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www.bioinformation.net Issue 6 **Hypothesis**

Supplementary material:

Table 1: Energies of docking results calculated using Autodock 4.0.

Ligand	Standard	CKRKC	CRGRC	CRTRC	CGRRC	CKRRC	CRRKC	CTRRC
Estimated free energy of binding, ΔG_{bind} (kcal/mol)	-6.14	-8.39	-7.35	-7.06	-7.04	-7.01	-6.83	-6.15
Estimated inhibition constant, Ki (μM)	31.54	0.707	4.12	6.66	6.96	7.32	9.83	30.9
Docking energy (kcal/mol)	-14.33	-13.59	-10.94	-11.15	-10.81	-11.72	-11.81	-10.37
Final intermolecular energy (kcal/mol)	-11.63	-11.32	-10.18	-9.98	-8.51	-10.16	-8.73	-8.85
Final internal energy of ligand (kcal/mol)	-2.70	-2.27	-0.76	-1.17	-2.3	-1.56	-3.08	-1.52
Torsional free energy, (kcal/mol)	6.86	4.39	2.74	3.29	2.74	4.12	4.12	3.29
Rotatable bonds	34	18	15	17	15	20	19	16

Table 2: Residues in the active site of DEN-2 NS3-NS2B protease that form hydrogen bond with the standard ligand and ligand CKRKC. Catalytic triads are shown in boldface.

Residue	Standard Ligand	Ligand CKRKC
Ile36	√	√
His51	√	√
Val52	√	
Lys73	√	√
Asp75		√
Leu128		√
Phe130	√	√
Ser131	√	√
Pro132	√	√
Asn152	√	√

Table 3: List of contact residues in the active site of DEN-2 NS3-NS2B protease that interact with the standard ligand and ligand CKRKC. Catalytic triads are shown in bold letter.

Residue	Standard Ligand	Ligand CKRKC
Ile36	√	√
Trp50	√	
His51	√	√
Val52	√	√
Arg54		√
Lys73	√	√
Lys74		√
Asp75	√	√
Leu128	√	√
Phe130	√	√
Ser131	√	√
Pro132	√	√
Ser135	√	√
Tyr150		√
Gly151	√	
Asn152	√	√
Gly153	√	√
Val154	√	√