

Supplementary-S2

Table 2. Interactions of HSP and amino acid residues of SUR1 receptor.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-6.75	-0.16	-8.07	- Conventional hydrogen bonds: 'Ring - C' C4-O C2'''-H C3'''-H C4'''-H C1'''-O 'Ring - B'C3'-H - Carbon hydrogen bonds: 'Ring - B'C'-H 'Ring - B'C'-H C1''-H - Alkyl hydrophobic interaction: C6''' - Pi-alkyl hydrophobic interaction: O - Miscellaneous sulfur interaction: C4'''-O	Chain A: THR`297`HG1'(1.85 Å) Chain B: ALA`172`O'(2.95 Å) Chain C: MET`169`O'(2.44 Å) Chain C: MET`169`O'(2.62 Å) Chain B: GLY`295`HN'(2.62 Å) Chain B: GLU`288`OE1'(2.83 Å) Chain B: SER`212`O' (3.71 Å) Chain B: GLU`288`O' (3.47 Å) Chain A: GLY`295`O' (3.19 Å) Chain C: ILE`296' (4.83 Å) Chain A: VAL`290' (5.22 Å) Chain C: MET`169''SD' (3.24 Å)

ALA; Alanine, GLU; Glutamic acid, GLY; Glycine, ILE; Isoleucine, MET; Methionine, SER; Serine, THR; Threonine, VAL; Valine..

Table 3. Interactions of GB and amino acid residues of SUR1 receptor.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-6.83	-0.21	-9.04	- Conventional hydrogen bonds: C7-O C7'-O - Carbon hydrogen bonds: C1'-SO C2-OC - Alkyl hydrophobic interaction: O OC OC - Pi-alkyl hydrophobic interaction: O, O - Pi-alkyl sigma interaction: O	Chain B: GLY`295`HN'(1.91 Å) Chain D: GLY`295`HN'(2.43 Å) Chain D: THR`294`CB'(2.76 Å) Chain C: GLN`173`OE1'(3.20 Å) Chain A: ALA`172' (3.65 Å) Chain C: MET`169' (5.02 Å) Chain C: ALA`172' (3.50 Å) Chain B: ALA`172' (5.23 Å) Chain C: MET`169' (4.98 Å) Chain D: ILE`296' CG2' (3.92 Å)

ALA; Alanine, GLN; Glutamine, GLY; Glycine, ILE; Isoleucine, MET; Methionine, THR; Threonine.

Table 4. Interactions of HSP and amino acid residues of NF- κ B.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-4.92	-0.11	-5.61	- Conventional hydrogen bonds: C2'''-OH C4''-O C4''-OH C3'-O(B) C3'-OH(B) - Carbon hydrogen bonds: C1'''-O C3'''-O - Alkyl hydrophobic interaction: C6'''	Chain A: ARG`187'O'(2.16 Å) Chain A: LYS`218'HZ1'(1.85 Å) Chain A: GLN`247'OE1'(1.86 Å) Chain B: LYS`572'HZ2'(1.77 Å) Chain B: GLN`606'OE1'(2.27 Å) Chain A: LYS`218'CE'(2.80 Å) Chain A: ARG`187'CD'(3.49 Å) Chain A: LYS`218'(4.16 Å)

ARG; Arginine, GLN; Glutamine, LYS; Lysine.

Table 5. Interactions of GB and amino acid residues of NF- κ B.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-4.70	-0.14	-6.80	- Conventional hydrogen bonds: C2-O C1'-SO -Carbon hydrogen bonds : C -Pi-alkyl hydrophobic interaction O : -Pi-Pi T-shaped hydrophobic interaction:O -Pi-sulfur interaction: C1'-S	Chain B: LYS`572'HZ3'(2.07 Å) Chain B: GLN`606'HE21'(2.64 Å) Chain B: LYS`541'O'(2.82 Å) Chain B: LYS`572'(4.45 Å) Chain B: PHE`607'(4.73 Å) Chain B: Chain B: PHE`607'(4.73 Å)

GLN; Glutamine, LYS; Lysine, PHE; Phenylalanine.

Table 6. Interactions of HSP and amino acid residues of CASPASE-3.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
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-8.44	-0.20	-9.34	- Conventional hydrogen bonds: C4'''-OH C4'''-O C3'''-OH C2''-O C2''-OH C3'-O (B) C3'-OH (B) - Carbon hydrogen bonds: C2-O (C) - Pi-alkyl hydrophobic interaction: C6'''	Chain C: THR`255'OG1'(2.30 Å) Chain A: THR`62'HG1'(2.77 Å) Chain A: THR`62'OG1'(2.12 Å) Chain C: LEU`168'HN'(2.26 Å) Chain C: THR`166'O'(2.34 Å) Chain A: LEU`168'HN'(2.69 Å) Chain A: GLU`167'OE1'(1.75 Å) Chain A: THR`166'CB1'(3.61 Å) Chain A: HIS`121'(4.09 Å)
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GLU; Glutamic acid, HIS; Histidine, LEU; Leucine, THR; Threonine.

Table 7. Interactions of GB and amino acid residues of CASPASE-3.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-6.35	-0.19	-8.31	- Conventional hydrogen interaction: C1'-SO C7'-NH C1''-NH - Carbon hydrogen interaction: C1'-SO C7-O	Chain A: LEU`168'HN'(2.56 Å) Chain A: THR`166'OG1'(2.16 Å) Chain A: THR`166'OG1'(1.97 Å) Chain A: GLU`167'CA'(3.25 Å) Chain A: THR`166'CA'(2.81 Å)

GLU; Glutamic acid, LEU; Leucine, THR; Threonine.

Table 8. Interactions of HSP and amino acid residues of BCL2.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-6.07	-0.14	-6.31	- Conventional hydrogen bonds: C5-OH(A) C3'(B) - Pi-anion interaction: O (B) - Pi-sulfur interaction: O(A)	Chain A: PHE`144'O'(2.18 Å) Chain A: ASP`95'OD1'(1.93 Å) Chain A: GLU`98'OE1'(4.19 Å) Chain A: MET`170'(5.70 Å)

ASP; Aspartic acid, GLU; Glutamic acid, MET; Methionine, PHE; Phenylalanine.

Table 9. Interactions of GB and amino acid residues of BCL2.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
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-6.67	-0.20	-8.56	- Conventional hydrogen bonds: C4'-NH C1'-SO C7'-NH - Carbon hydrogen bonds: C2-OH - Alkyl hydrophobic interaction: C4'' C3'' C3' - Pi-anion interaction: O	Chain A: PHE`144'O'(3.02 Å) Chain A: ARG`91'HE'(2.23 Å) Chain A: LYS`87'O'(3.05 Å) Chain A: SER`145'OG'(3.47 Å) Chain A: VAL`86'(5.24 Å) Chain A: TRP`188'(5.08 Å) Chain A: LEU`90'(5.31 Å) Chain A: GLU`98'OE2'(4.35 Å)
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ARG; Arginine, GLU; Glutamic Acid, LEU; Leucine LYS; Lysine, PHE; Phenylalanine, SER; Serine, TRP; Tryptophan, VAL; Valine.

Table 10. Interactions of HSP and amino acid residues of DGAT1.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-7.07	-0.16	-8.46	- Conventional hydrogen bonds: C3'''-OH C2'''-OH C2-O (C) - Pi-donor hydrogen interaction: O - Alkyl hydrophobic interaction: C4' (B) - Pi-sigma hydrophobic interaction: C6''' C - Miscellaneous pi-sulfur interaction O :	Chain B: LEU`355'O'(2.17 Å) Chain B: LEU`355'O'(2.37 Å) Chain A: CYS`92'SG'(3.01 Å) Chain A: CYS`92'SG'(3.66 Å) Chain A: LEU`89'(4.09 Å) Chain A: TYR`339'(4.11 Å) Chain A: TYR`339'(3.48 Å) Chain B: TRP`91'CZ3'(3.48 Å) Chain A: CYS`92'SG'(5.12 Å)

CYS; Cysteine, LEU; Leucine, TRP; Tryptophan, TYR; Tyrosine.

Table 11. Interactions of HSP and amino acid residues of CEBP/α.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-6.64	-0.15	-7.54	- Conventional hydrogen bonds: C4''-O C1''-O C3'-OH(B) - Alkyl hydrophobic interaction: C4'(B) - Pi-alkyl hydrophobic interaction: O(B) O(A)	Chain C: ARG`306'HH22'(3.56 Å) Chain C: ASN`307'HD22'(1.94 Å) Chain A: GLN`312'OE1'(2.10 Å) Chain A: LEU`315'(4.19 Å) Chain A: VAL`308'(5.47 Å) Chain A: VAL`308'(5.15 Å)

ARG; Arginine, ASN; Asparagine, GLN; Glutamine, LEU; Leucine, VAL; Valine.

Table 12. Interactions of HSP and amino acid residues of PPARγ.

Binding energy	Ligand efficiency	Intermole energy	Ligand atoms (ring)	Docked amino acid residue (bond length)
-4.61	-0.11	-8.83	- Conventional hydrogen bonds: Ring - B'C3'-OH Ring - B'C3'-O C2-O C6''-O C2'''-OH C2'''-OH C3''-OH - Carbon hydrogen bond: C6''-H - Alkyl hydrophobic interaction: C4' - Pi-alkyl hydrophobic interaction: C4' - Pi-Pi T-shaped interaction: Ring - B'O'	Chain B: GLU`324'OE2'(1.85 Å) Chain B: ARG`397'HH22'(2.12 Å) Chain A: GLN`444'HE21'(2.564 Å) Chain A: GLN`444'HE21'(2.75 Å) Chain B: ASP`396'OD1'(1.97 Å) Chain B: ASP`396'O'(1.99 Å) Chain A: PRO`366'O'(2.02 Å) Chain A: ASP`441'OD1'(3.21 Å) Chain B: VAL`446'(5.19 Å) Chain B: TYR`320' (5.18 Å) Chain B: TYR`320' (4.67 Å)
ARG; Arginine, ASP; Aspartic acid, GLN; Glutamine, GLU; Glutamic acid, PRO; Proline, TYR; Tyrosine, VAL; Valine.				