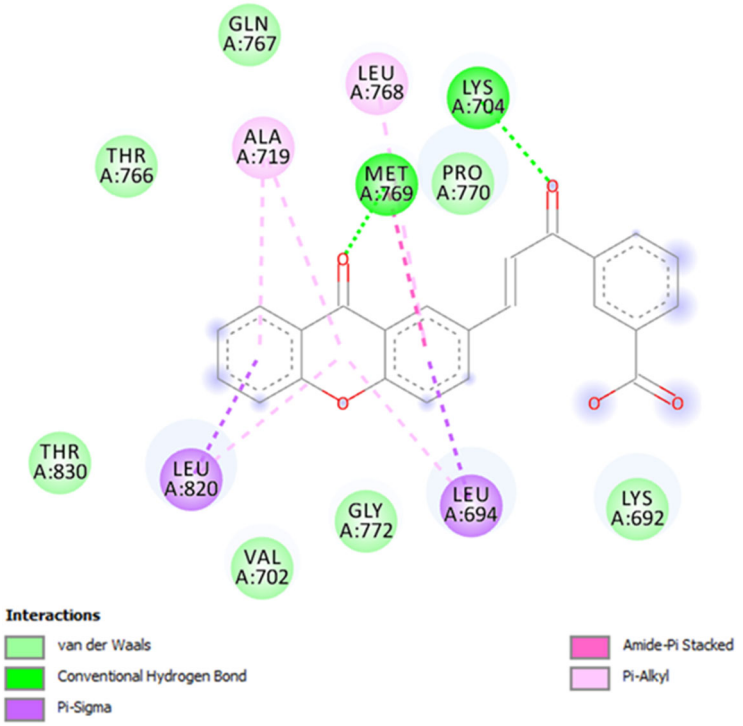

Fig S19. Non-covalent interactions between compound $3CO_2H$ and the active site of EGFR

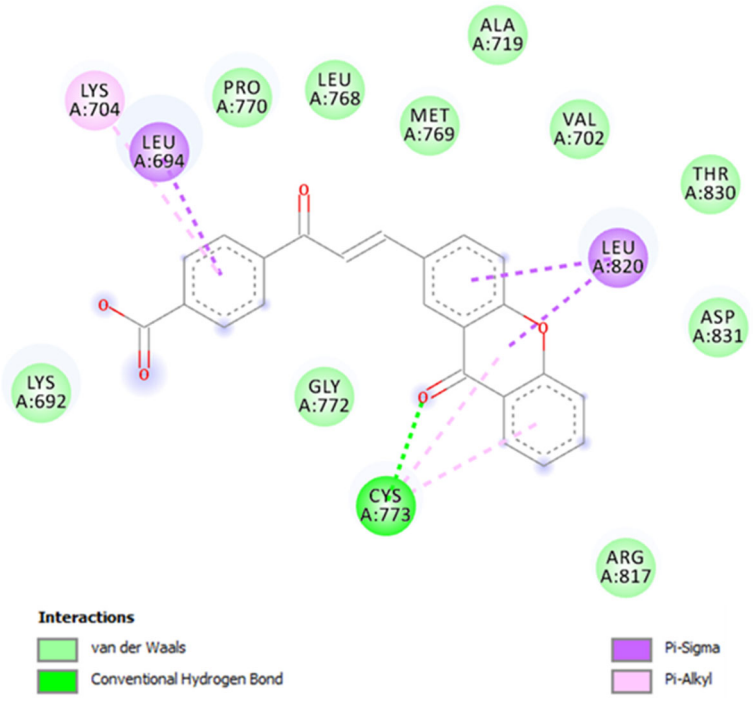

Fig S20. Non-covalent interactions between compound $4CO_2H$ and the active site of EGFR

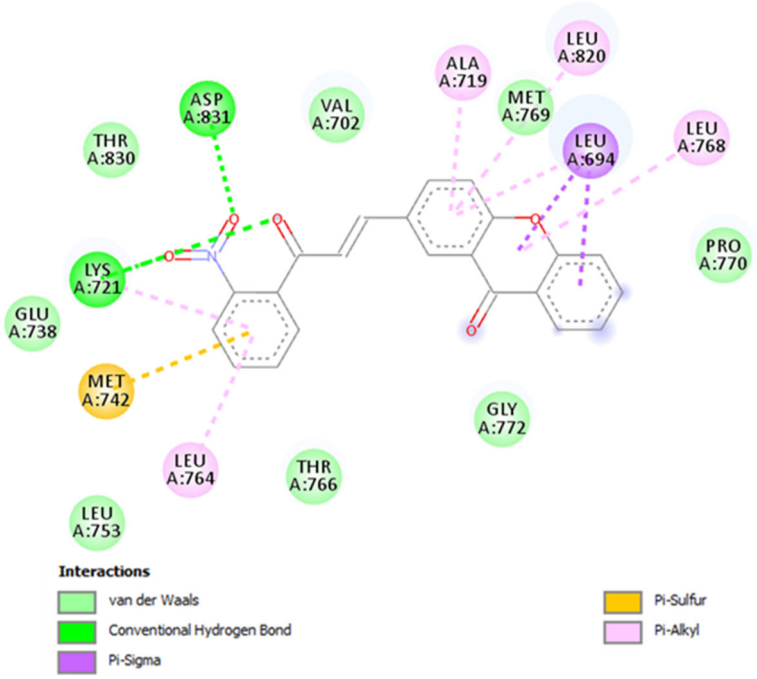

Fig S21. Non-covalent interactions between compound $2NO_2$ and the active site of EGFR

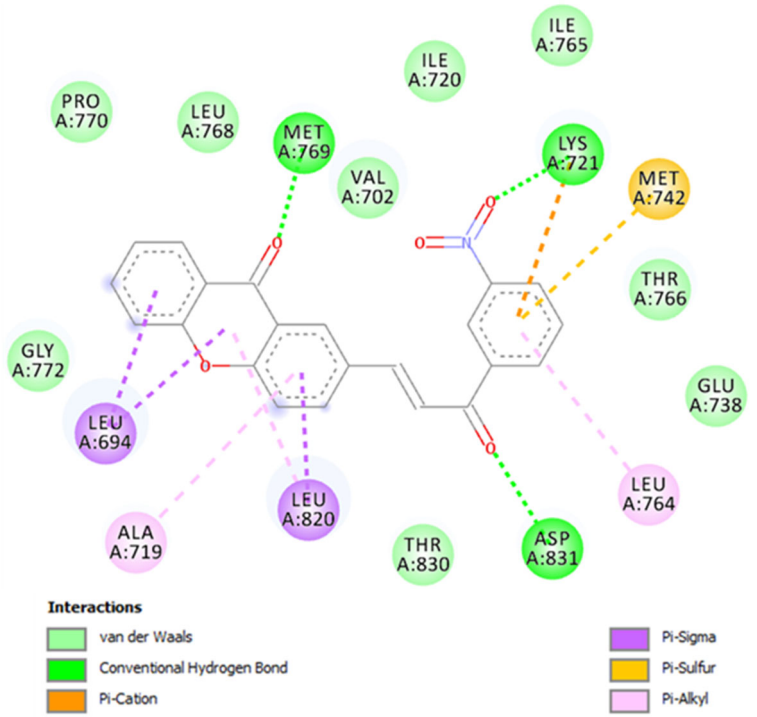

Fig S22. Non-covalent interactions between compound $3NO_2$ and the active site of EGFR

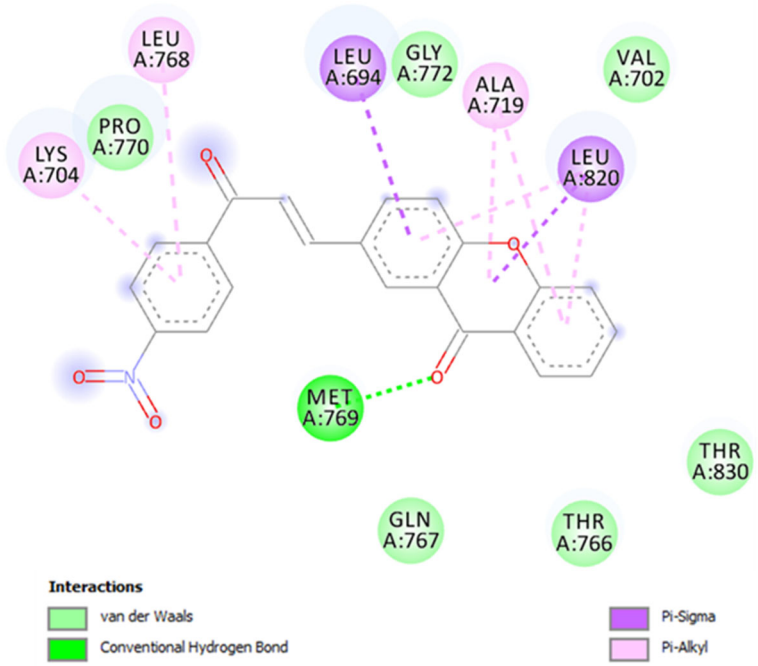

Fig S23. Non-covalent interactions between compound $4NO_2$ and the active site of EGFR

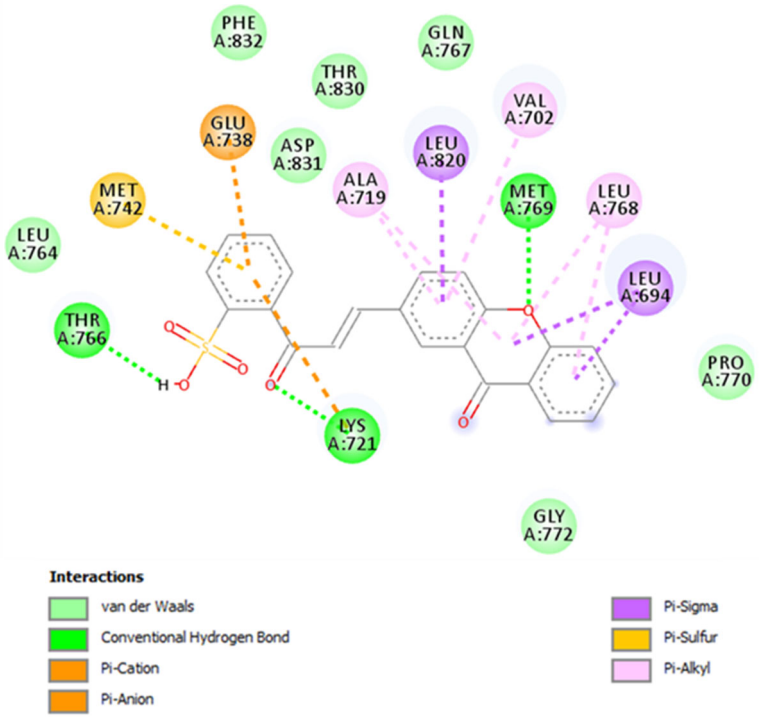

Fig S24. Non-covalent interactions between compound $2SO_3H$ and the active site of EGFR

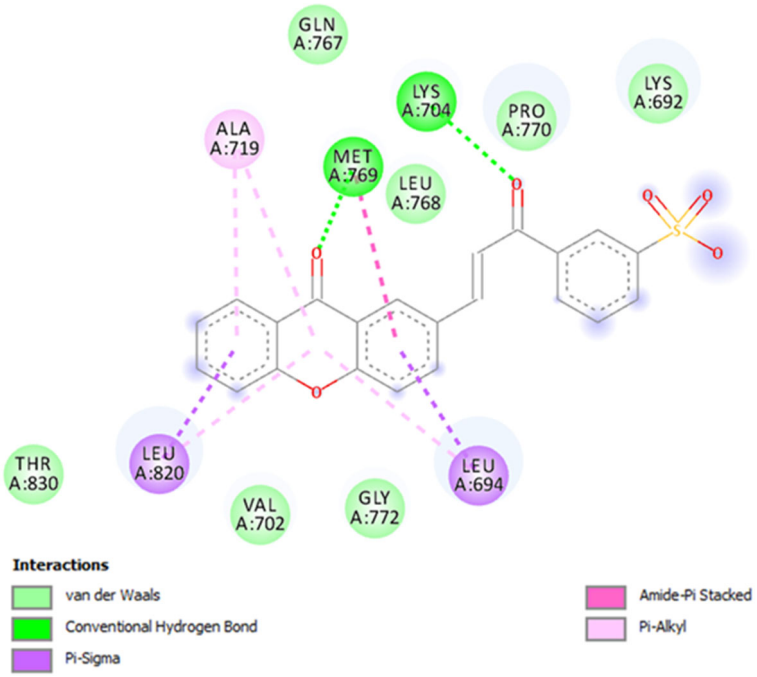

Fig S25. Non-covalent interactions between compound $3SO_3H$ and the active site of EGFR

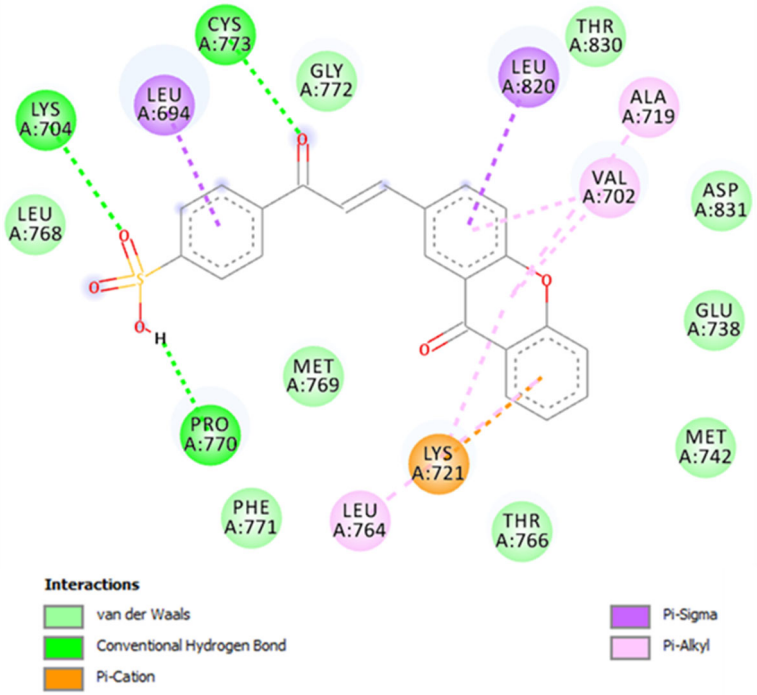

Fig S26. Non-covalent interactions between compound $4SO_3H$ and the active site of EGFR

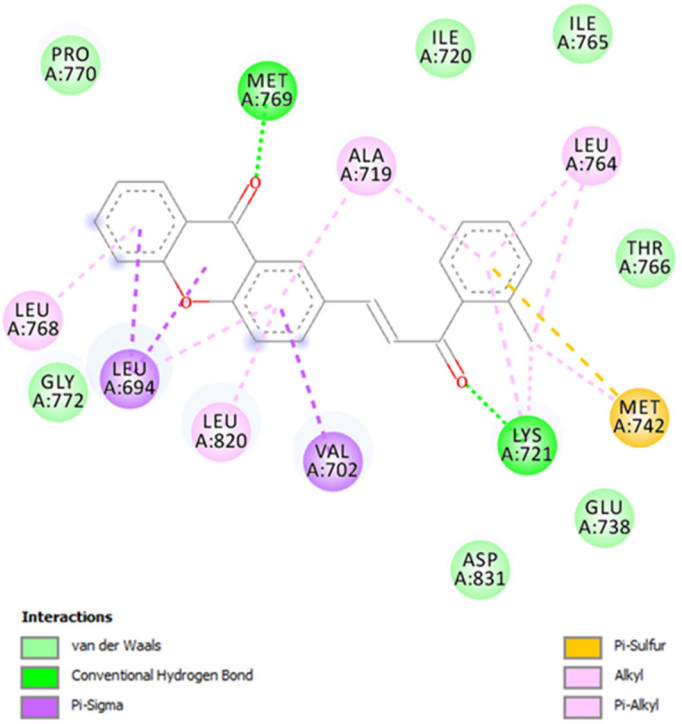

Fig S27. Non-covalent interactions between compound $2CH_3$ and the active site of EGFR

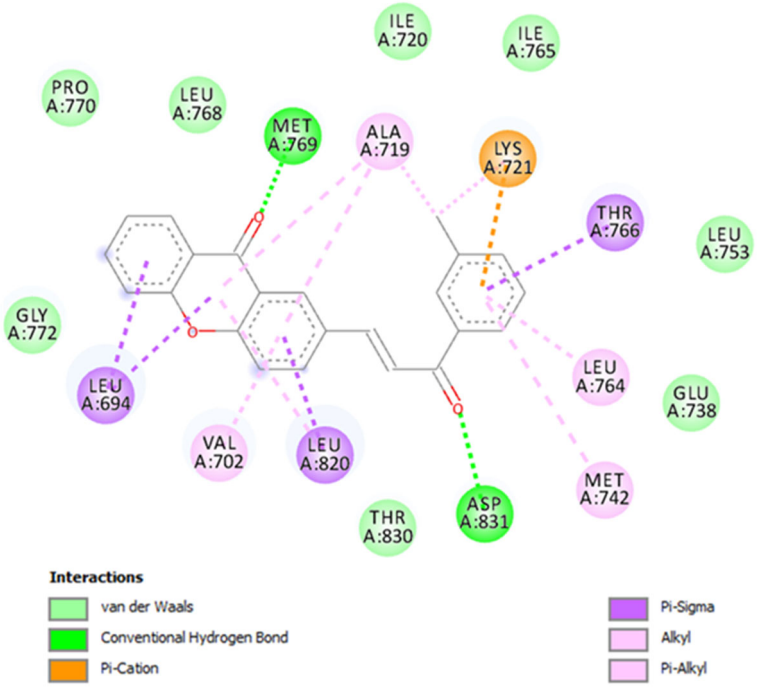

Fig S28. Non-covalent interactions between compound $3CH_3$ and the active site of EGFR

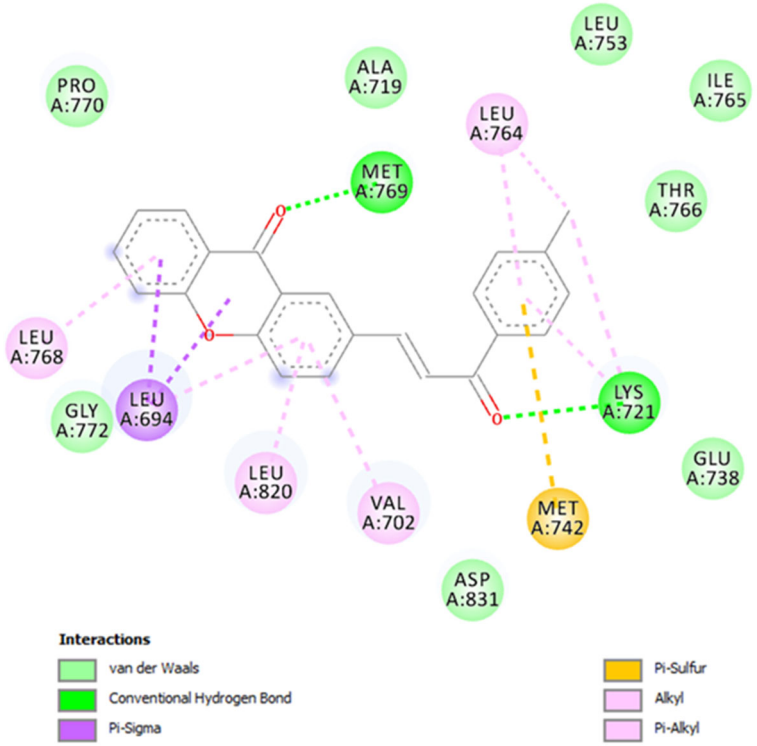

Fig S29. Non-covalent interactions between compound $4CH_3$ and the active site of EGFR

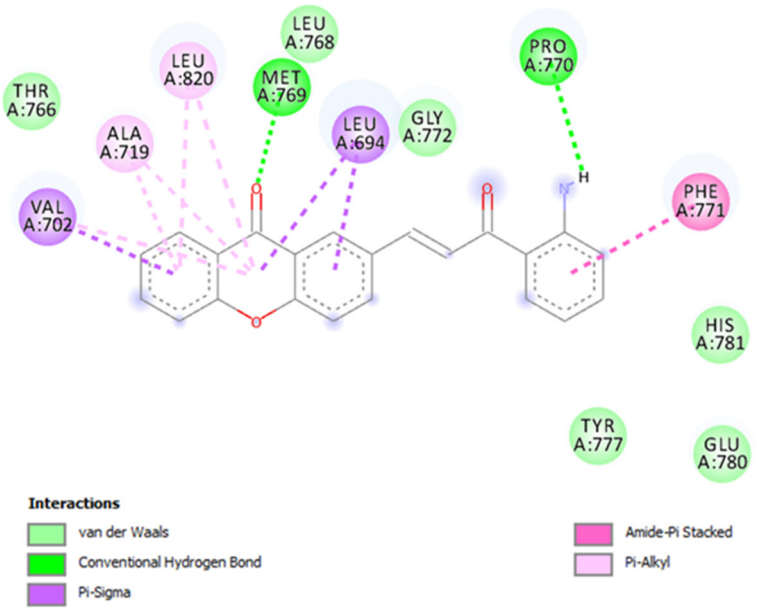

Fig S30. Non-covalent interactions between compound $2NH_2$ and the active site of EGFR

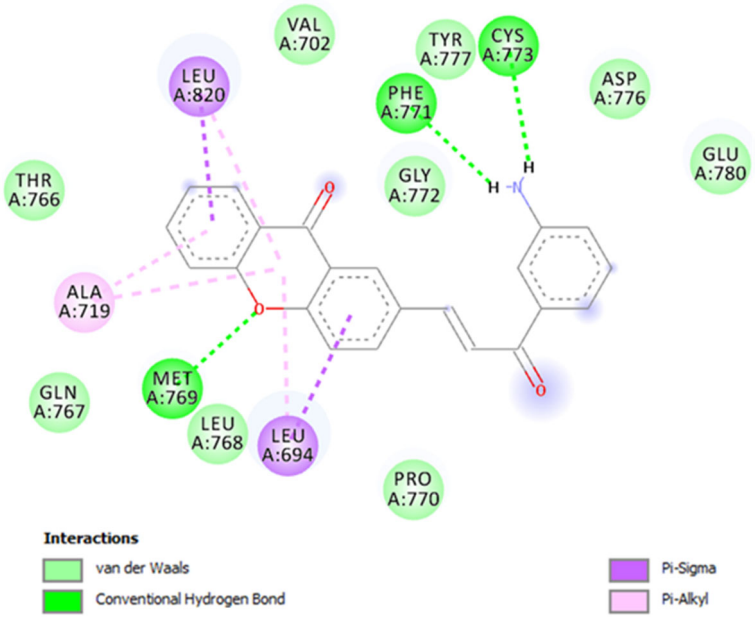

Fig S31. Non-covalent interactions between compound $3NH_2$ and the active site of EGFR

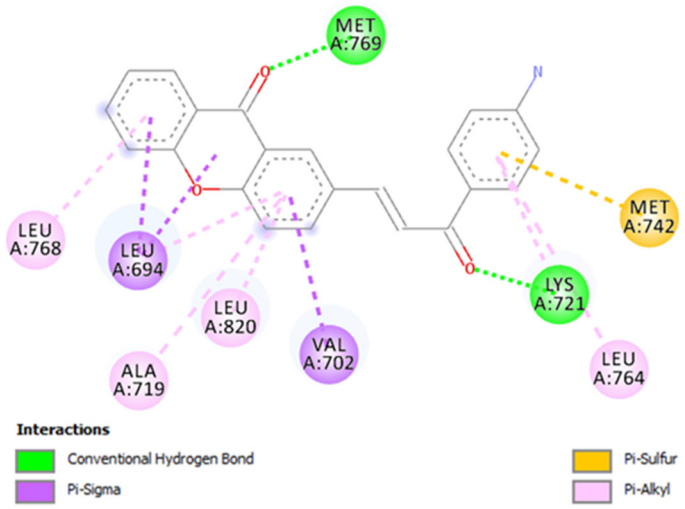

Fig S32. Non-covalent interactions between compound $4NH_2$ and the active site of EGFR

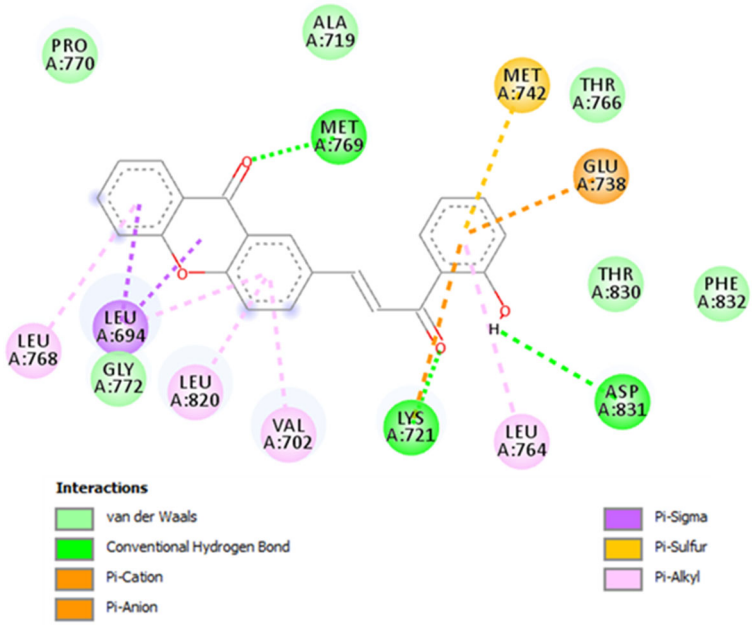

Fig S33. Non-covalent interactions between compound 2OH and the active site of EGFR

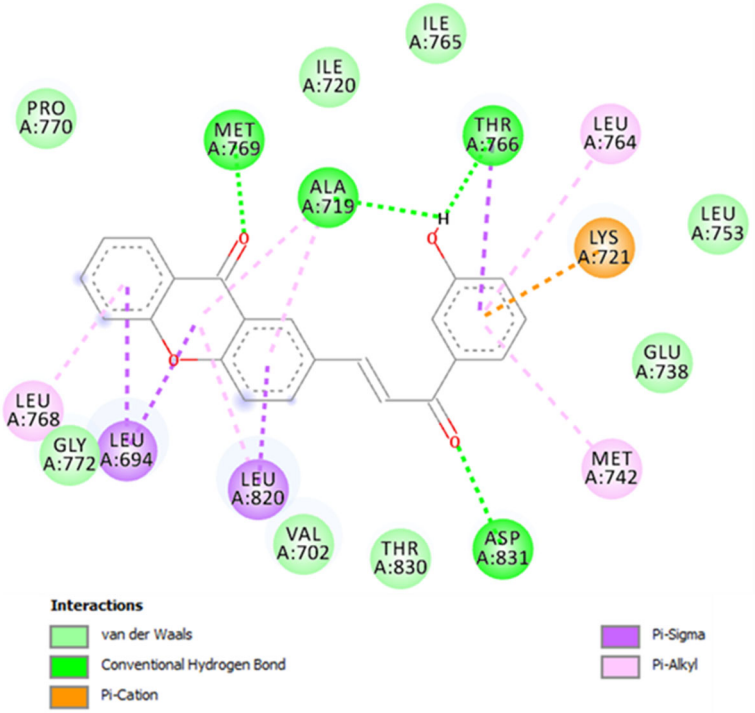

Fig S34. Non-covalent interactions between compound 3OH and the active site of EGFR

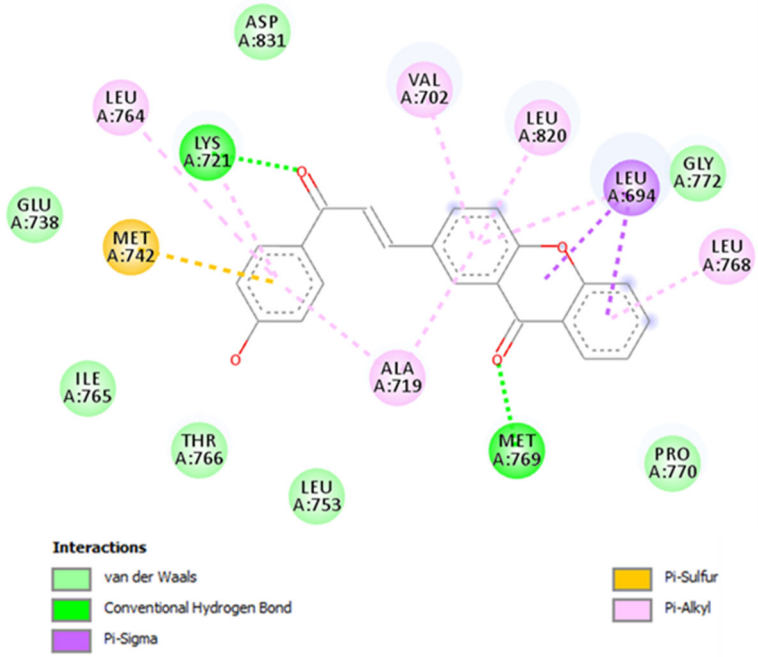

Fig S35. Non-covalent interactions between compound 4OH and the active site of EGFR

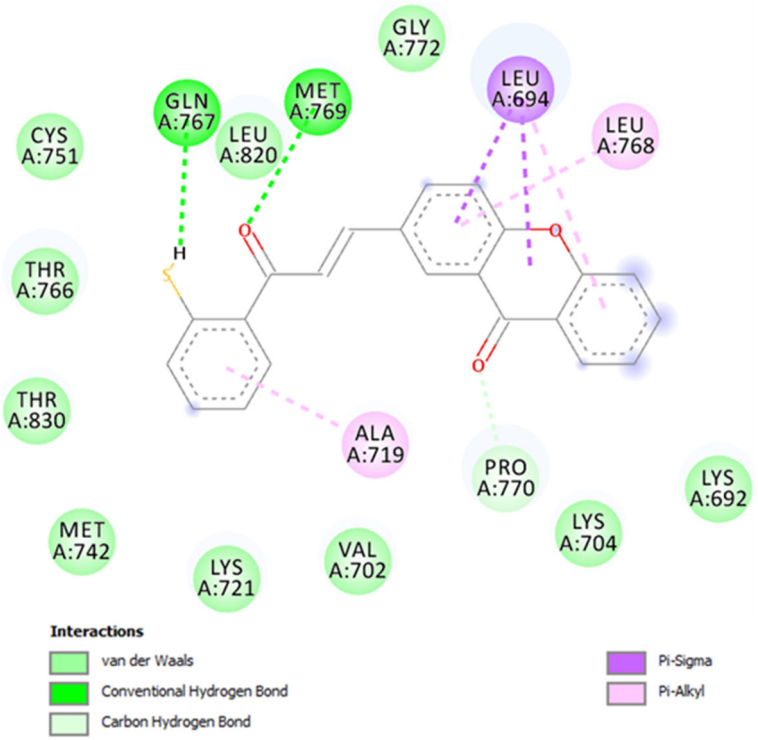

Fig S36. Non-covalent interactions between compound 2SH and the active site of EGFR

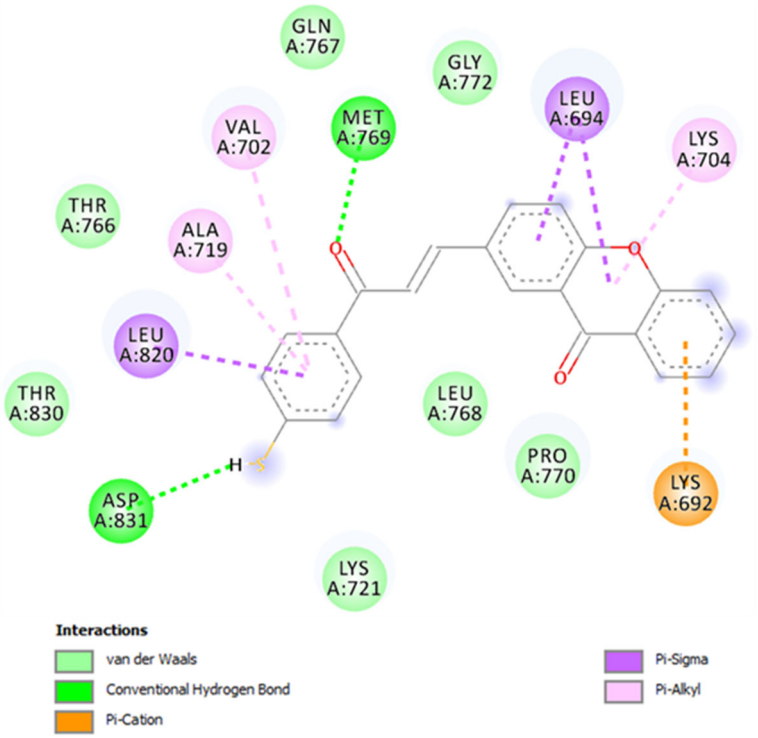

Fig S37. Non-covalent interactions between compound 4SH and the active site of EGFR

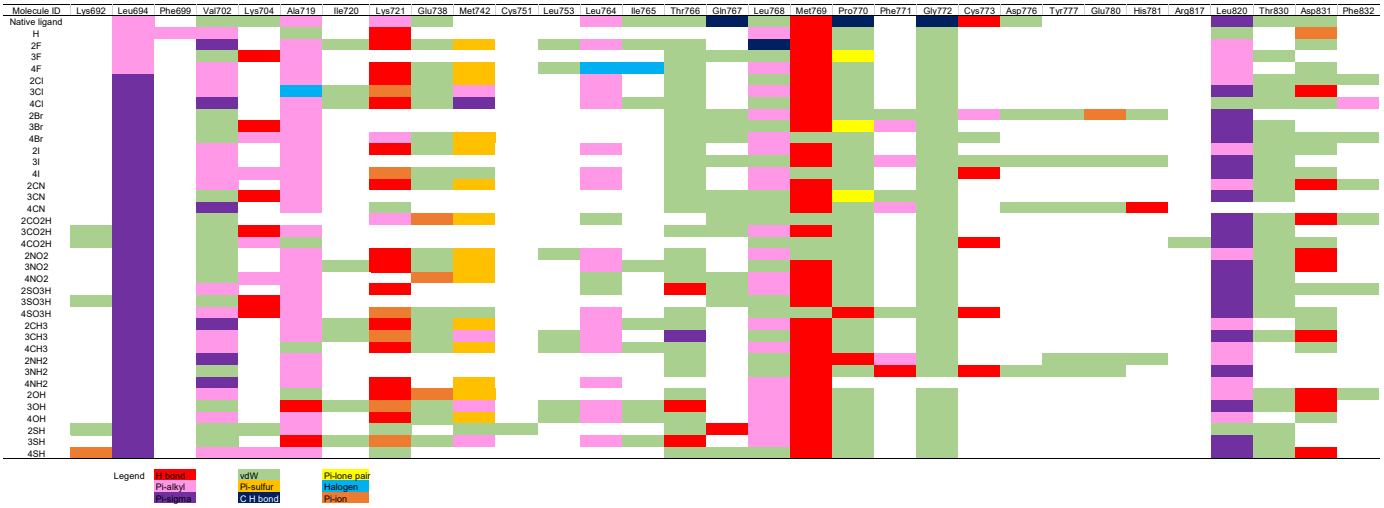

Fig S38. Non-covalent interactions diagram of xanthone-chalcones in the active site of EGFR