Molecular modelling of the adipokinetic hormone receptor from the stick insect Carausius morosus, and its endogenous agonist

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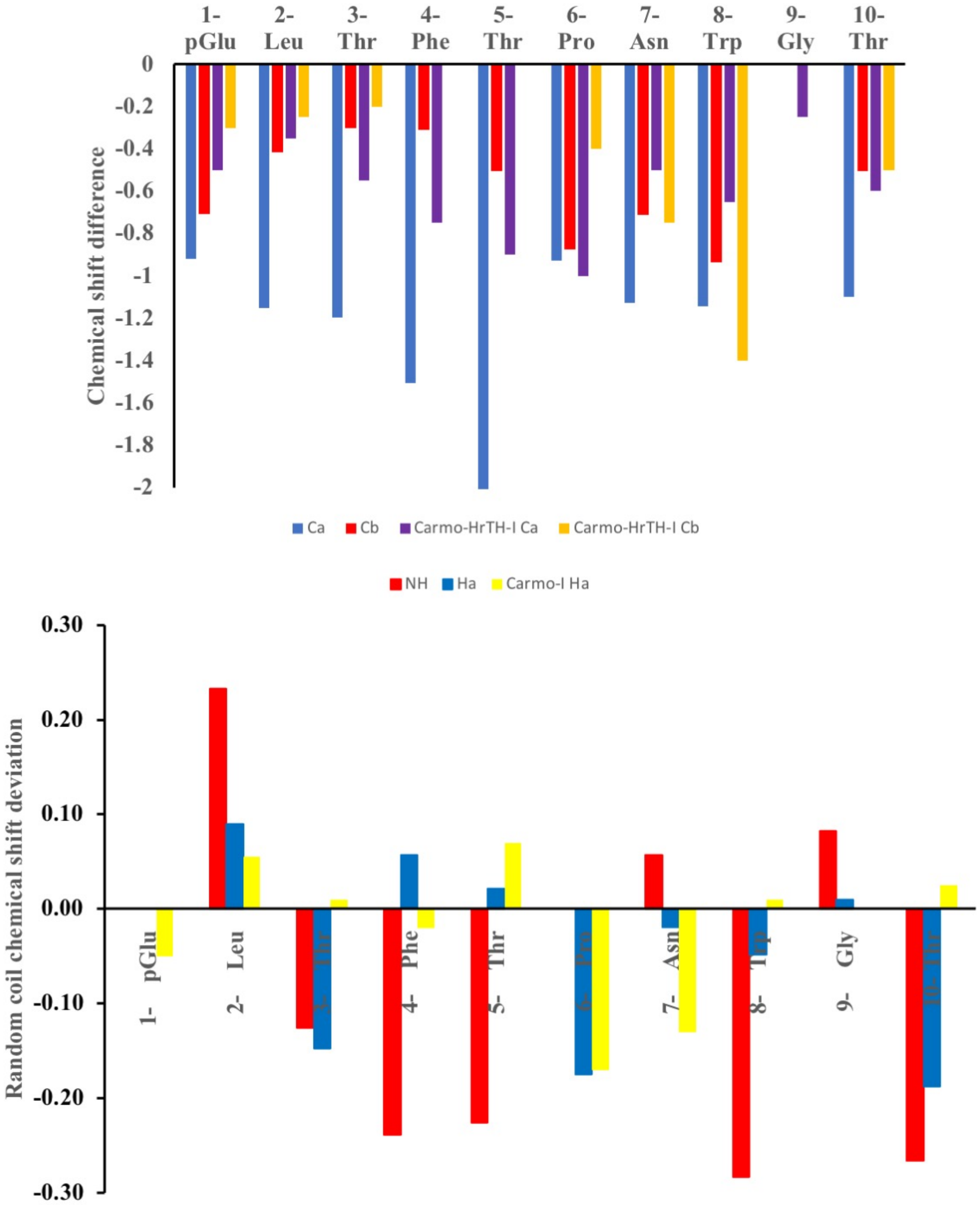
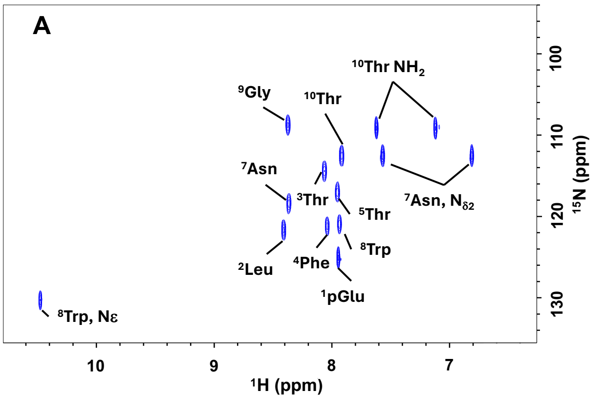


Figure S1. Random coil chemical shift differences of Carmo-HrTH-I and II (a) C_α and C_β and (b) NH, N_α. Data for Carmo-HrTH-I in D_2O solution is taken from reference {Munte, 2008 #435}



B **Statistical information for the averaged refined Carmo-HrTH-II* NMR structure in DPC micelles**

Assignments	**Total**	244
	Intra residue	117
	Inter	127
	Sequential	104
	Short range (seq)	23
Atomic backbone RMSD (Å) from 10 lowest energy structures (residue 1-10)		0.54
Violations from experimental restraints		
Number of restraints used		244
NOE violations (> 0.4 Å)		4
Average violation (Å)		0.44
Molprobity statistics		
Clashes (> 0.4 Å)		4
Ramachandran outliers (%)		0
Ramachandran favoured (%)		87.5
MolProbity score		3.02
Cβ deviations > 0.25		0
Bad bonds		0
Bad angles		0

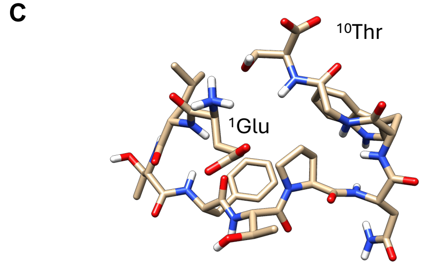


Figure S2 (A) ^{15}N HSQC spectra of Carmo-HrTH-II in DPC micelles. Experiments were performed at 298 K. **(B)** statistical parameters used for the structure calculation and Molprobity validation outcome and **(C)** averaged structure of Carmo-HrTH-II.

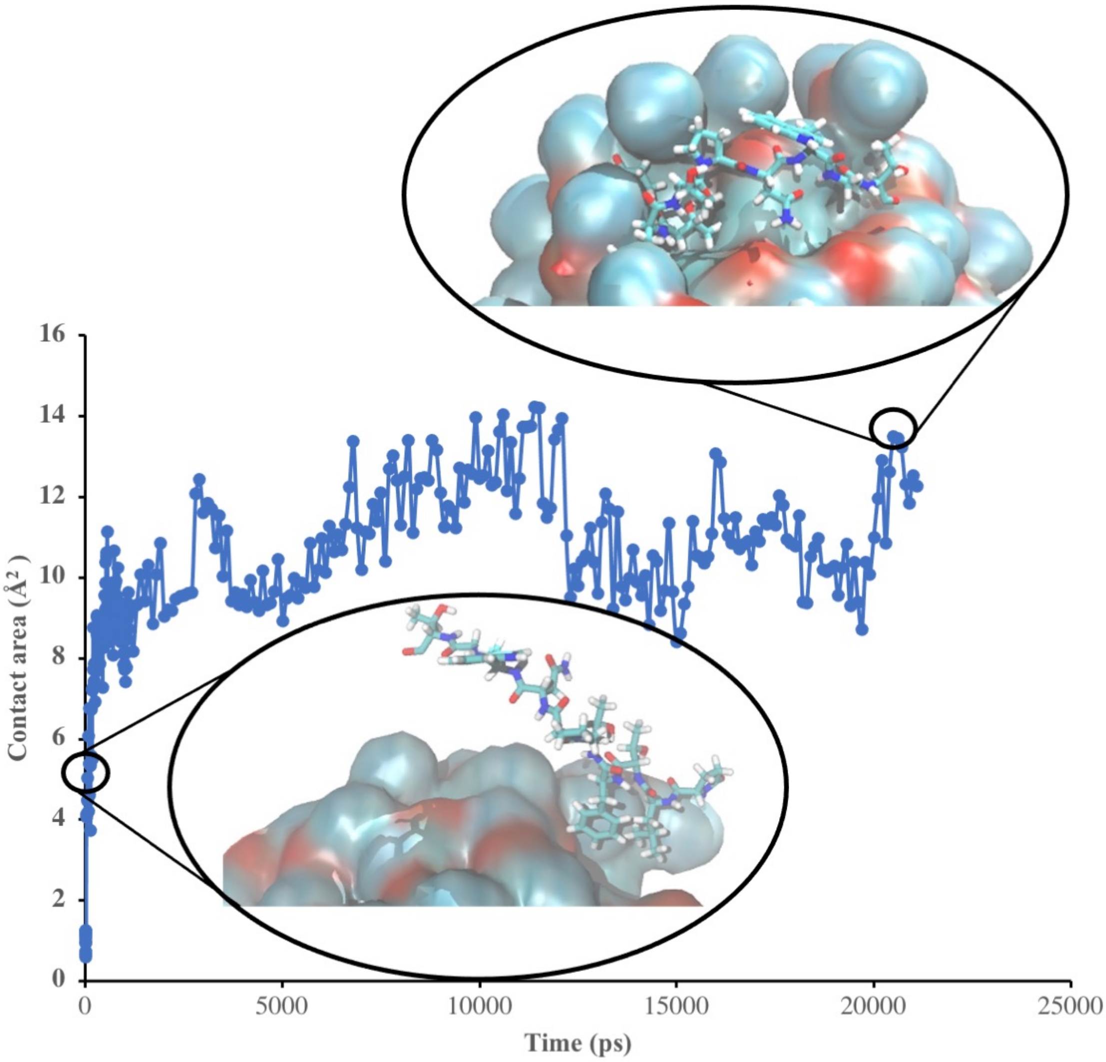


Figure S3. Surface contact area between DPC micelle and Carmo-HrTH-II during MD simulation. Two snapshots of the structure are shown. For clarity, water is not shown and the DPC is shown as an electrostatic surface.

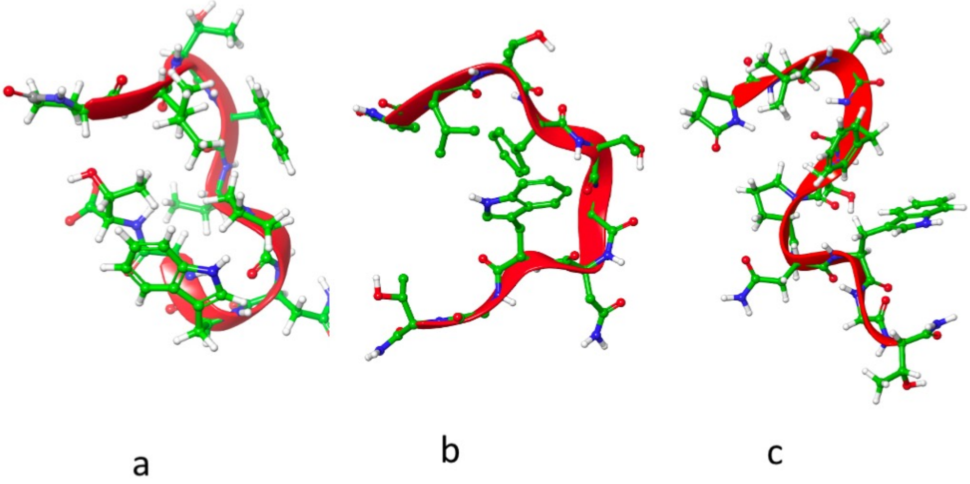


Figure S4. Comparison of Carmo-HrTH-II (a) Average structure from NMR, (b) Predominant structure in DPC micelle solution, (c) Docked structure after MD.

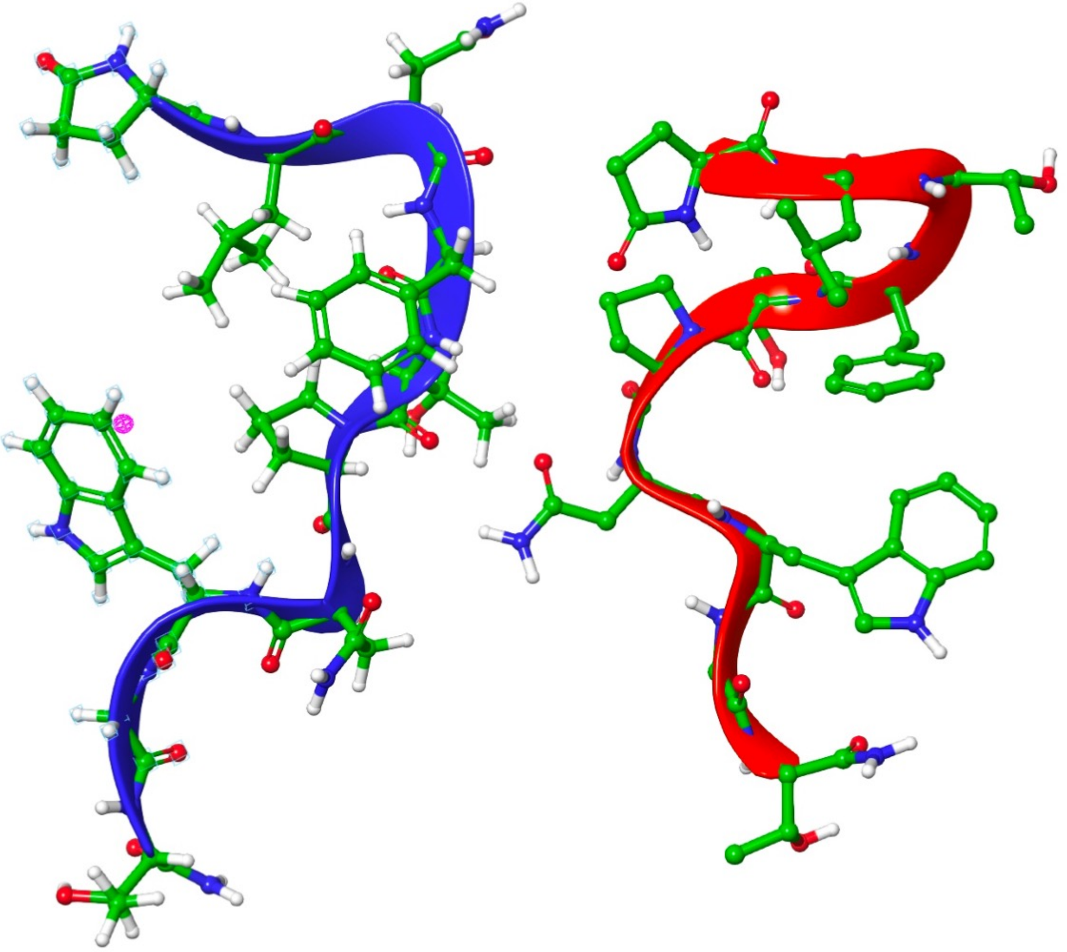
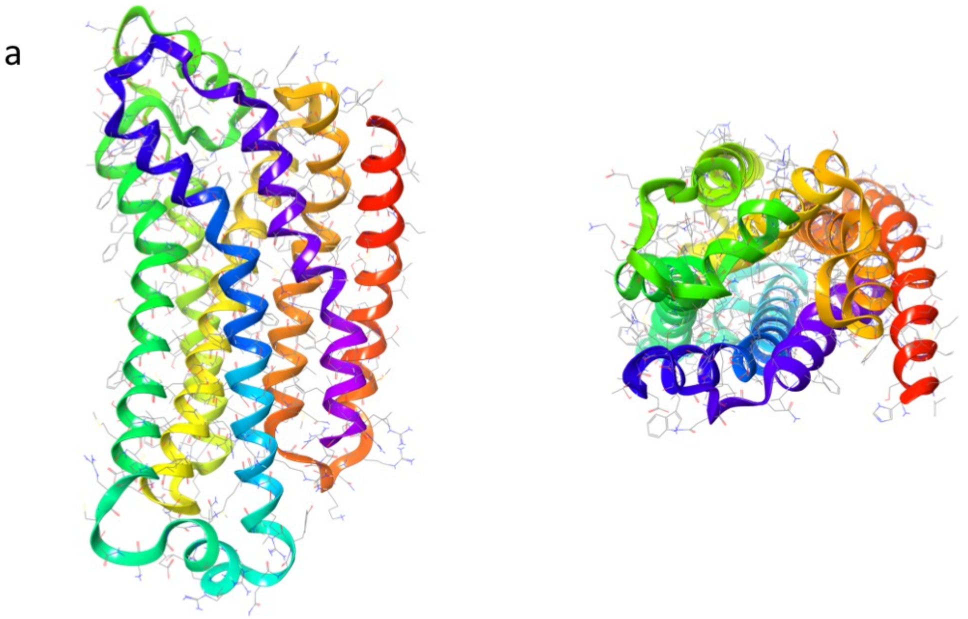
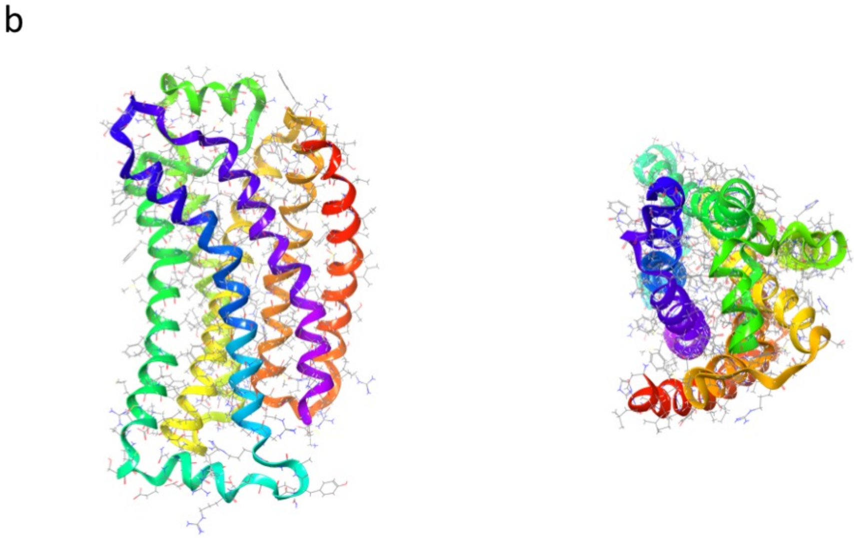


Figure S5. Carmo-HrTH-II (red ribbon) and Locmi-AKH-I (blue ribbon).



Carmo-AKHR open model.



Carmo-AKHR closed model.

Figure S6. Side and top view of Carmo-AKHR model (a) ‘Open’ inactive conformation and (b) ‘Closed’ active conformation

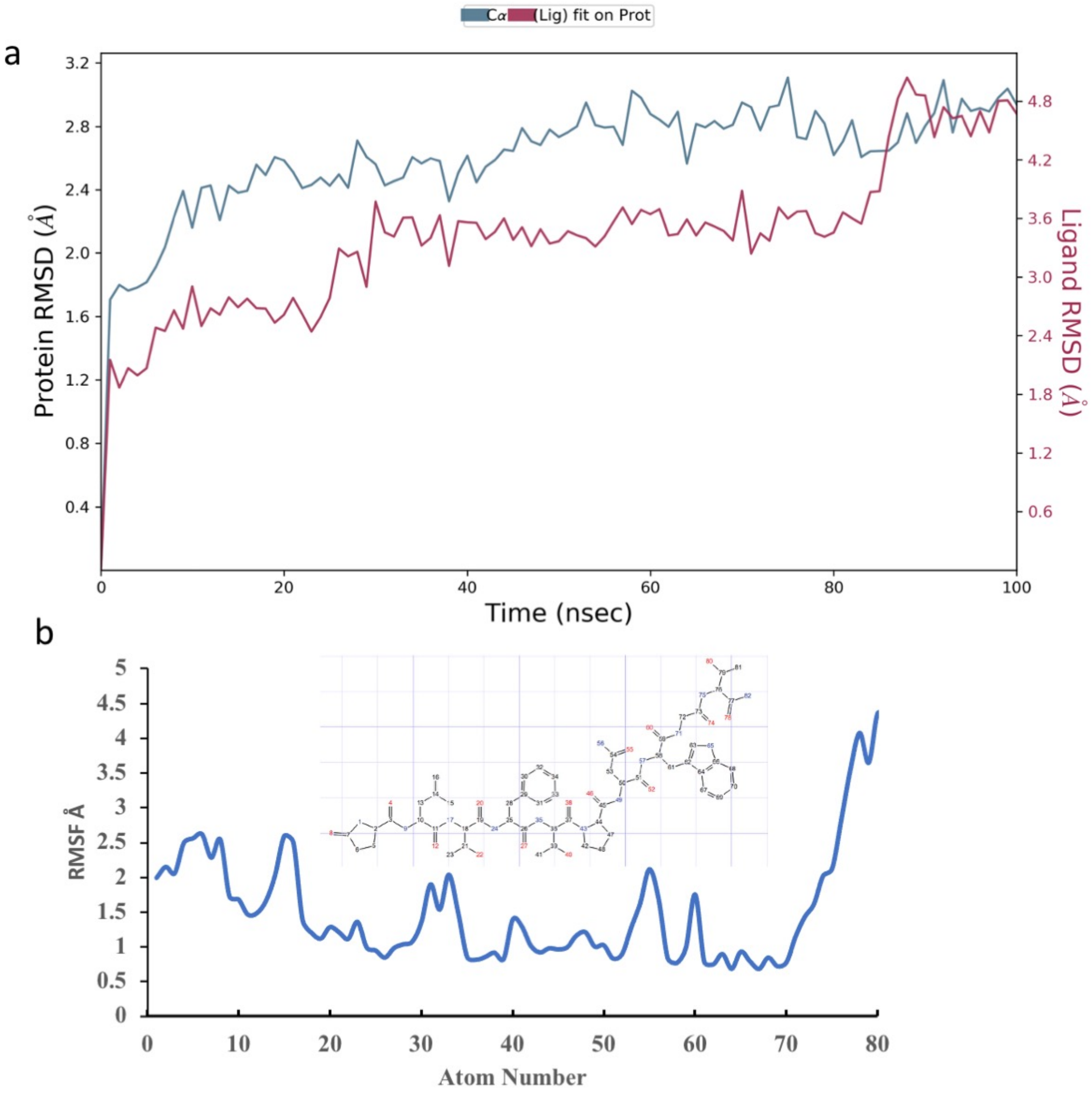


Figure S7 (a) RMSD of Carmo-HrTH-II/CarmoAKHR complex. b) RMSF of Carmo-HrTH-II.

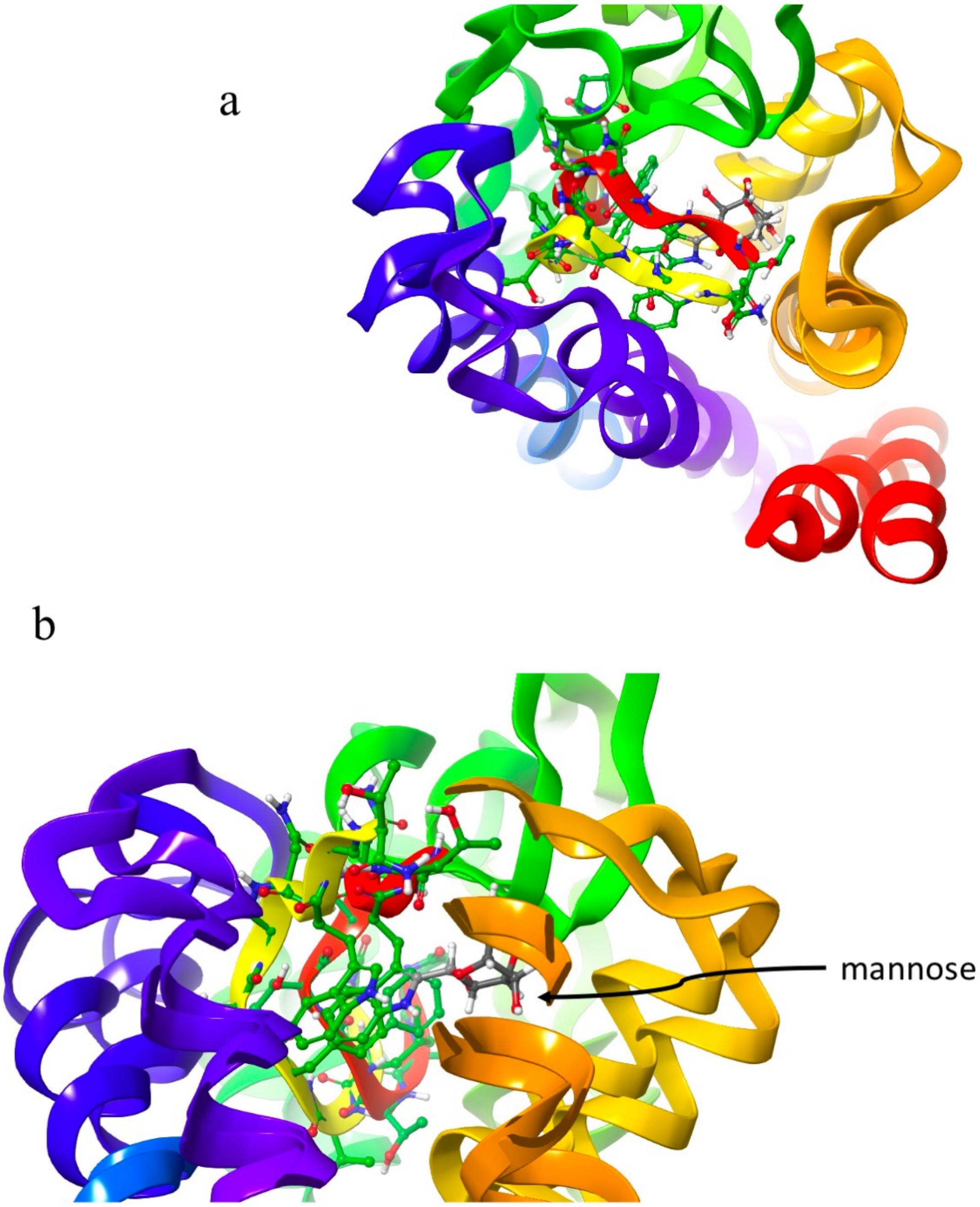


Fig S8. Overlay of Carmo-HrTH-I (red) and II (yellow) in the binding pocket of Carmo-AKHR. (a) top view, (b) side view.

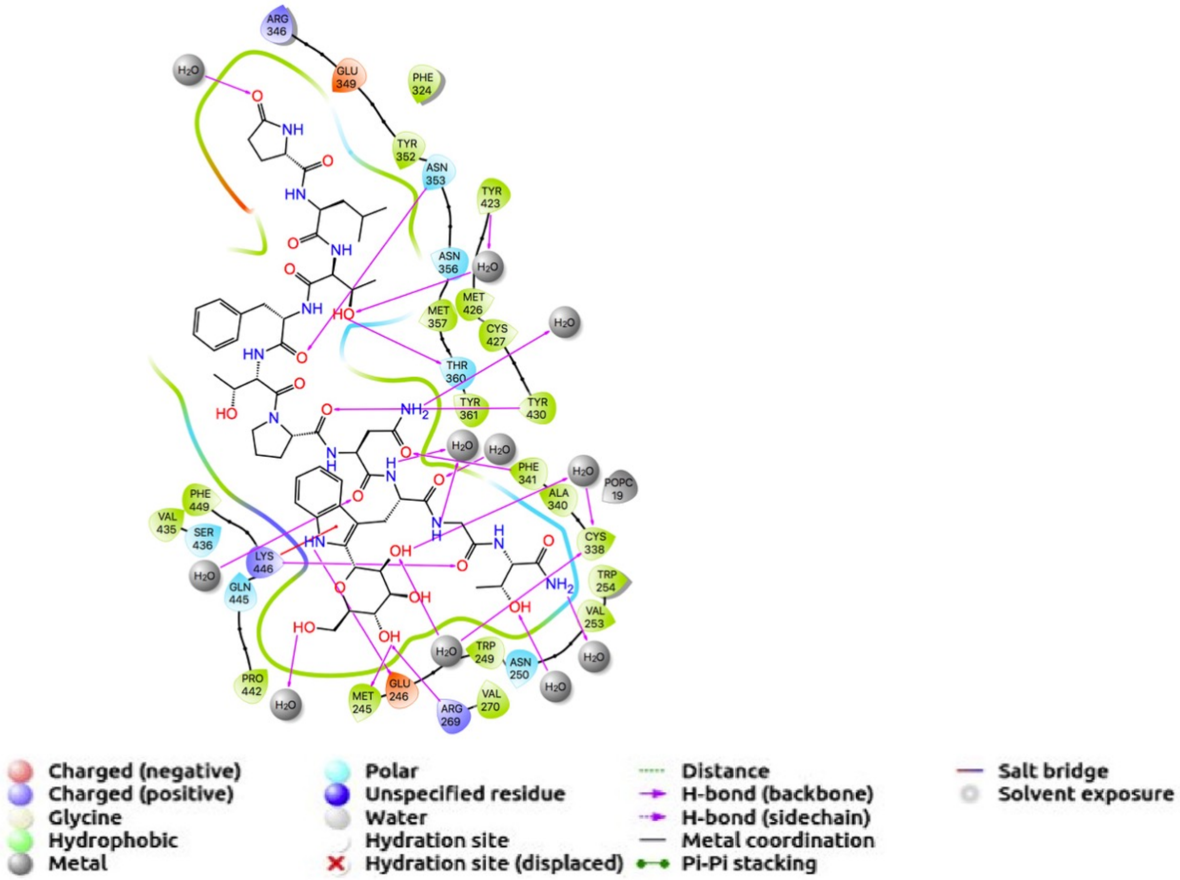


Figure S9. Ligand interaction diagram of Carmo-HrTH-I docked to Carmo-AKHR.

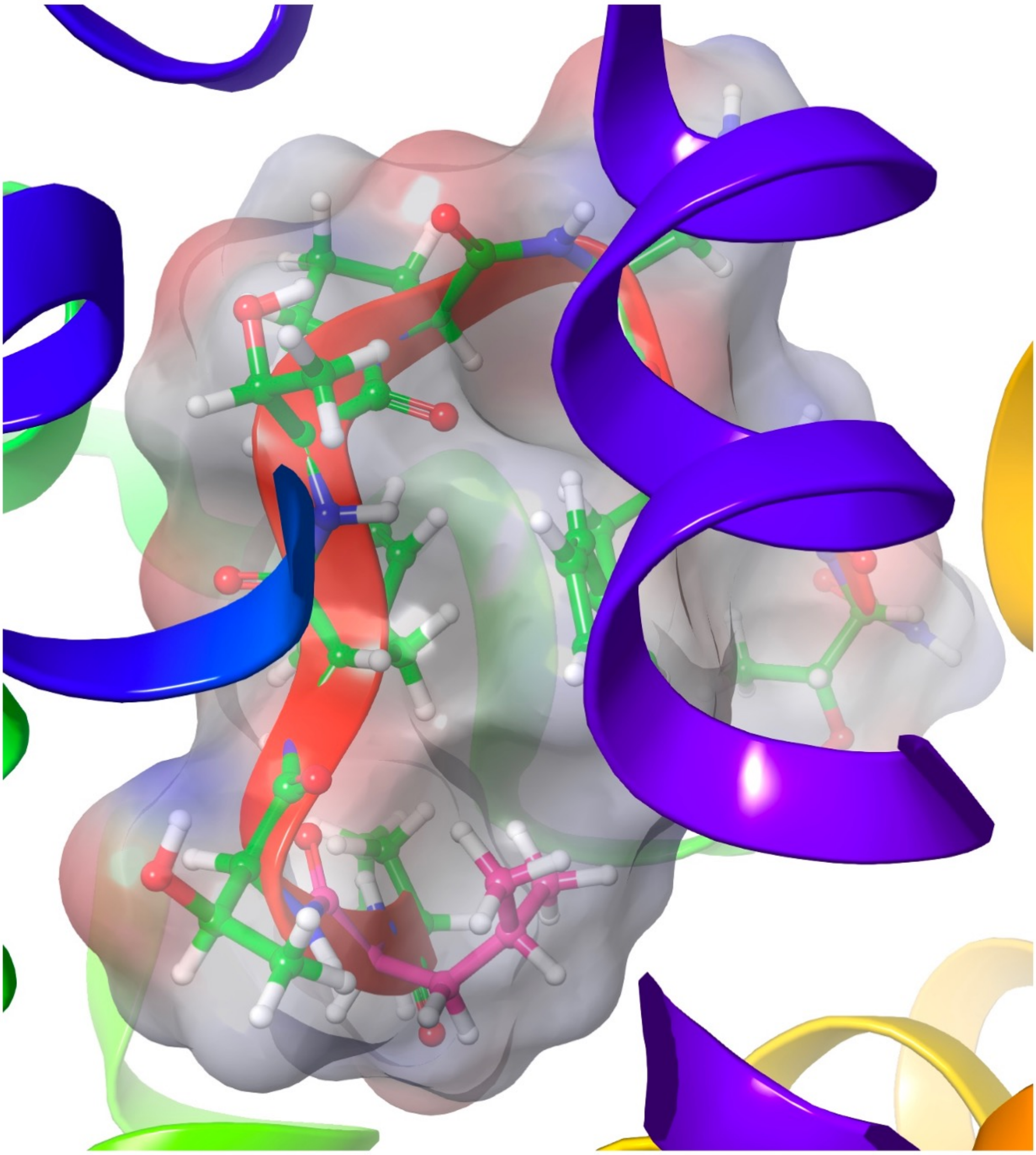


Figure S10. Carmo-AKHR binding pocket. Leucine 2 is displayed in pink. For clarity some of the helices are not shown

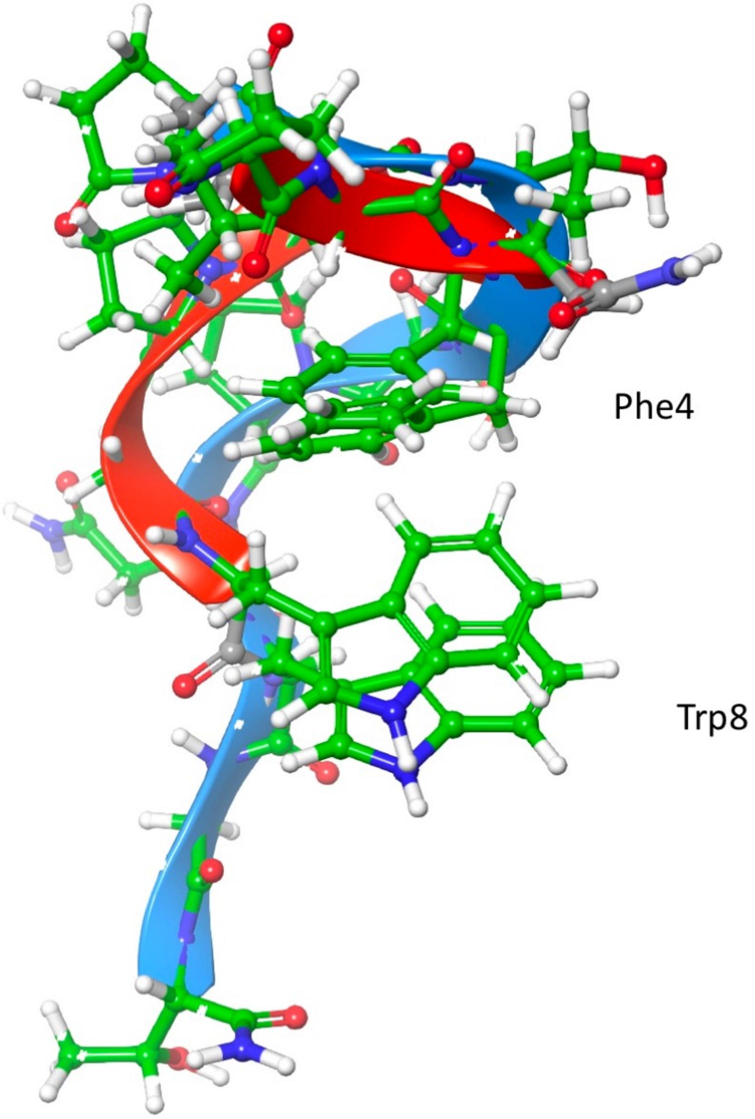


Figure S11. Overlay of Panbo-RPCH (red) and Carmo-HrTH-II (blue) in Carmo-AKHR binding site., showing the orientation of Phe4 and Trp8.

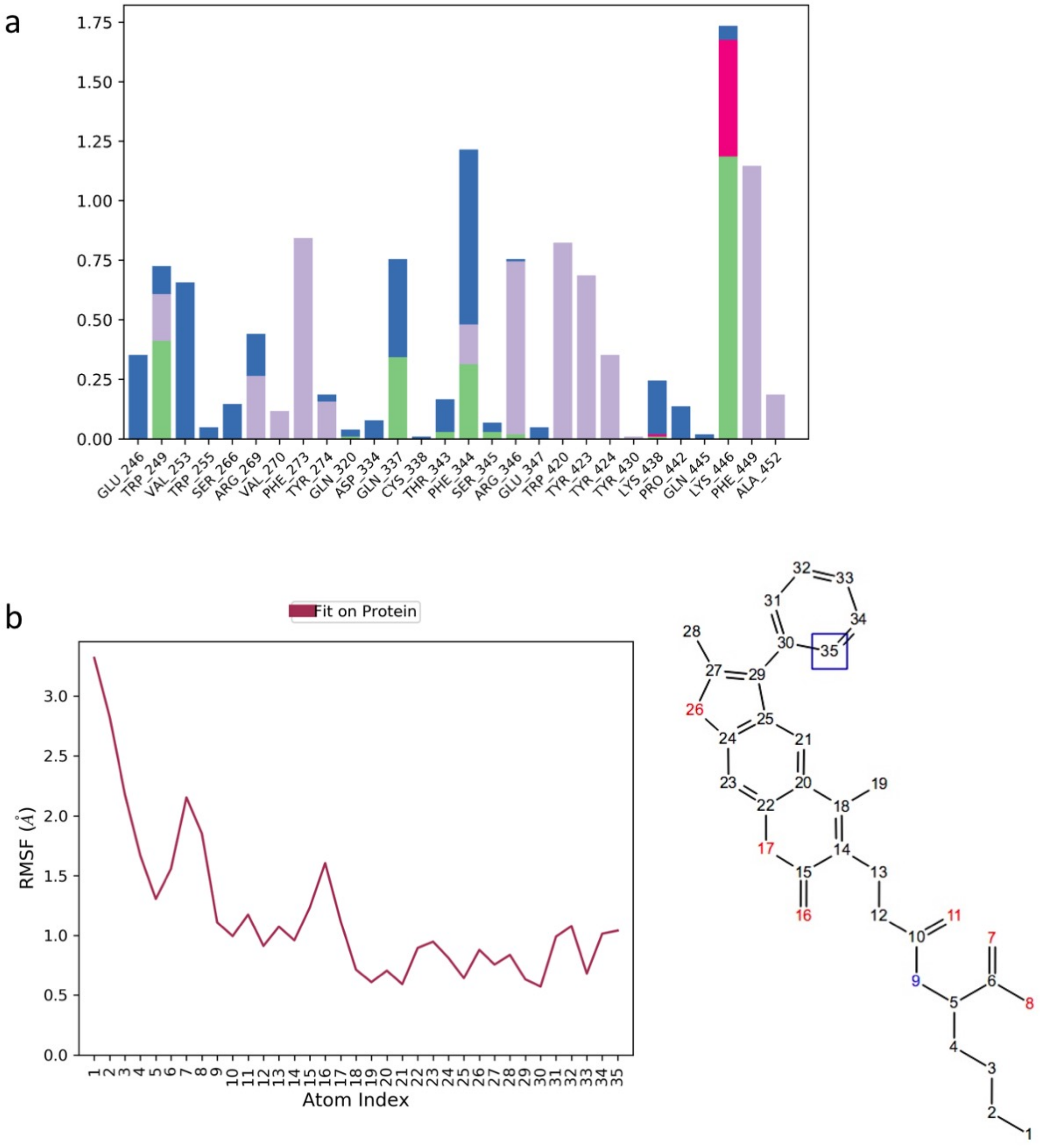
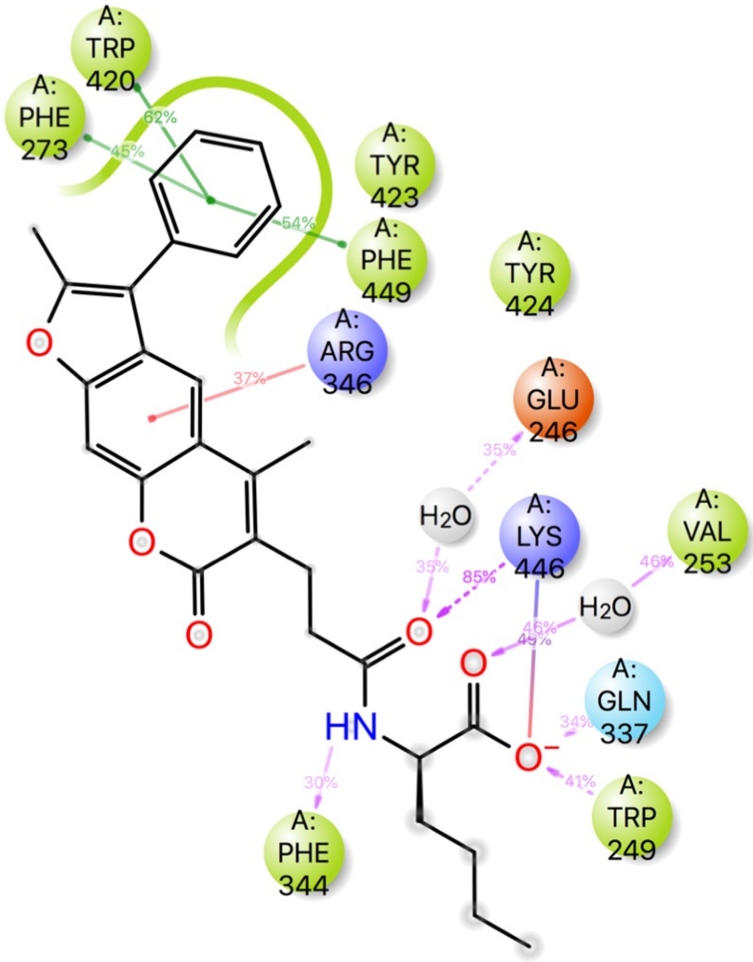


Figure S12. (a) RMSF of Cpd 2429 docked to Carmo-AKHR.(b) Protein ligand interactions as a % of simulation time. The interactions are colour coded: Green = H-bonds; Grey = Hydrophobic; Red = Ionic and Blue = Water bridge.



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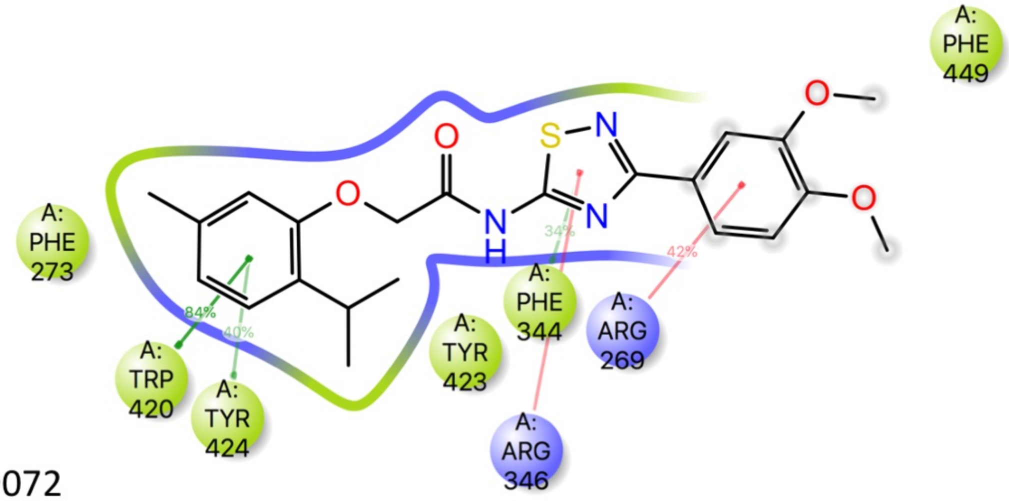

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Figure S13. Simulation interaction diagram of compounds 2429 and 9072.

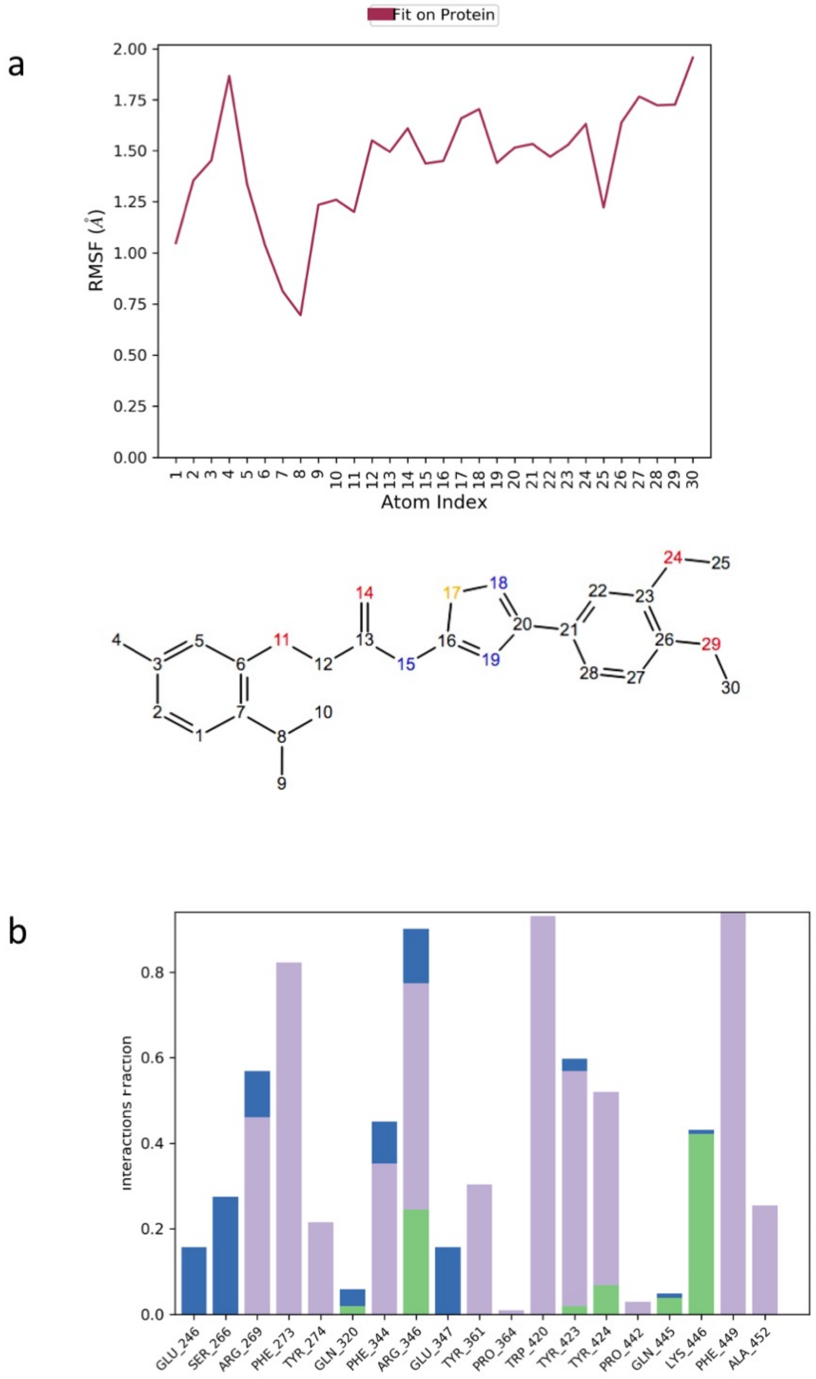

Figure S14. (a) RMSF of Cpd 9072 docked to Carmo-AKHR.(b) Protein ligand interactions as a % of simulation time. The interactions are colour coded: Green = H-bonds; Grey = Hydrophobic; Red = Ionic and Blue = Water bridge.