Supplementary Material

Umamaheswari, A., *et al*. 2010. Identification of potential *Leptospira* phosphoheptose isomerase inhibitors through virtual high-throughput screening. *Genomics Proteomics Bioinformatics* 8(4): 246-255.

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Figures S1-S3; Table S1

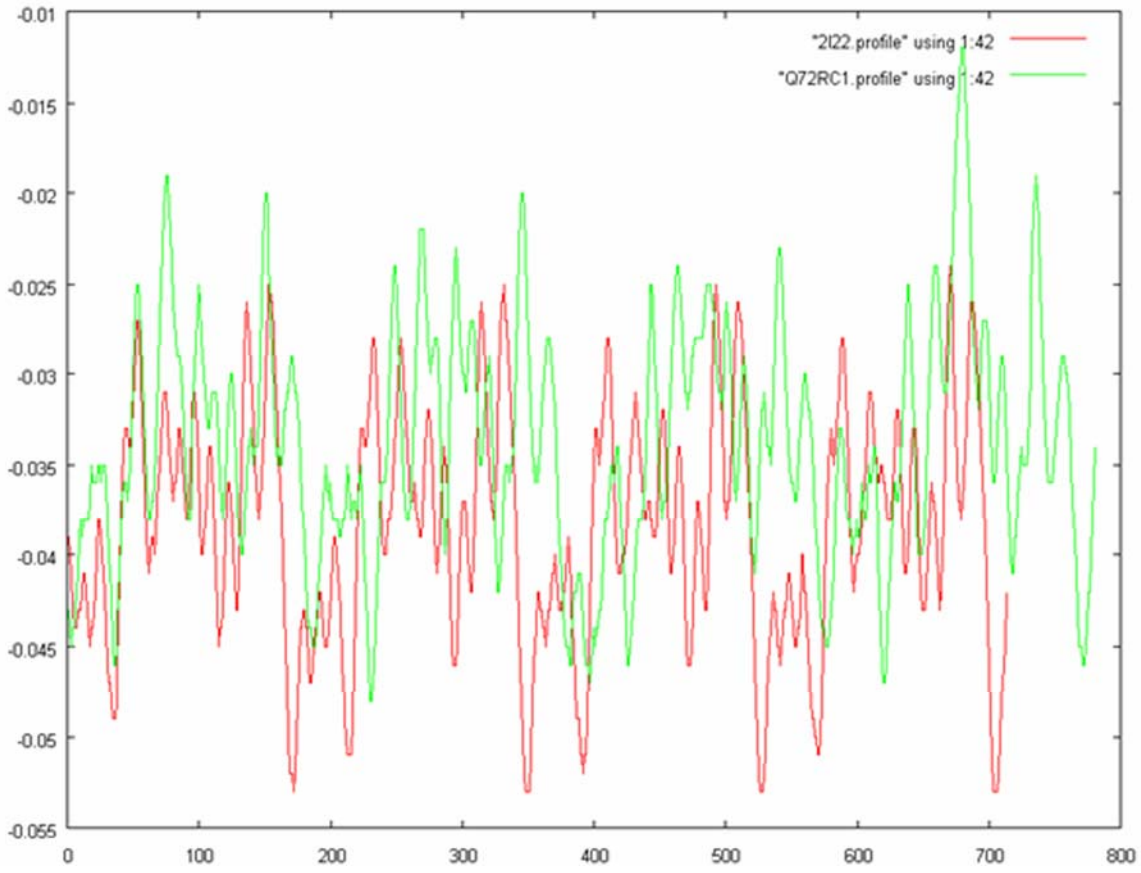
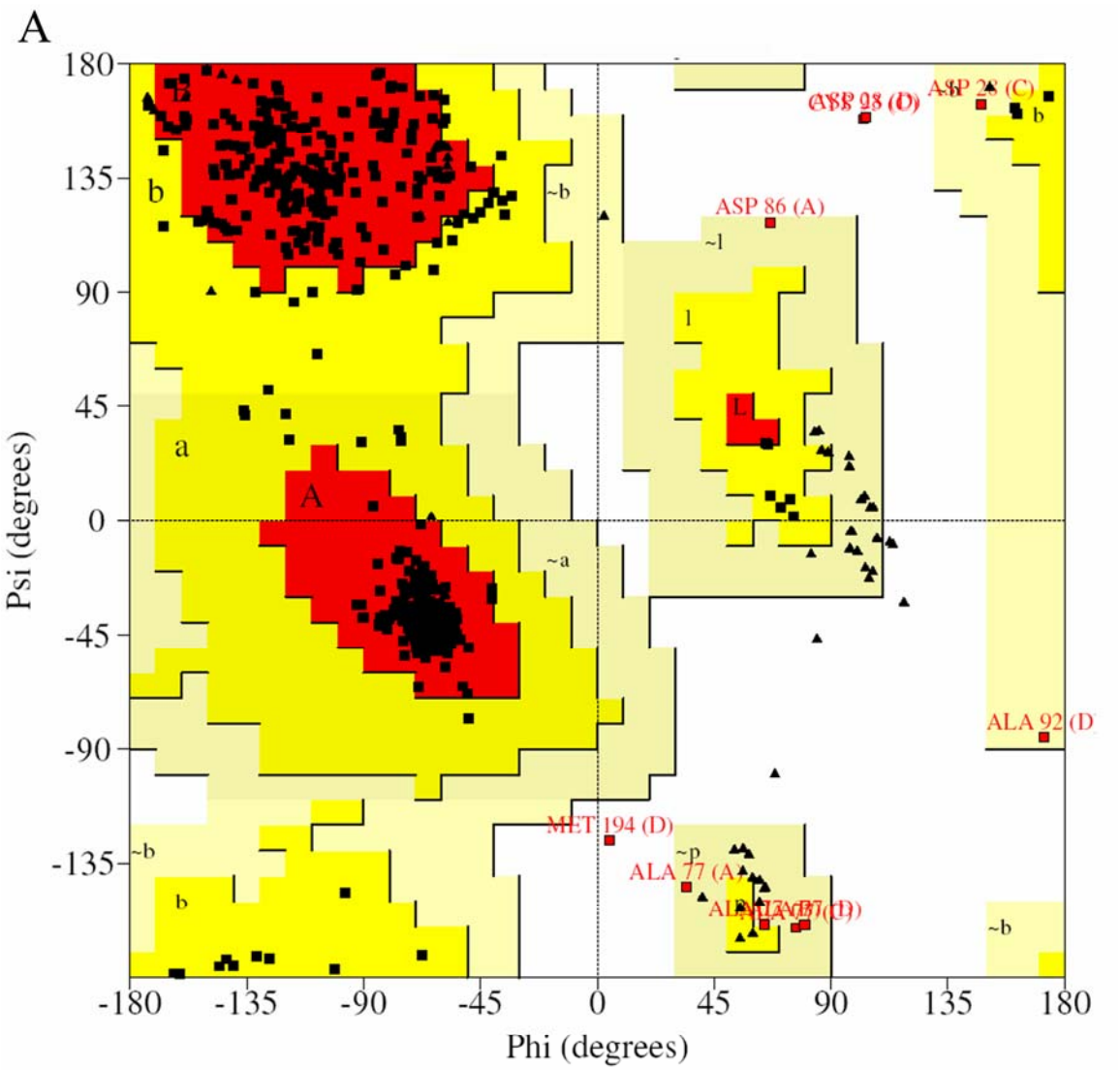


Figure S1 Graphical representation of discrete optimized protein energy (DOPE) score profiles for the model (green) and templates (PDB ID: 2I22) (red).

A



Plot statistics

Residues in most favoured regions [A,B,L]	631	91.2%
Residues in additional allowed regions [a,b,l,p]	51	7.4%
Residues in generously allowed regions [~a,~b,~l,~p]	7	1.0%
Residues in disallowed regions	3	0.4%
Number of non-glycine and non-proline residues	692	100.0%
Number of end-residues (excl. Gly and Pro)	8	
Number of glycine residues (shown as triangles)	72	
Number of proline residues	8	
Total number of residues	780	

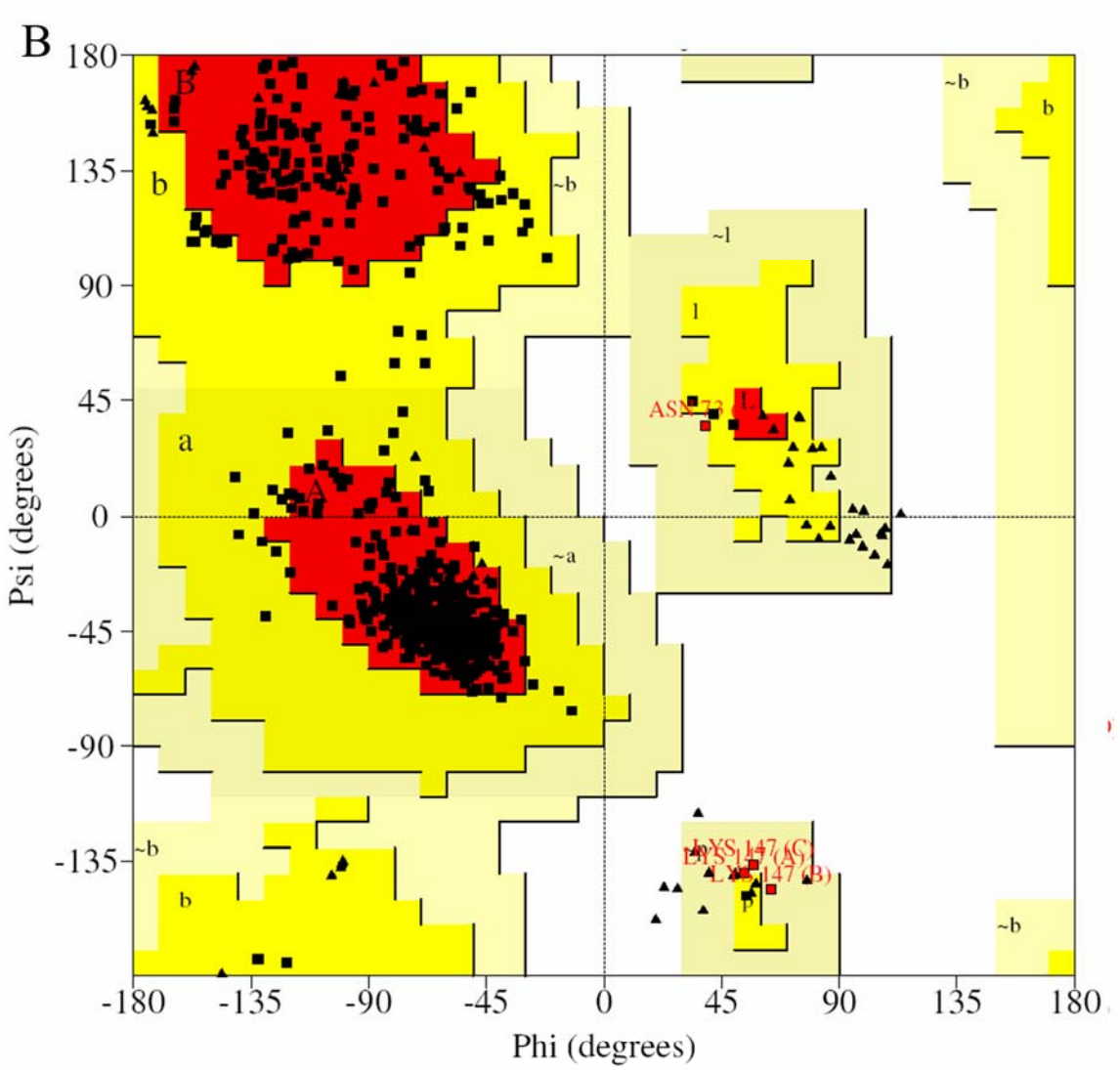


Figure S2 **A**. Procheck evaluation report of GmhA 3D model. **B**. Procheck evaluation report of Template 2I22.

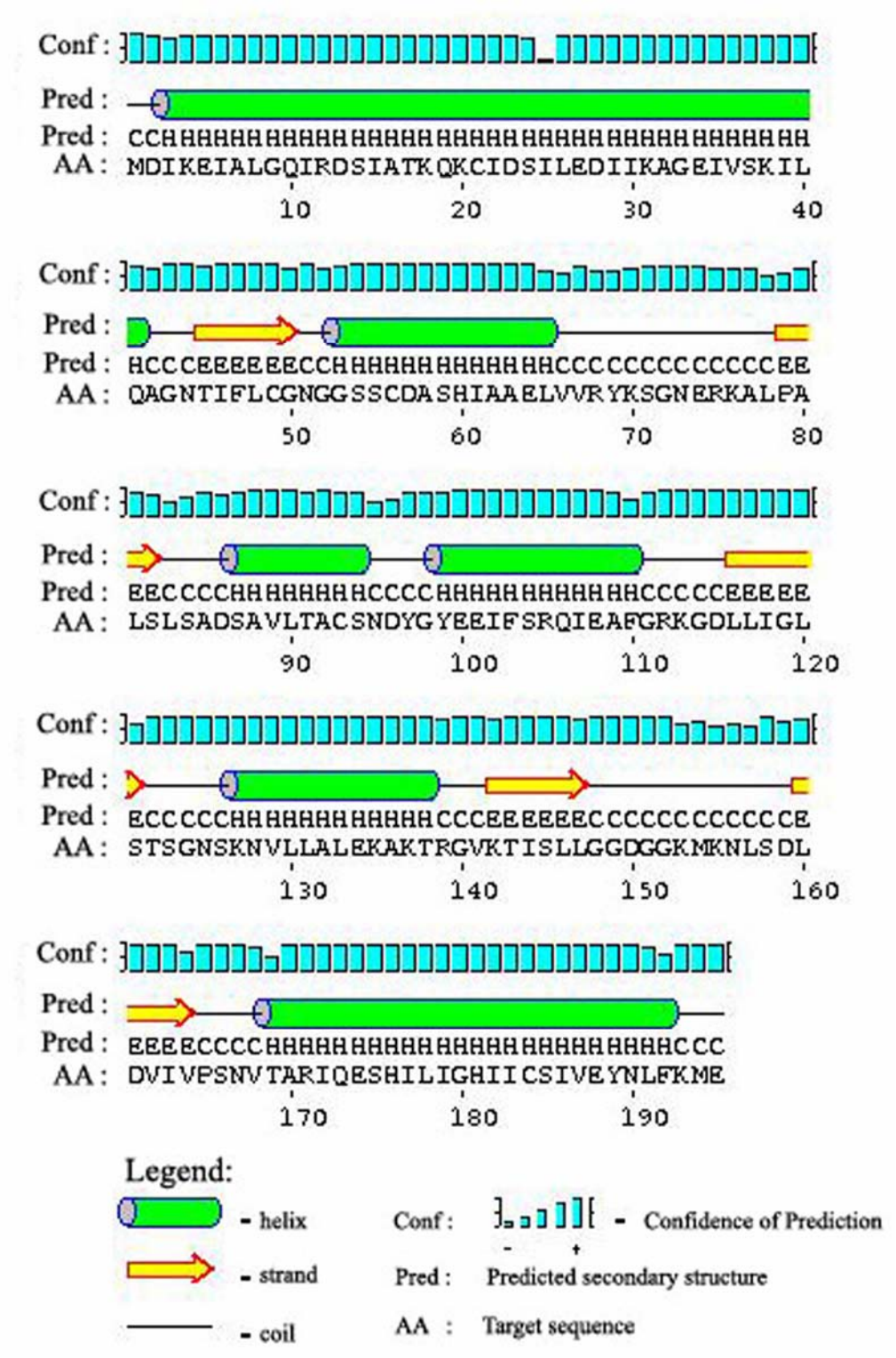
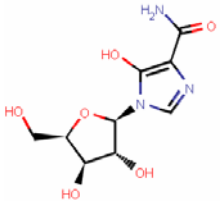
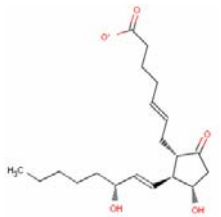
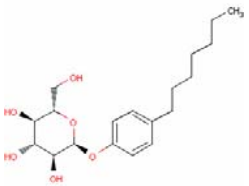
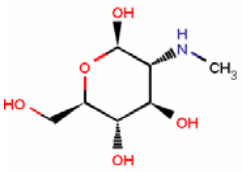
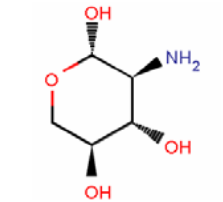
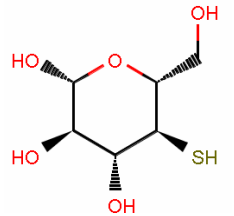
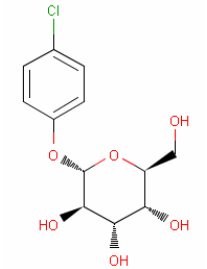
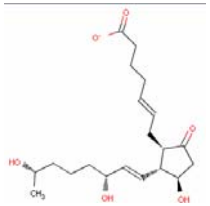
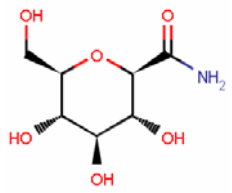
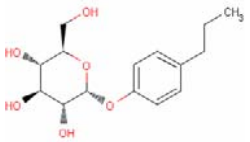
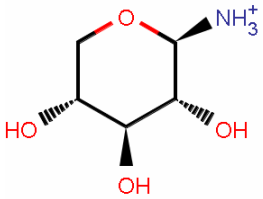
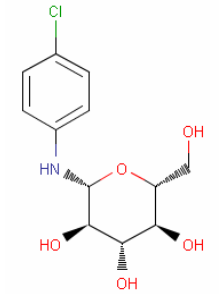


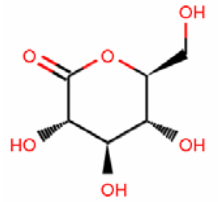
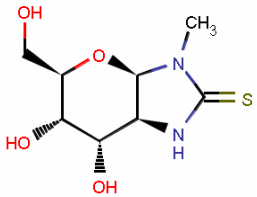
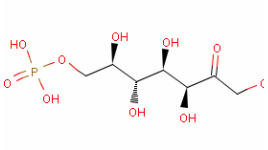
Figure S3 Secondary structure prediction diagram for the GmhA.

Table S1 Structure, smiles and docking scores of predicted 14 novel competitive inhibitors designed for GmhA of *Leptospira* serovars

No.	Lead structure	Lead smiles	M.W. (Dalton)	Glide score (Kcal/mol)	Glide score after Glu64→Asp64
1		NC(=O)C1=C(O)N(C=N1)[C@@H]2O[C@H](CO)[C@H](O)[C@H]2O	259.22	−8.39	−7.09
2		CCCCC[C@@H](O)\C=C\[C@@H]1[C@@H](O)CC(=O)[C@H]1C\C=C\CCC([O-])=O	351.46	−8.04	−6.08
3		CCCCCCCC1=CC=C(O[C@@H]2O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]2O)C=C1	354.44	−7.93	−6.88
4		CN[C@H]1[C@H](O)O[C@H](CO)[C@@H](O)[C@@H]1O	193.2	−7.66	−5.80

5		N[C@@H]1[C@@H](O)OC[C@H](O)[C@H]1O	149.15	−7.60	−6.87
6		OC[C@H]1O[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1S	196.22	−7.56	−6.47
7		OC[C@@H]1O[C@@H](OC2=CC=C(Cl)C=C2)[C@H](O)[C@@H](O)[C@H]1O	290.7	−7.55	−5.97
8		C[C@H](O)CCC[C@@H](O)\C=C\[C@H]1[C@H](O)CC(=O)[C@@H]1C\C=C\CCCC([O-])=O	367.46	−7.52	−7.11

9		NC(=O)[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O	207.18	−7.52	−6.16
10		CCCC1=CC=C(O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)C=C1	298.34	−7.51	−6.64
11		[NH3+][C@@H]1OC[C@@H](O)[C@H](O)[C@H]1O	148.14	−7.50	−7.81
12		OC[C@H]1O[C@@H](NC2=CC=C(Cl)C=C2)[C@H](O)[C@@H](O)[C@@H]1O	289.72	−7.47	−6.38

13		OC[C@@H]1OC(=O)[C@@H](O)[C@H](O)[C@H]1O	178.14	−7.43	−4.93
14		CN1[C@@H]2O[C@H](CO)[C@@H](O)[C@@H](O)[C@@H]2NC1=S	234.28	−7.41	−5.99
15		**OCC(=O)[C@@H](O)[C@H](O)[C@H](O)[C@H](O)COP(O)(O)=O**	**290**	**−3.41**	**−3.18**
	(Substrate S7P)				