Insights into the interaction of LVV-hemorphin-7 with Angiotensin II Type 1 Receptor

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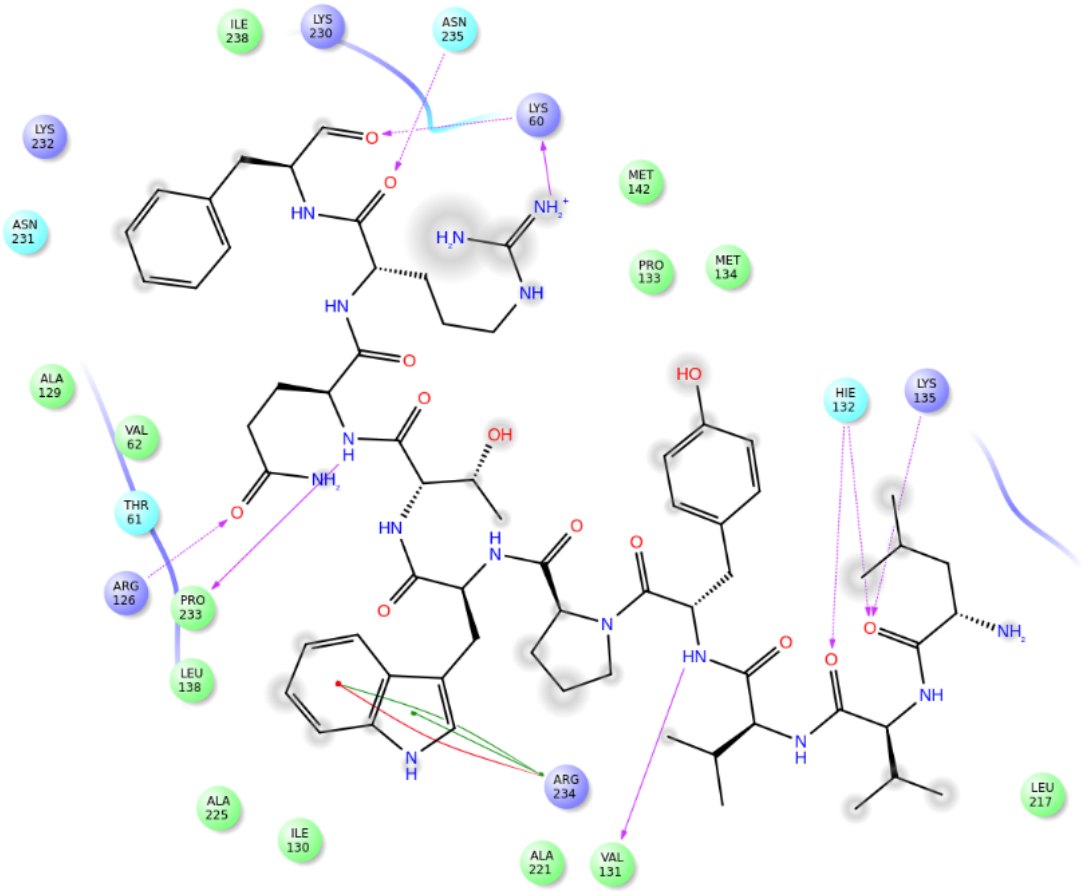
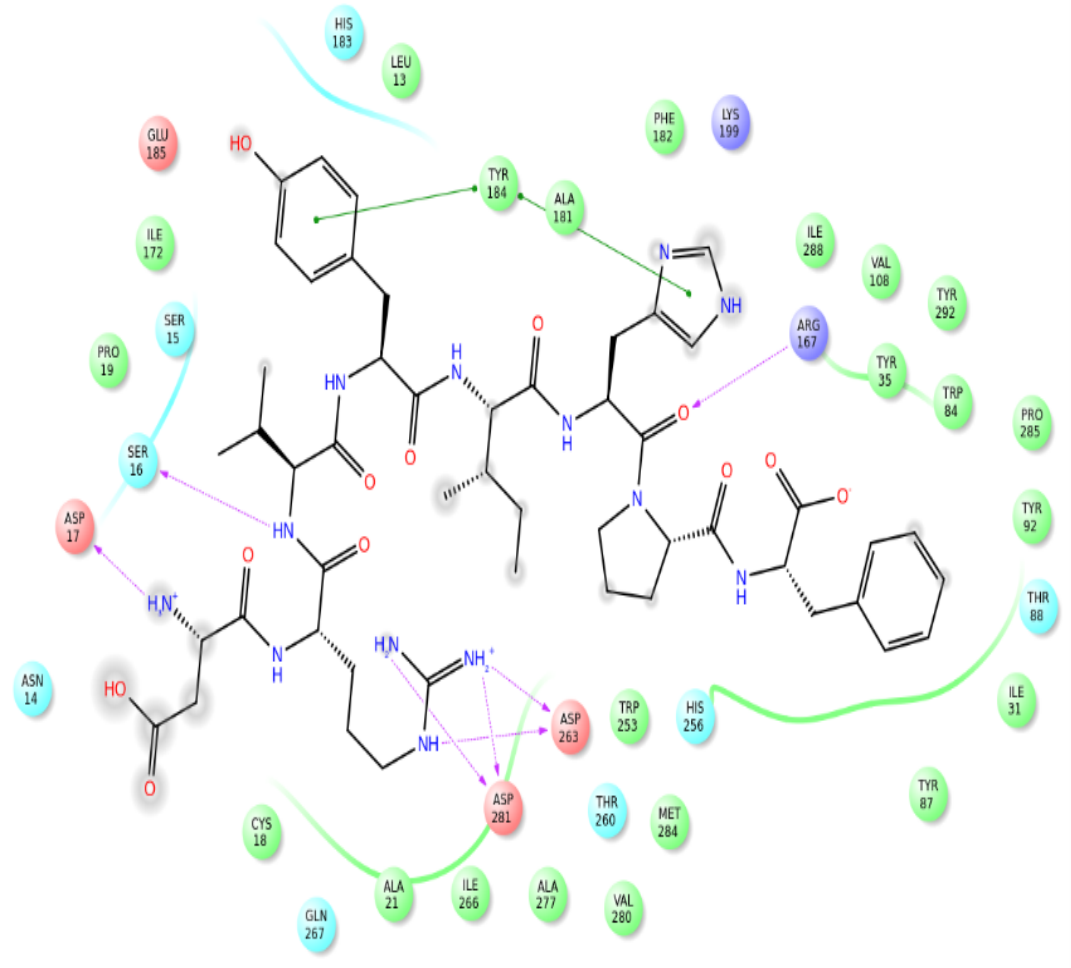
Supplementary Materials

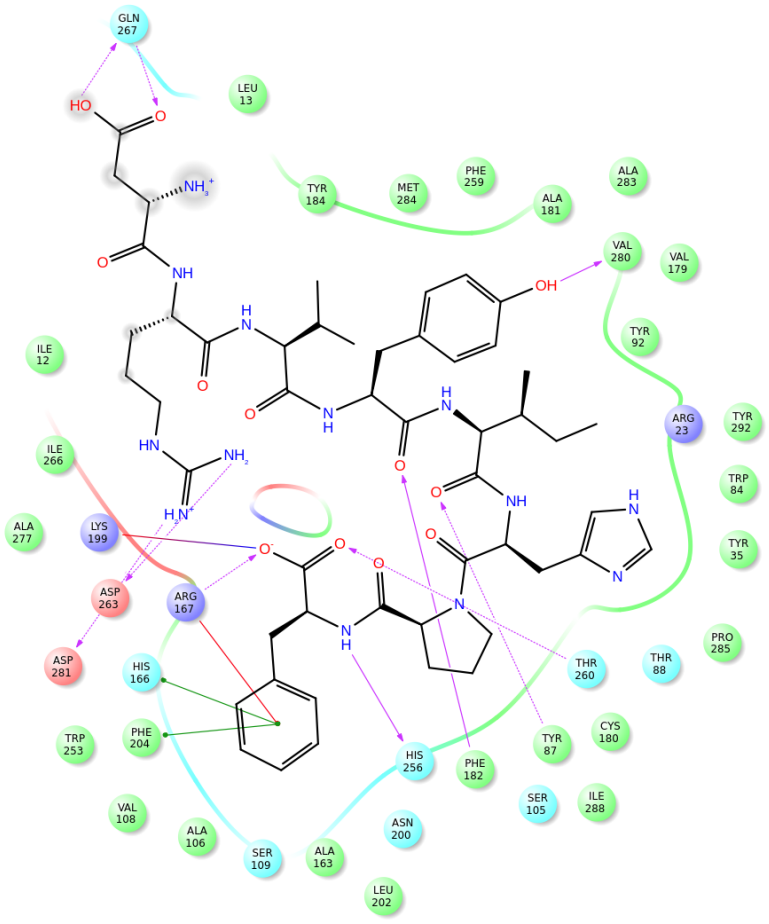


Supplementary Figure S1. 2D ligand interaction diagram of LVV-H7 bound to AT1R. AT1R (PDB ID: 4ZUD) residues that interacted with LVV-H7 in the intracellular binding site. Colored circles represent AT1R amino acids that interact with bound peptide. Red circles indicate negatively charged amino acids, dark blue colors indicate positively charged amino acids, light blue circles indicate polar amino acids, and green circles indicate hydrophobic amino. Hydrogen bonds are shown with purple arrows–dashed arrows for hydrogen bonds involving amino acid side chain and regular arrows for hydrogen bonds involving amino acid backbone. π–π interactions are represented with green lines.

Supplementary Figure S2. Histograms of the percentage of simulation time where an AT1R residue maintained contact with: (**A**) LVV-H7 in the AT1R-LVV-H7 complex; (**B**) AngII in the AT1R-AngII complex; (**C**) AngII in the AT1R-LVV-H7-AngII complex.



Supplementary Figure S3. 2D ligand interaction diagram of AngII bound to AT1R. AT1R (PDB ID: 4ZUD) residues that interacted with AngII in the orthosteric binding site. Colored circles represent AT1R amino acids that interact with bound peptide. Red circles indicate negatively charged amino acids, dark blue colors indicate positively charged amino acids, light blue circles indicate polar amino acids, and green circles indicate hydrophobic amino. Hydrogen bonds are shown with purple arrows–dashed arrows for hydrogen bonds involving amino acid side chain and regular arrows for hydrogen bonds involving amino acid backbone. π–π interactions are represented with green lines.



Supplementary Figure S4. 2D ligand interaction diagram of AngII bound to AT1R-LVV-H7 complex. AT1R residues that interacted with AngII in the orthosteric binding site. Colored circles represent AT1R amino acids that interact with bound peptide. Red circles indicate negatively charged amino acids, dark blue colors indicate positively charged amino acids, light blue circles indicate polar amino acids, and green circles indicate hydrophobic amino. Hydrogen bonds are shown with purple arrows–dashed arrows for hydrogen bonds involving amino acid side chain and regular arrows for hydrogen bonds involving amino acid backbone. π–π interactions are represented with green lines.