

Supplementary material:

Table 1: Sequence identity (%) matrix of HSP90 homolog for all aligned regions

1	100.000	68.063	63.874	66.492	61.780
2	68.063	100.000	65.183	64.921	62.565
3	63.874	65.183	100.000	64.660	79.581
4	66.492	64.921	64.660	100.000	65.969
5	61.780	62.565	79.581	64.969	100.000

Table 2: RMSD (Å) matrix for the superimposed structures of HSP90 homolog for all aligned regions

1	0.000	1.701	1.805	2.100	2.046
2	1.701	0.000	0.861	1.828	1.674
3	1.805	0.861	0.000	1.937	1.761
4	2.100	1.828	1.937	0.000	1.003
5	2.046	1.674	1.761	1.003	0.000

1: *Homo sapiens*; 2: *Entamoeba histolytica*; 3: *Trypanosoma brucei*; 4: *Leishmania donovani*; 5: *Plasmodium falciparum*

Table 3: Analogs of Geldanamycin

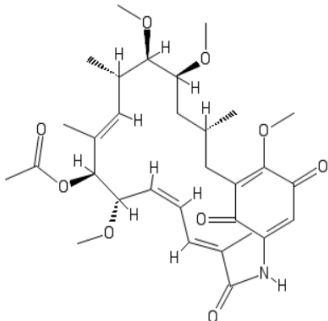
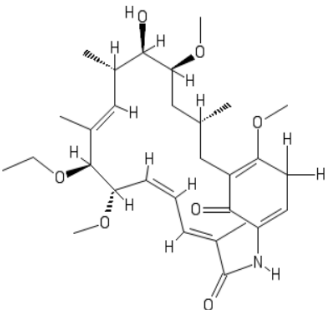
GA-Analog 1	GA-Analog 2
	
<chem>O([C@H]1C[C@@H](CC2=C(OC)C(=O)C=C(N(C(=O)\C(=C(\C(=C/[C@H](OC)[C@@H](OC(=O)C)/C(=C/[C@H]([C@H]1O)C)C)[H])C)[H])[H])C)C(=O)[H])C2=O)C)C</chem>	<chem>O([C@H]1C[C@@H](CC2=C(OC)C(=O)C=C(N(C(=O)\C(=C(\C(=C/[C@H](OC)[C@@H](OCC)/C(=C/[C@H]([C@H]1O)[H])C)[H])C)[H])[H])C)C(=O)[H])C2=O)[H])C)C</chem>

Table 4: Binding affinity (kcal/mol) of analogs of Geldanamycin and HSP90 homologs

Target	GA	Analog1	Analog2
Human	-4.68	-4.33	-4.86
Plasmodium	-5.09	-5.23	-5.08
Leishmania	-4.57	-4.76	-4.82
Trypanosoma	-5.42	-4.50	-5.08
E.Histolytica	-4.76	-4.54	-7.15

Table 5: Drug likeliness properties of analogs of Geldanamycin

DRUG	Mol.wt.	H-bond donor	H-bond acceptor	LogP	Molar refractivity
Geldanamycin	560.00	4	9	1.803	146.247
Analog1	573.00	1	9	3.565	152.524
Analog2	531.00	2	7	4.205	147.204

Table 6: Interaction analysis of docked structure of HSP90 with Geldanamycin and its analogs

HSP90 species	Geldanamycin (Residues involved in close contact)	Analog1 (Residues involved in close contact)	Analog2 (Residues involved in close contact)
Human	I426, H450, P423, W431, D424, K449, N428, T427, I428	S627, Q623, A628, R734, G797, L794, S795	I647, E475, L 569, W650, N476
Plasmodium	L560, W512, K 565, C562, Q550, K553, F623, K561, E566, Q622	K462, F 363, A366, N463, M370, N402, E459, F460	K561, K563, E550, F623, K565, L560, E622, G624
Trypanosoma	E510, K509, T429, K 432, S428, R431	E512, E510, K509, K432,	V279, P278, H303, W284, T301, Q401, K281, L 398, L 402
Leishmania	I11, L14, Q8, T94, I95	I 95, 119, L368, 371, I 370, I18, T21	E398, M395, T298, A297, M296, P295, K 278, W286, V276, T298
Entamoeba	E452, K469, D470, L453, E420, S419, R 455, N421, K422	I30, W35, A33, L29, V 389, L29, V389, L 387	K377, P 335, E 312, P 339, S308, D310, F340, N309, W311