

Supplementary Information -3-

Colorectal anti-cancer activity of a novel class of triazolic triarylmethanes derivatives

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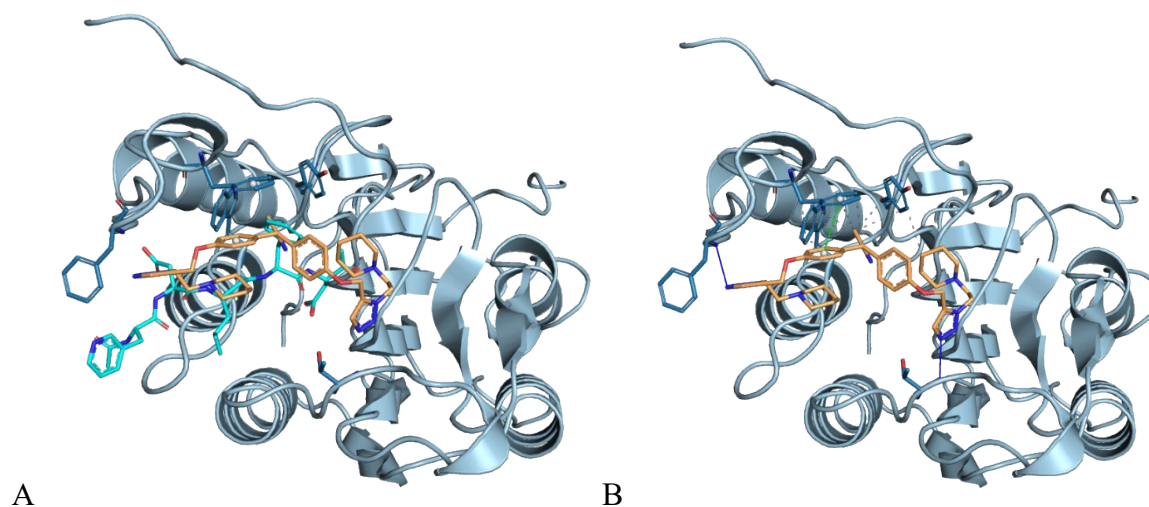
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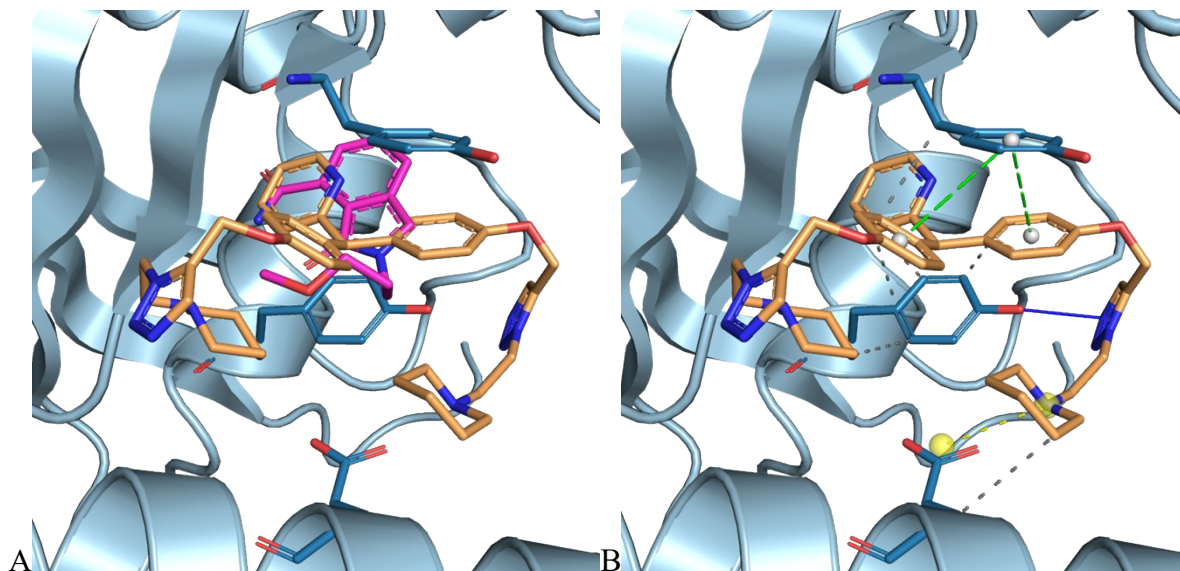
Predicted binding modes of compounds **9b** in the in the caspase-3 and PARP binding sites



Predicted binding modes of compounds **9b** (in orange) in the caspase-3 binding site (PDB ID: 6CKZ) (A) in comparison with the 6CKZ co-crystallized ligand (in cyan) and (B) with detailed information about the interactions established with the caspase-3 binding site obtained using PLIP (blue line: hydrogen bonds; green dotted lines: π -stacking; grey dotted lines: hydrophobic)

Interaction	6CKZ binding site residues	6CKZ bound ligand	Compound 9b
Hydrophobic	Y18	✓	
	N53		✓
	Q79		✓
	W80	✓	
	I84	✓	
	L210	✓	✓
	L264	✓	✓
	K268	✓	
	V270	✓	
	Y272	✓	✓
D292	✓	✓	
Hydrogen bonds	R200		✓
	K297	✓	
π -stacking	W80	✓	✓
π -cation	R273	✓	
salt bridges	D274	✓	✓

Detailed interactions established between the 6CKZ bound ligand or compound **9b** and the caspase 3 binding site residues (the shared interactions are colored in green).



Predicted binding modes of compounds **9b** (in orange) in the PARP binding site (PDB ID: 4ZZZ) (A) in comparison with the 4ZZZ co-crystallized ligand (in magenta) and (B) with detailed information about the interactions established with the PARP binding site obtained using PLIP (blue line: hydrogen bonds; green dotted lines: π -stacking; grey dotted lines: hydrophobic)

Interaction	4ZZZ binding site residues	4ZZZ bound ligand	Compound 9b
Hydrophobic	E763		✓
	Y896	✓	✓
	A898	✓	
	Y907	✓	✓
Hydrogen bonds	G863	✓	
	Y907		✓
π -stacking	Y896		✓
	Y907	✓	
salt bridges	G763		✓

Detailed interactions established between the 6CKZ bound ligand or compound **9b** and the caspase 3 binding site residues (the shared interactions are colored in green).