Supplementary Materials

for

In Silico Study of Inhibitory Capacity of Sacubitril/Valsartan toward Neprilysin and Angiotensin Receptor

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Table S1 The corresponding amino acid with its position in the structure of neprilysin, distance in Å between respective active cites of SAC and amino acid, its role in bond formation, and type of interaction during bond formation.

Amino acids from receptor	r (A)	Category	Type of interaction
ARG102	1.85	Hydrogen Bond	Conventional Hydrogen Bond
ARG102	1.74	Hydrogen Bond	Conventional Hydrogen Bond
ARG110	1.99	Hydrogen Bond	Conventional Hydrogen Bond
ARG110	2.22	Hydrogen Bond	Conventional Hydrogen Bond
ARG717	2.62	Hydrogen Bond	Conventional Hydrogen Bond
ARG717	1.77	Hydrogen Bond	Conventional Hydrogen Bond
ASN542	2.21	Hydrogen Bond	Conventional Hydrogen Bond
HIS711	2.92	Hydrogen Bond	Carbon Hydrogen Bond
ALA543	3.50	Hydrogen Bond	Carbon Hydrogen Bond
HIS583	2.86	Hydrogen Bond	π-Donor Hydrogen Bond
HIS587	4.19	Electrostatic	π -Cation
HIS587	4.85	Hydrophobic	π - π Stacked
HIS587	4.59	Hydrophobic	π - π T-shaped
TYR545	2.94	Other	π -Lone Pair

Table S2 The corresponding amino acid with its position in the structure of angiotensin receptor, distance in Å between respective active cites of VAL and amino acid, its role in bond formation, and type of interaction during bond formation.

Amino acids from receptor	r (A)	Category	Type of interaction
ARG167	1.93	Hydrogen Bond	Conventional Hydrogen Bond
ARG167	2.30	Hydrogen Bond	Conventional Hydrogen Bond
ARG167	3.62	Electrostatic	π -Cation
ARG167	5.26	Hydrophobic	π -Alkyl
VAL108	3.74	Electrostatic	π -Cation
VAL108	4.22	Hydrophobic	Alkyl
ALA163	3.90	Hydrophobic	π -σ
TRP84	5.63	Hydrophobic	π - π T-shaped
TRP84	4.58	Hydrophobic	π -Alkyl
TRP84	5.43	Hydrophobic	π -Alkyl
TRP84	4.46	Hydrophobic	π -Alkyl
LEU81	5.49	Hydrophobic	Alkyl
TYR35	5.18	Hydrophobic	π -Alkyl
PHE77	4.71	Hydrophobic	π -Alkyl
TYR87	4.88	Hydrophobic	π -Alkyl

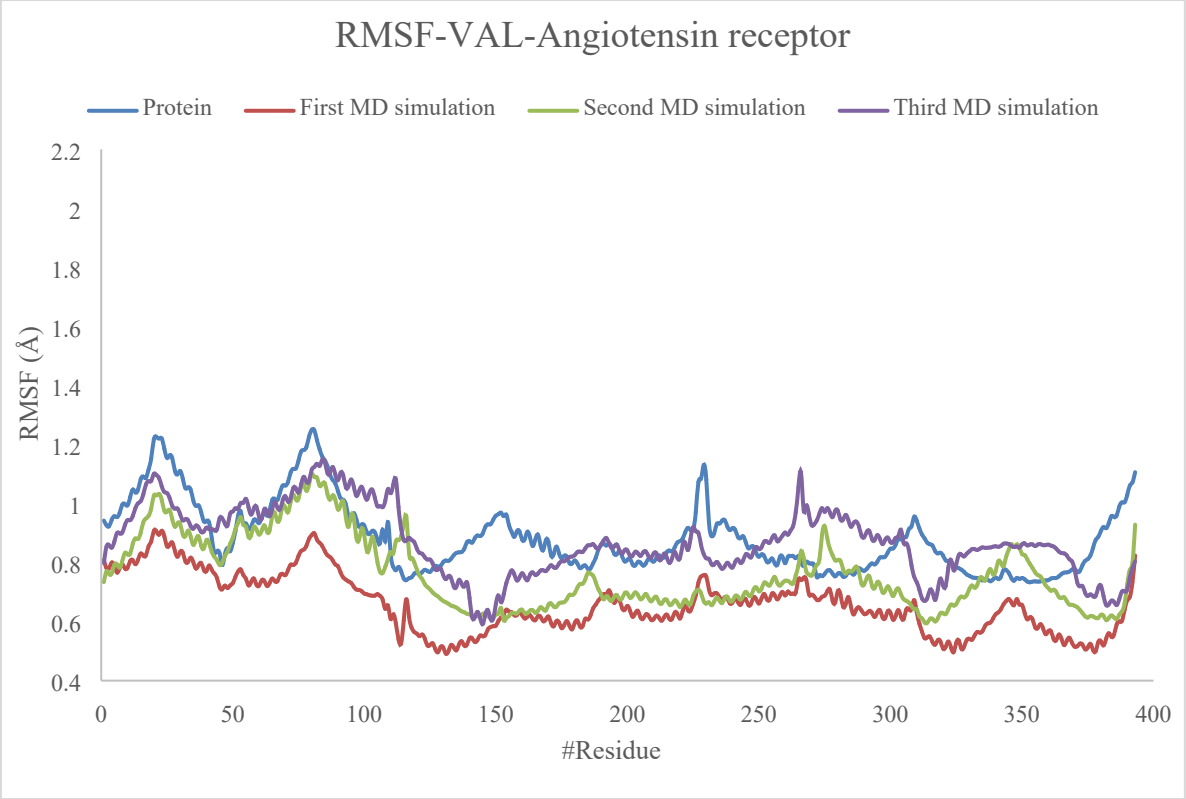

Figure S1. RMSF values obtained by MD simulations of angiotensin receptor and VAL-Angiotensin receptor complex

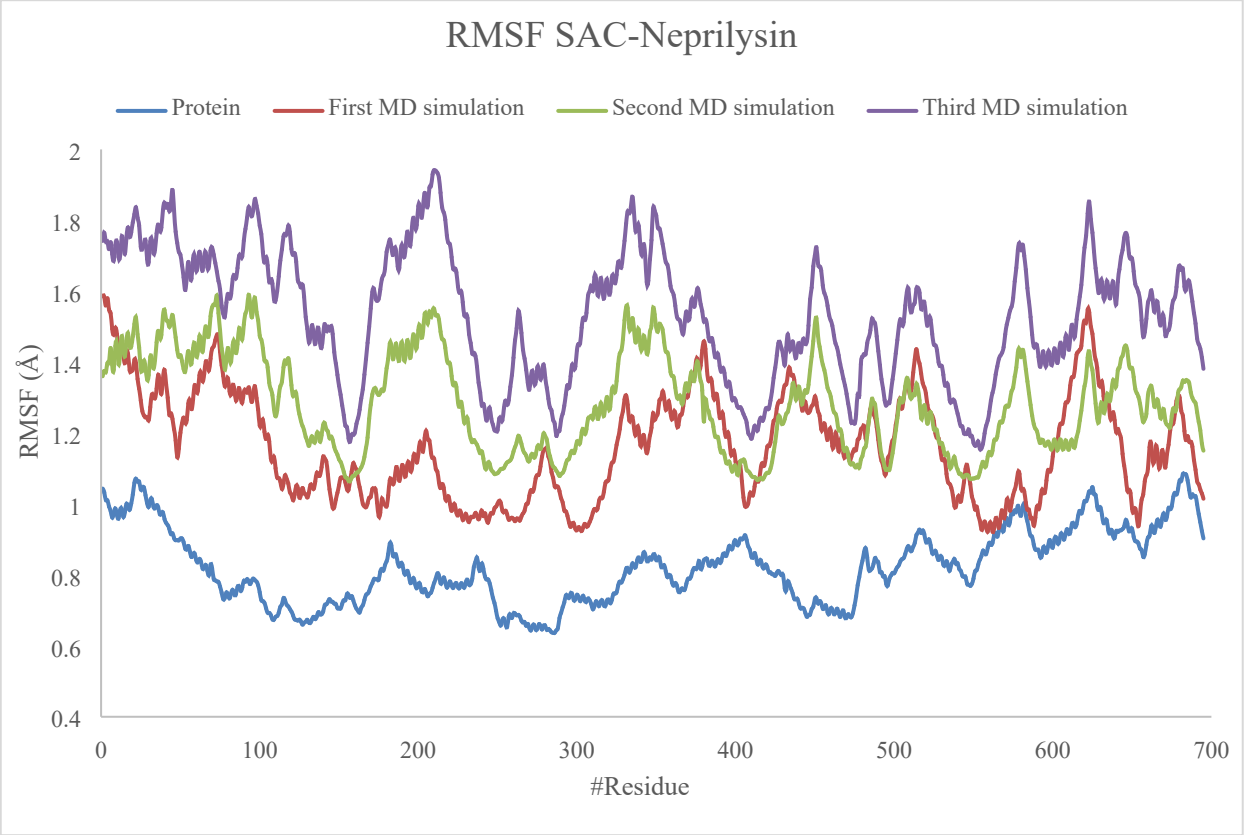

Figure S2. RMSF values obtained by MD simulations of neprilysin and SAC-Neprilysin system