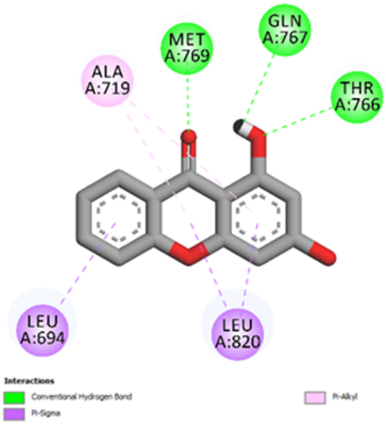
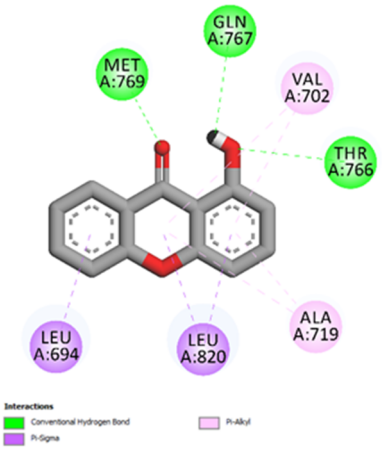
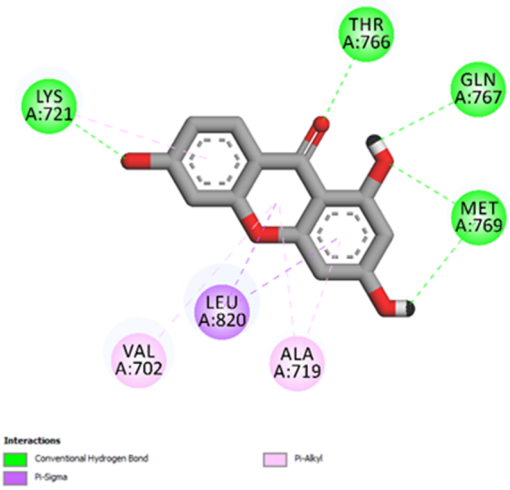
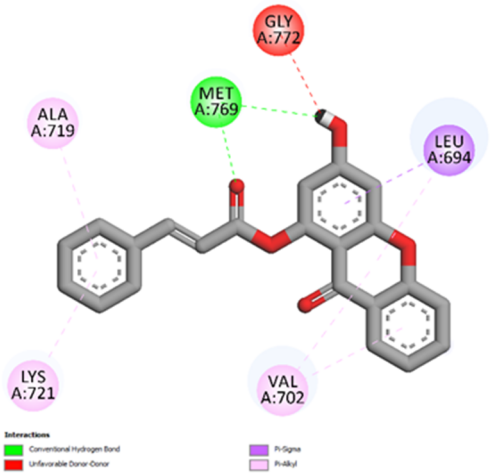
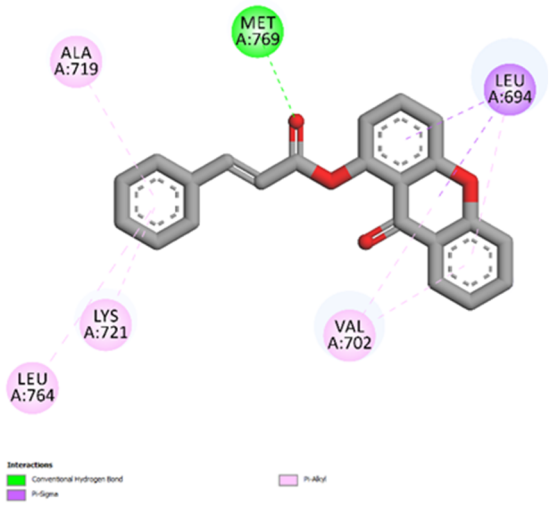
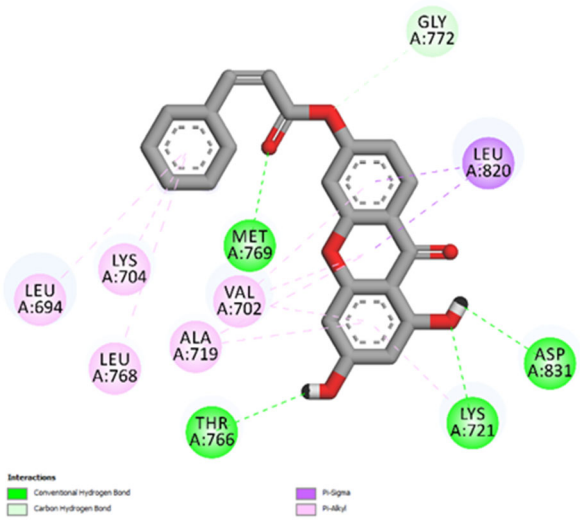
Supplementary Data

This supplementary data is a part of a paper entitled "Synthesis, Cytotoxicity Evaluation and Molecular Docking Studies of Xanthyl-Cinnamate Derivatives as Potential Anticancer Agents".

Table S1. 2D structure of ligand interaction with EGFR amino acid residues

Compound	2D structure of ligand interaction with EGFR amino acid residues	Interaction
3a		Hydrogen bond: MET769, GLN767, THR766 Hydrophobic bond: ALA719, LEU694, LEU820
3b		Hydrogen bond: MET769, GLN767, THR766 Hydrophobic bond: ALA719, VAL702, LEU694, LEU820
3c		Hydrogen bond: MET769, GLN767, THR766, LYS721 Hydrophobic bond: ALA719, VAL702, LEU820

Compound	2D structure of ligand interaction with EGFR amino acid residues	Interaction
4a		Hydrogen bond: MET769 Hydrophobic bond: ALA719, VAL702, LYS721, LEU694 Unfavorable donor-donor: GLY772
4b		Hydrogen bond: MET769 Hydrophobic bond: ALA719, VAL702, LYS721, LEU764, LEU694
4c		Hydrogen bond: MET769, THR766, LYS721, ASP831 Hydrophobic bond: ALA719, VAL702, LEU694, LYS704, LEU768, LEU820 Carbon hydrogen bond: GLY772

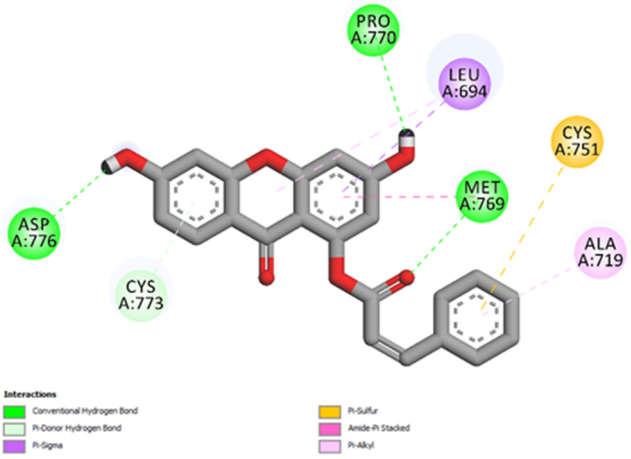
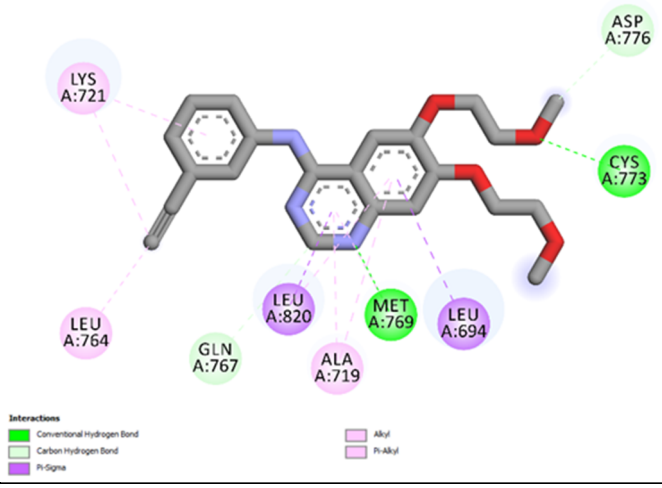
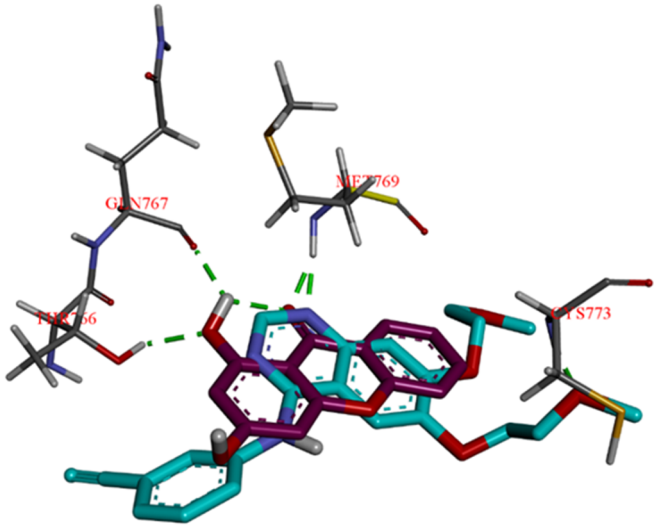
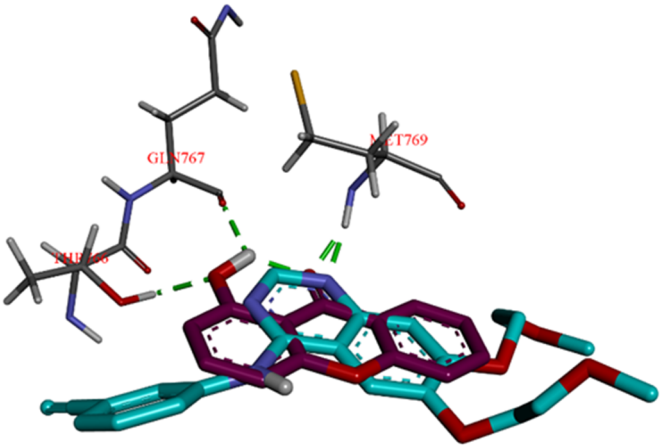
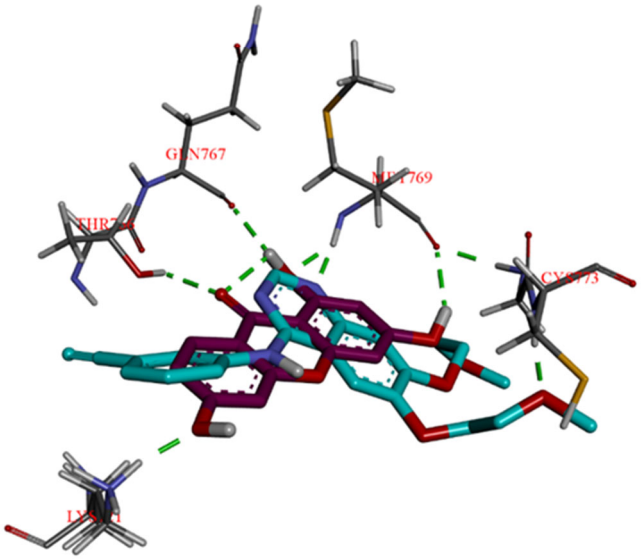
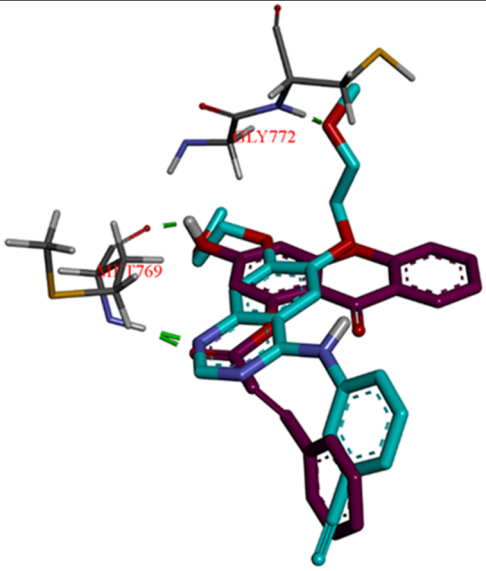
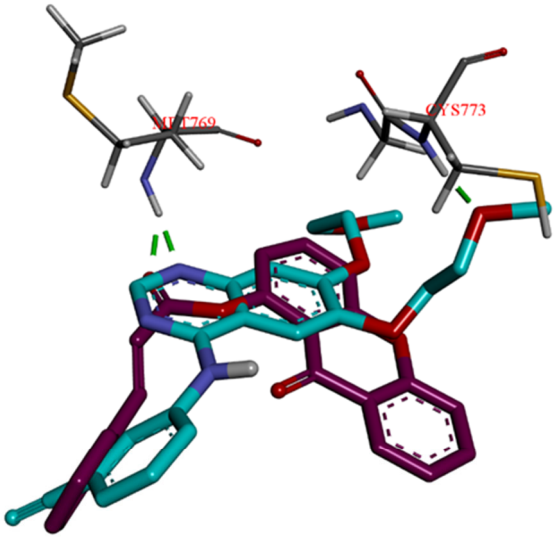
Compound	2D structure of ligand interaction with EGFR amino acid residues	Interaction
4d		Hydrogen bond: MET769, ASP776, PRO770 Hydrophobic bond: ALA719, LYS721, LEU764, LEU820, LEU694 π-sulfur: CYS751 π -donor hydrogen bond: CYS773
erlotinib		Hydrogen bond: MET769, CYS773 Hydrophobic bond: ALA719, LYS721, LEU764, LEU820, LEU694 Carbon hydrogen bond: GLN767, ASP776

Table S2. 3D structure molecular docking results of ligand molecule in EGFR protein overlay with erlotinib position

Compound	3D structure molecular docking results of ligand molecule (magenta) in EGFR protein overlay with erlotinib (cyan) position
3a	
3b	
3c	

Compound	3D structure molecular docking results of ligand molecule (magenta) in EGFR protein overlay with erlotinib (cyan) position
4a	
4b	
4c