Results Table

Rank	Est. Free Energy of Binding	Est. Inhibition Constant, Ki	vdW + Hbond + desolv Energy	Electrostatic Energy	Total Intermol. Energy	Frequency	Interact. Surface
1.	-4.98 kcal/ mol	223.41 uM	-4.79 kcal/ mol	-0.01 kcal/ mol	-4.80 kcal/ mol	23%	438.797
2.	-3.70 kcal/ mol	1.93 mM	-3.79 kcal/ mol	-0.15 kcal/ mol	-3.94 kcal/ mol	6%	414.442
3.	-3.67 kcal/ mol	2.04 mM	-3.47 kcal/ mol	-0.01 kcal/ mol	-3.48 kcal/ mol	18%	383.13
4.	-3.47 kcal/ mol	2.85 mM	-3.78 kcal/ mol	-0.10 kcal/ mol	-3.88 kcal/ mol	9%	375.666
5.	-3.46 kcal/ mol	2.89 mM	-3.91 kcal/ mol	-0.08 kcal/ mol	-3.98 kcal/ mol	2%	391.465
6.	-3.42 kcal/ mol	3.11 mM	-3.37 kcal/ mol	+0.01 kcal/ mol	-3.36 kcal/ mol	3%	366.656
7.	-3.32 kcal/ mol	3.67 mM	-3.39 kcal/ mol	-0.49 kcal/ mol	-3.89 kcal/ mol	9%	366.918
8.	-3.30 kcal/ mol	3.83 mM	-3.47 kcal/ mol	-0.16 kcal/ mol	-3.63 kcal/ mol	5%	374.662
9.	-3.17 kcal/ mol	4.72 mM	-2.90 kcal/ mol	-0.08 kcal/ mol	-2.98 kcal/ mol	1%	398.401
10.	-3.16 kcal/ mol	4.82 mM	-2.65 kcal/ mol	-0.32 kcal/ mol	-2.97 kcal/ mol	2%	329.486
11.	-3.04 kcal/ mol	5.87 mM	-3.95 kcal/ mol	-0.03 kcal/ mol	-3.98 kcal/ mol	5%	380.48
12.	-2.98 kcal/ mol	6.51 mM	-2.90 kcal/ mol	-0.11 kcal/ mol	-3.02 kcal/ mol	1%	378.244
13.	-2.96 kcal/ mol	6.78 mM	-3.08 kcal/ mol	-0.10 kcal/ mol	-3.17 kcal/ mol	1%	357.489
14.	-2.87 kcal/ mol	7.86 mM	-2.97 kcal/ mol	-0.41 kcal/ mol	-3.38 kcal/ mol	1%	381.492
15.	-2.86 kcal/ mol	8.03 mM	-2.71 kcal/ mol	-0.05 kcal/ mol	-2.75 kcal/ mol	1%	345.838
16.	-2.83 kcal/ mol	8.40 mM	-2.81 kcal/ mol	-0.51 kcal/ mol	-3.31 kcal/ mol	5%	383.057
17.	-2.59 kcal/ mol	12.56 mM	-1.91 kcal/ mol	-0.56 kcal/ mol	-2.47 kcal/ mol	3%	318.092
18.	-2.58 kcal/ mol	12.76 mM	-3.00 kcal/ mol	-0.26 kcal/ mol	-3.26 kcal/ mol	1%	399.508
19.	-2.39 kcal/ mol	17.72 mM	-2.29 kcal/ mol	-0.54 kcal/ mol	-2.83 kcal/ mol	1%	383.24
20.	-2.24 kcal/ mol	22.72 mM	-2.85 kcal/ mol	+0.12 kcal/ mol	-2.73 kcal/ mol	1%	328.289
21.	-2.24 kcal/ mol	22.92 mM	-2.66 kcal/ mol	+0.01 kcal/ mol	-2.66 kcal/ mol	1%	331.706
22.	-2.18 kcal/ mol	25.35 mM	-2.71 kcal/ mol	-0.26 kcal/ mol	-2.96 kcal/ mol	1%	369.988

Docking Parameters

Protein Clean

tstep	0.2
qstep	5.0
dstep	5.0
rmstol	2.0
ga_pop_size	150
ga_num_evals	2500000
ga_num_generations	540000
ga_run	100

Interaction Table

hydrogen bonds	polar	hydrophobic	pi- pi	cation- pi	other
none	O2 ( ) [3.38] – ARG27 (CB)	C5 ( ) [3.52] – ILE24 (CG2)	*none*	H14 ( ) [3.68] – TYR33 (CE1)	O3 ( ) [3.40] – ILE24 (CB, CG2)
	H14 ( ) [3.69] – ARG27 (CB, CD)	C6 ( ) [3.43] – ILE24 (CG2)		H1 ( ) [2.34] – TRP51 (CD2, CE2, CE3, CH2, CZ2, CZ3)	H15 ( ) [3.35] – ILE24 (CB, CG2)
		C5 ( ) [3.76] – TYR33 (CD1, CE1)			O4 ( ) [3.78] – ILE24 (CG2)
		C8 ( ) [3.48] – TRP51 (CD2, CE3, CZ3)			O2 ( ) [3.36] – TYR33 (CE1)
		C1 ( ) [3.61] – TRP51 (CH2)			N1 ( ) [3.30] – TRP51 (CE3, CH2, CZ2, CZ3)
		C1 ( ) [3.68] – VAL56 (CB)			O5 ( ) [3.71] – THR55 (CG2)
					O4 ( ) [3.56] – PRO58 (CD, CG)
					H15 ( ) [3.56] – PRO58 (CD, CG)

Interactions

24: ILE
27: ARG
33: TYR
51: TRP
55: THR
56: VAL
58: PRO

Computational Methods

Docking calculations were carried out using DockingServer (*http:// www.dockingserver.com*). Gasteiger partial charges were added to the ligand atoms. Non- polar hydrogen atoms were merged, and rotatable bonds were defined.
Docking calculations were carried out on ***NAG.pdb*** protein model. Essential hydrogen atoms, Kollman united atom type charges, and solvation parameters were added with the aid of AutoDock tools (*Morris, Goodsell et al., 1998*). Affinity (grid) maps of ×× Å grid points and 0.375 Å spacing were generated using the Autogrid program (*Morris, Goodsell et al., 1998*). AutoDock parameter set- and distance- dependent dielectric functions were used in the calculation of the van der Waals and the electrostatic terms, respectively.
Docking simulations were performed using the Lamarckian genetic algorithm (LGA) and the Solis & Wets local search method (*Solis and Wets, 1981*). Initial position, orientation, and torsions of the ligand molecules were set randomly. All rotatable torsions were released during docking. Each docking experiment was derived from 100 different runs that were set to terminate after a maximum of 2500000 energy evaluations. The population size was set to 150. During the search, a translational step of 0.2 Å, and quaternion and torsion steps of 5 were applied.

References

E. Hazai, S. Kovacs, L. Demko, Z. Bikadi
DockingServer (www.dockingserver.com)
Virtua Drug Ltd., Budapest, Hungary

T. A. Halgren
Merck molecular force field. I. Basis, form, scope, parametrization, and performance of MMFF94
Journal of Computational Chemistry **17 (5-6)**, 490-519 (1998)

G. M. Morris, D. S. Goodsell, et al.
Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function
Journal of Computational Chemistry **19 (14)**, 1639-1662 (1998)

F. J. Solis and R. J. B. Wets
Minimization by Random Search Techniques
Mathematics of Operations Research **6 (1)**, 19-30 (1981)

Image Gallery

This software includes code developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana- Champaign.

References, please cite:

W. Humphrey, A. Dalke, and K. Schulten
VMD - Visual Molecular Dynamics
J. Mol. Graph. **14**, 33-38 (1996)

N-acetylglucosamine docking parameters to VisP *S.* Typhimurium modeled structure.

Results Table

Rank	Est. Free Energy of Binding	Est. Inhibition Constant, Ki	vdW + Hbond + desolv Energy	Electrostatic Energy	Total Intermol. Energy	Frequency	Interact. Surface
1.	-2.69 kcal/ mol	10.64 mM	-4.85 kcal/ mol	-0.08 kcal/ mol	-4.93 kcal/ mol	11%	426.921
2.	-2.67 kcal/ mol	10.99 mM	-3.80 kcal/ mol	-0.12 kcal/ mol	-3.93 kcal/ mol	18%	373.792
3.	-2.47 kcal/ mol	15.52 mM	-3.00 kcal/ mol	-0.11 kcal/ mol	-3.11 kcal/ mol	17%	411.997
4.	-2.35 kcal/ mol	18.79 mM	-4.12 kcal/ mol	+0.05 kcal/ mol	-4.06 kcal/ mol	7%	423.29
5.	-2.29 kcal/ mol	21.00 mM	-4.58 kcal/ mol	-0.07 kcal/ mol	-4.65 kcal/ mol	10%	469.379
6.	-2.06 kcal/ mol	30.75 mM	-3.20 kcal/ mol	-0.08 kcal/ mol	-3.28 kcal/ mol	3%	412.409
7.	-1.75 kcal/ mol	52.12 mM	-2.90 kcal/ mol	-0.87 kcal/ mol	-3.77 kcal/ mol	2%	435.958
8.	-1.66 kcal/ mol	60.41 mM	-3.12 kcal/ mol	-0.93 kcal/ mol	-4.05 kcal/ mol	4%	406.202
9.	-1.52 kcal/ mol	77.51 mM	-4.65 kcal/ mol	-0.14 kcal/ mol	-4.79 kcal/ mol	1%	437.015
10.	-0.93 kcal/ mol	208.35 mM	-2.37 kcal/ mol	+0.23 kcal/ mol	-2.14 kcal/ mol	3%	354.806
11.	-0.80 kcal/ mol	258.57 mM	-3.10 kcal/ mol	-0.10 kcal/ mol	-3.20 kcal/ mol	2%	417.624
12.	-0.18 kcal/ mol	738.44 mM	-2.43 kcal/ mol	-0.32 kcal/ mol	-2.75 kcal/ mol	1%	417.777
13.	-0.13 kcal/ mol	798.73 mM	-2.56 kcal/ mol	+0.14 kcal/ mol	-2.42 kcal/ mol	1%	359.325
14.	-0.12 kcal/ mol	821.77 mM	-3.35 kcal/ mol	-0.28 kcal/ mol	-3.63 kcal/ mol	1%	413.4
15.	+0.17 kcal/ mol		-1.89 kcal/ mol	-0.06 kcal/ mol	-1.95 kcal/ mol	1%	386.46
16.	+0.65 kcal/ mol		-1.39 kcal/ mol	-0.29 kcal/ mol	-1.68 kcal/ mol	1%	442.364
17.	+1.54 kcal/ mol		-1.76 kcal/ mol	-0.89 kcal/ mol	-2.65 kcal/ mol	1%	362.723
18.	+1.71 kcal/ mol		-2.08 kcal/ mol	-0.05 kcal/ mol	-2.13 kcal/ mol	4%	464.03
19.	+2.14 kcal/ mol		-0.53 kcal/ mol	-0.11 kcal/ mol	-0.64 kcal/ mol	3%	460.711
20.	+2.39 kcal/ mol		+0.18 kcal/ mol	+0.05 kcal/ mol	+0.23 kcal/ mol	3%	483.123
21.	+3.91 kcal/ mol		-0.89 kcal/ mol	-0.37 kcal/ mol	-1.26 kcal/ mol	2%	419.047
22.	+4.18 kcal/ mol		-0.49 kcal/ mol	-0.32 kcal/ mol	-0.81 kcal/ mol	1%	351.61
23.	+5.50 kcal/ mol		+0.76 kcal/ mol	+0.01 kcal/ mol	+0.77 kcal/ mol	3%	469.707

Docking Parameters

Protein Clean

tstep	0.2
qstep	5.0
dstep	5.0
rmstol	2.0
ga_pop_size	150
ga_num_evals	2500000
ga_num_generations	540000
ga_run	100

Interaction Table

hydrogen bonds	polar	hydrophobic	pi- pi	cation- pi	other
none	O ( ) [2.71] – ASN43 (*ND2, OD1*) H ( ) [2.07] – ASN43 (*ND2, OD1*) N ( ) [3.69] – ASN43 (*ND2*)	CA ( ) [3.76] – VAL75 (*CG1*) C ( ) [3.28] – VAL75 (*CG1*)	*none*	*none*	O ( ) [3.63] – LYS10 (*CD, CE*) H ( ) [3.27] – VAL34 (*CB, CG1, CG2*) O ( ) [3.52] – VAL34 (*CG1, CG2*) O ( ) [3.22] – THR41 (*CG2*) H ( ) [3.51] – THR41 (*CG2*) H ( ) [2.88] – ASN43 (*CB, CG*) C ( ) [3.23] – ASN43 (*CG, ND2, OD1*) O ( ) [3.43] – ASN43 (*CG*) C ( ) [3.26] – SER74 (*CB*) N ( ) [3.89] – VAL75 (*CG1*) ... – ...

Interactions

10: LYS
34: VAL
41: THR
43: ASN
74: SER
75: VAL
76: GLU

Computational Methods

Docking calculations were carried out using DockingServer (*http:// www.dockingserver.com*). Gasteiger partial charges were added to the ligand atoms. Non- polar hydrogen atoms were merged, and rotatable bonds were defined.
Docking calculations were carried out on ***N- acetylmuramic acid*** protein model. Essential hydrogen atoms, Kollman united atom type charges, and solvation parameters were added with the aid of AutoDock tools (*Morris, Goodsell et al., 1998*). Affinity (grid) maps of ×× Å grid points and 0.375 Å spacing were generated using the Autogrid program (*Morris, Goodsell et al., 1998*). AutoDock parameter set- and distance- dependent dielectric functions were used in the calculation of the van der Waals and the electrostatic terms, respectively.
Docking simulations were performed using the Lamarckian genetic algorithm (LGA) and the Solis & Wets local search method (*Solis and Wets, 1981*). Initial position, orientation, and torsions of the ligand molecules were set randomly. All rotatable torsions were released during docking. Each docking experiment was derived from 100 different runs that were set to terminate after a maximum of 2500000 energy evaluations. The population size was set to 150. During the search, a translational step of 0.2 Å, and quaternion and torsion steps of 5 were applied.

References

E. Hazai, S. Kovacs, L. Demko, Z. Bikadi
DockingServer (www.dockingserver.com)
Virtua Drug Ltd., Budapest, Hungary

T. A. Halgren
Merck molecular force field. I. Basis, form, scope, parametrization, and performance of MMFF94
Journal of Computational Chemistry **17 (5-6)**, 490-519 (1998)

G. M. Morris, D. S. Goodsell, et al.
Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function
Journal of Computational Chemistry **19 (14)**, 1639-1662 (1998)

F. J. Solis and R. J. B. Wets
Minimization by Random Search Techniques
Mathematics of Operations Research **6 (1)**, 19-30 (1981)

Image Gallery

This software includes code developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana- Champaign.

References, please cite:

W. Humphrey, A. Dalke, and K. Schulten
VMD - Visual Molecular Dynamics
J. Mol. Graph. **14**, 33-38 (1996)

N-acetylmuramic acid docking parameters to VisP *S.* Typhimurium modeled structure.