Table S1: Binding Parameters :

Following parameters were used for docking and subsequent binding energy calculations.

Flexible Receptor Atom Property	Receptor.Positions, Gold.Protein.RotatedAtoms
In Situ Ligand Minimization	False
In Situ Ligand Minimization Minimization Algorithm	Smart Minimizer
In Situ Ligand Minimization Minimization Max Steps	1000
In Situ Ligand Minimization Minimization RMS Gradient	0.001
In Situ Ligand Minimization Minimization Energy Change	0.0
Ligand Conformational Entropy	False
Maximum Alignment RMSD	0.5
Conformation Generation	
Conformation Method	FAST
Maximum Conformations	1000
Ligand Conformational Entropy Minimization	
Ligand Conformational Entropy Minimization Minimization Algorithm	Smart Minimizer
Ligand Conformational Entropy Minimization Minimization Max Steps	500
Ligand Conformational Entropy Minimization Minimization RMS Gradient	0.1
Ligand Conformational Entropy Minimization Minimization Energy Change	0.0
Implicit Solvent Model	None
Dielectric Constant	1
Implicit Solvent Dielectric Constant	80
Generalized Born Lambda Constant	
Minimum Hydrogen Radius	1.0
Use Non-polar Surface Area	True
Non-polar Surface Constant	0.92
Non-polar Surface Coefficient	0.00542
Salt Concentration	0.0
Input Atomic Radii	van der Waals radii
Use Molecular Surface	True
Nonbond List Radius	14.0
Nonbond Higher Cutoff Distance	12.0
Nonbond Lower Cutoff Distance	10.0
Electrostatics	Spherical Cutoff
Kappa	0.34
Order	4
Estimate Entropy	True
Entropy Temperature	298.15
Partial Charge Estimation	default
Parallel Processing	False
Parallel Processing Batch Size	25
Parallel Processing Server	localhost
Parallel Processing Server Processes	2
Parallel Processing Preserve Order	True
Entropy Mode	Translational and Rotational Only