

Supplementary Materials to:

# In vivo, in vitro and in silico studies on AA3266, an opioid peptide with selective cytotoxicity

By:

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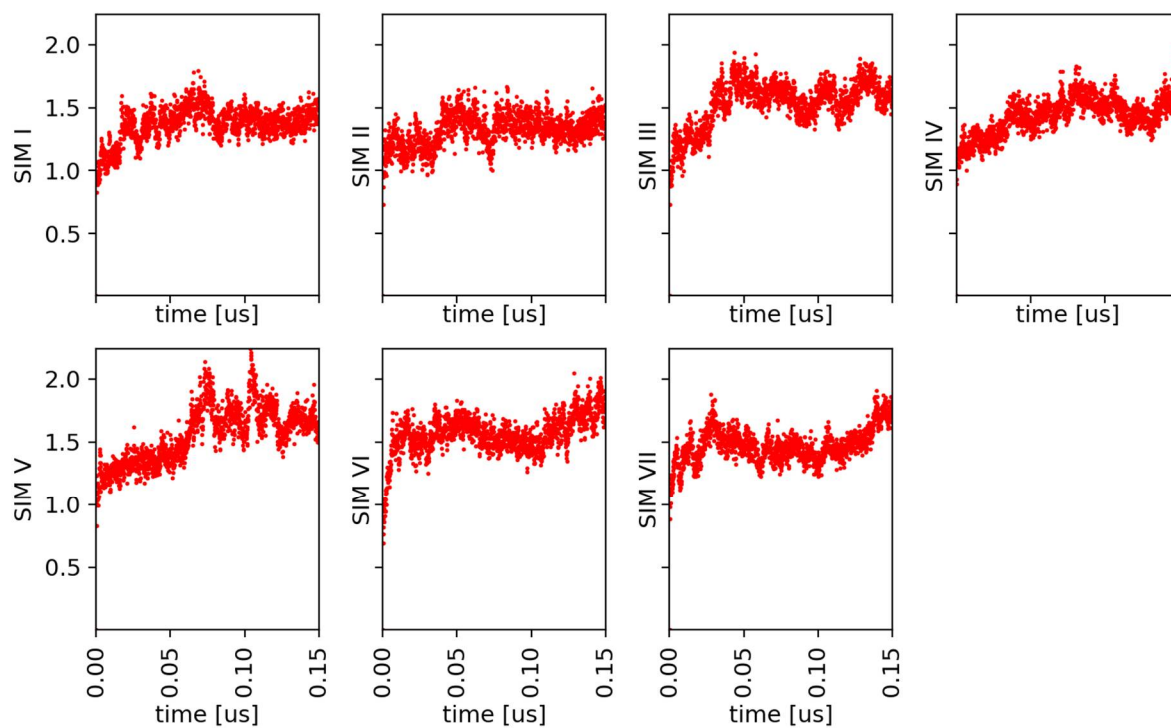
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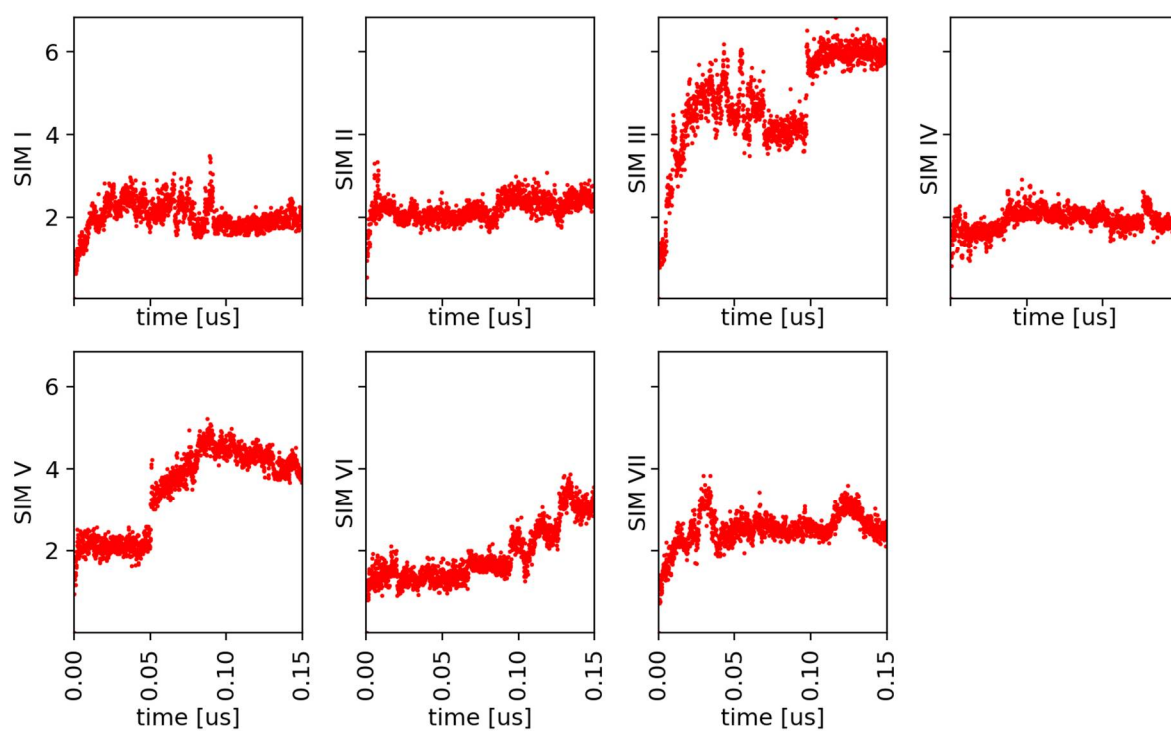
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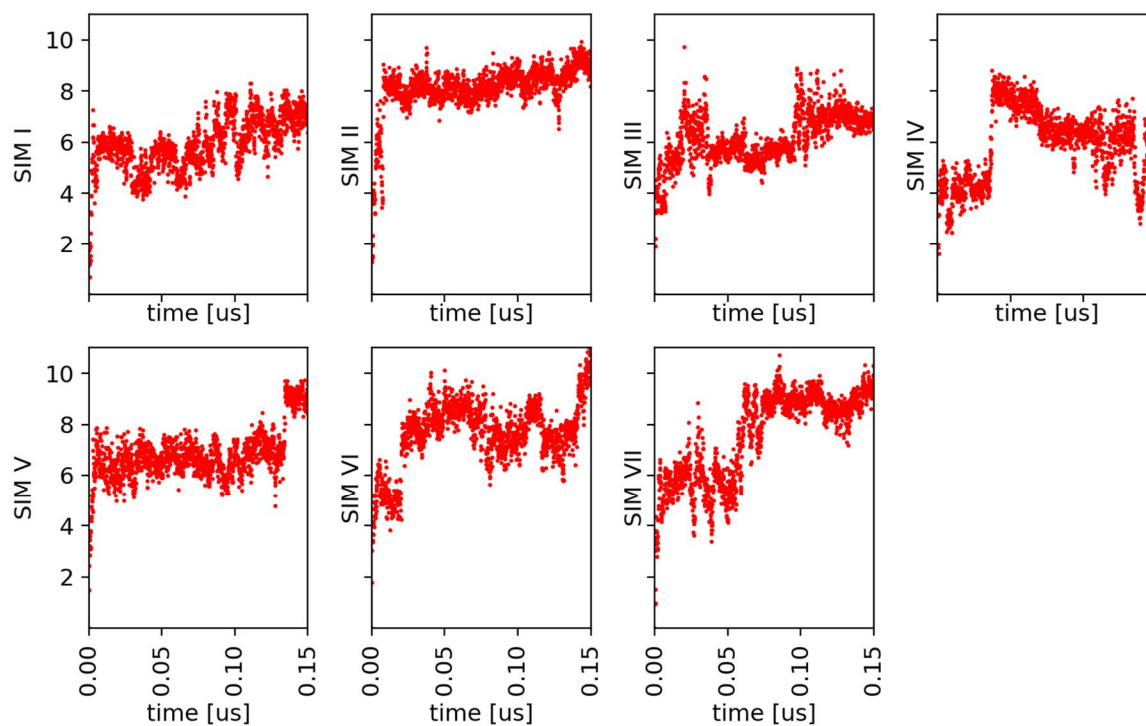
**Figure S1.** RMSD plot of the protein in the simulations of AA3266/MOR complexes.

*RMSD is given in Angstroms.*



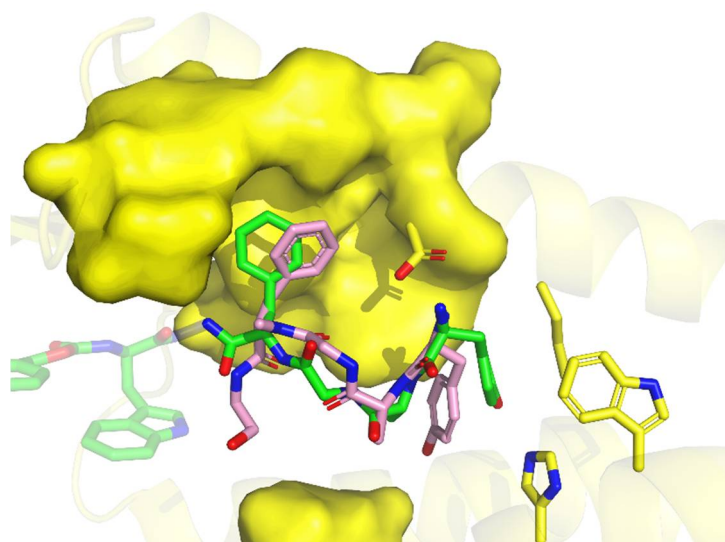
**Figure S2.** RMSD plot of the Tyr-D-Ala-Gly-Phe- fragment in the simulations of AA3266/MOR complexes.

*RMSD is given in Angstroms.*



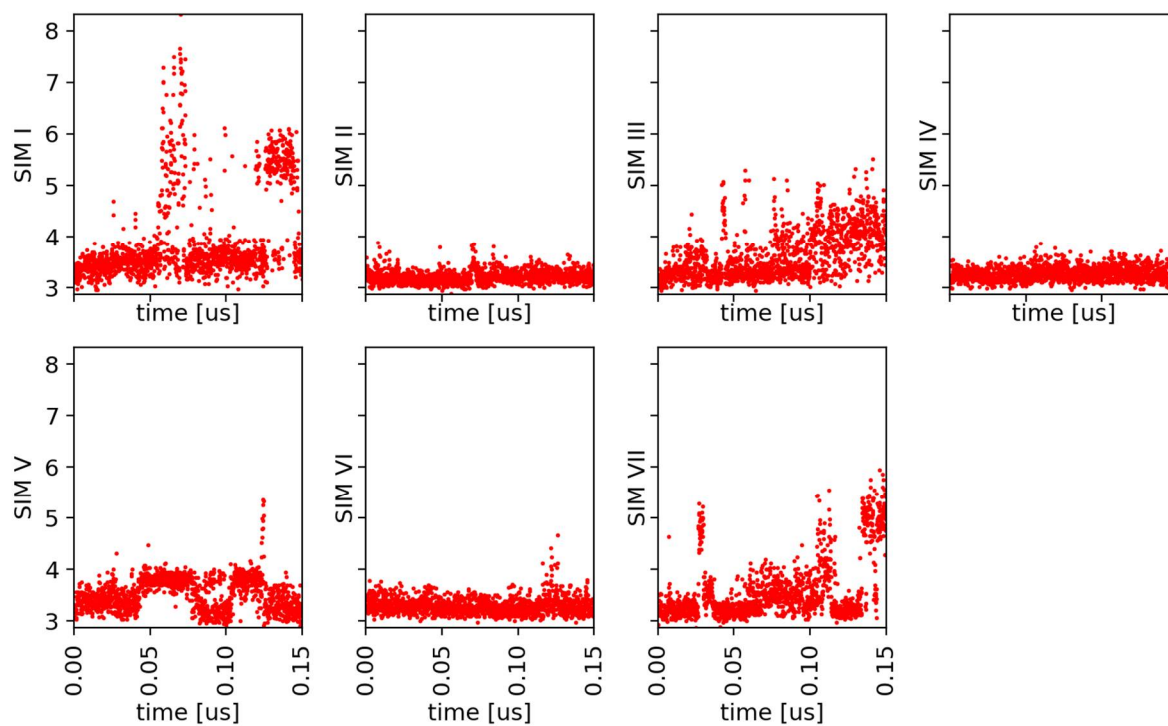
**Figure S3.** RMSD plot of the -NH-NH<-Z-D-Trp fragment in the simulations of AA3266/MOR complexes.

*RMSD is given in Angstroms.*



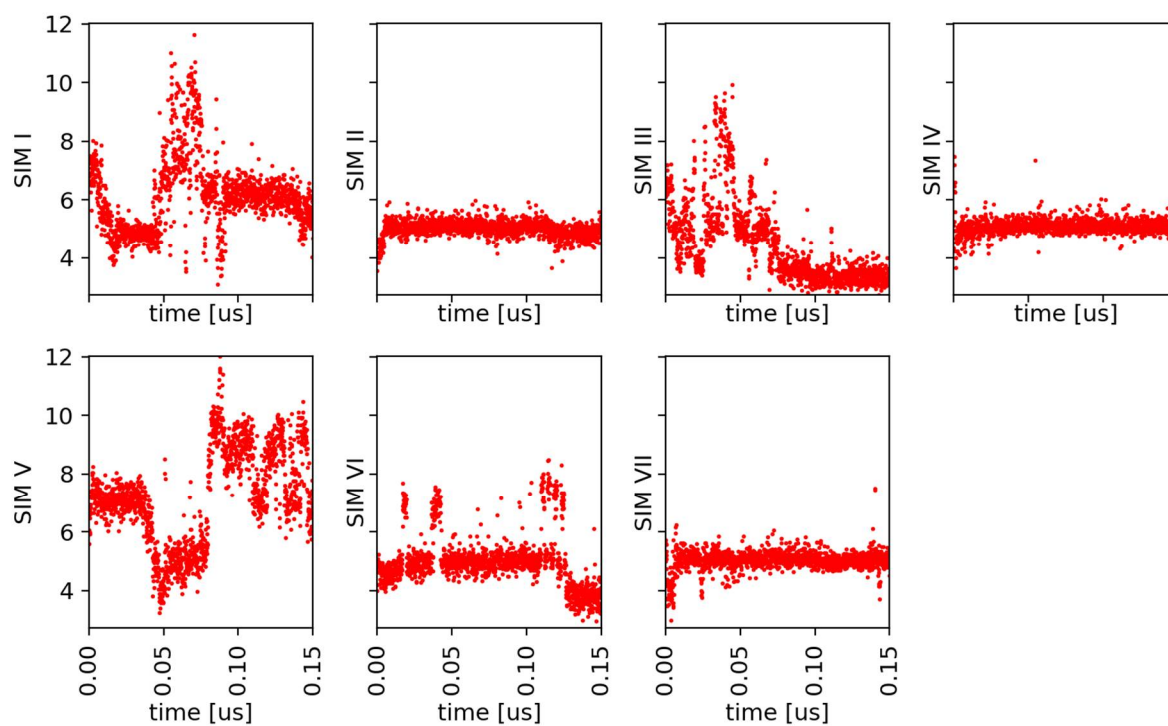
**Figure S4.** Superposition of MOR-1 binding pose and experimental position of DAMGO in 6DDF PDB structure.

*AA3266 is in green, DAMGO in pink. The receptor is shown in a simplified manner (yellow).*



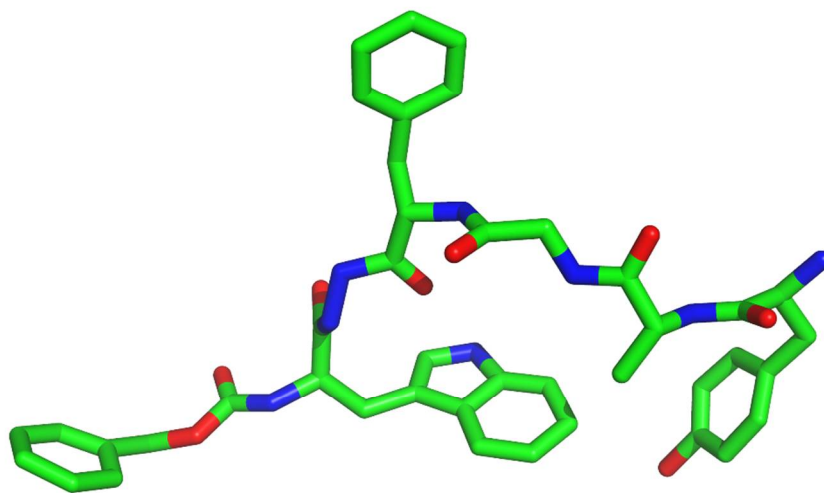
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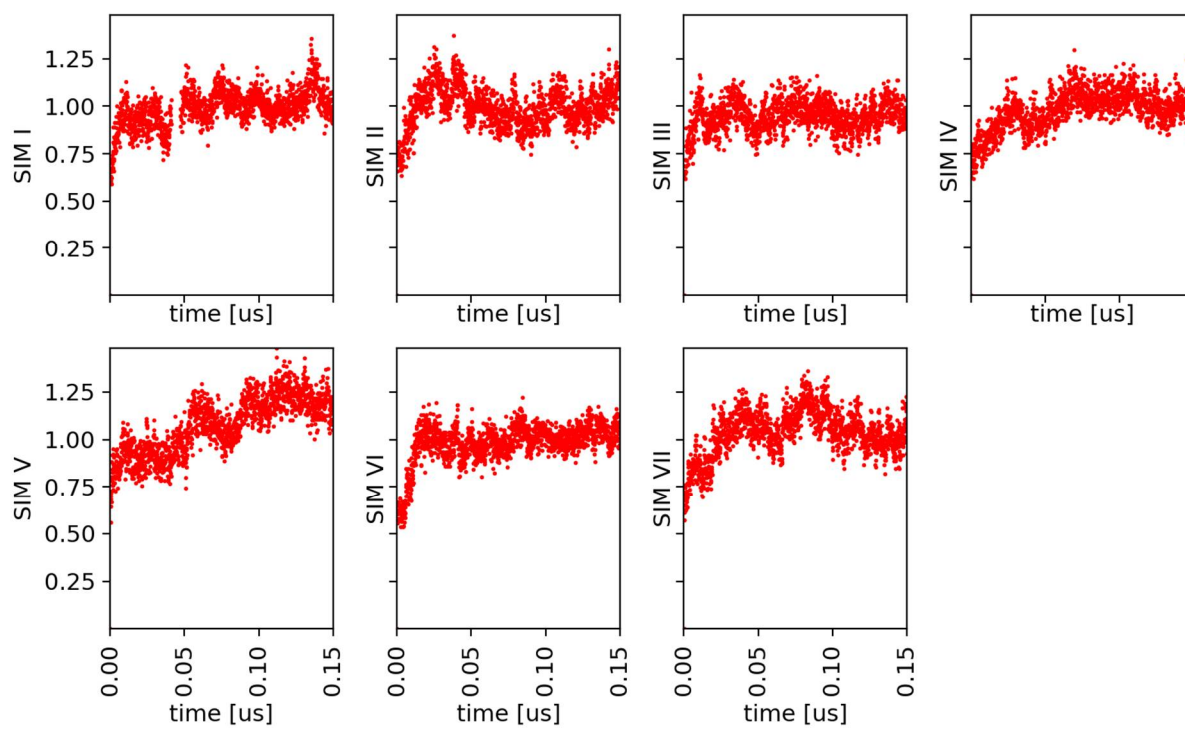


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*Distance is given in Angstroms.*

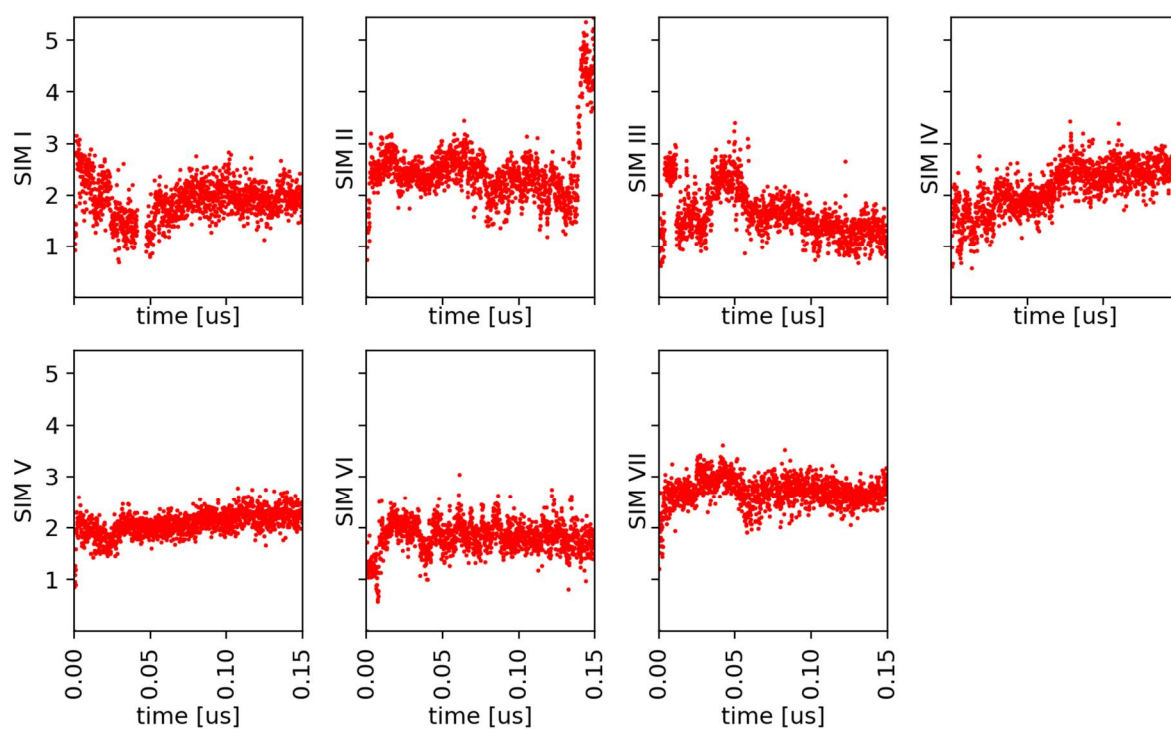


**Figure S7.** Conformation of AA3266 in **MOR-b** binding pose.



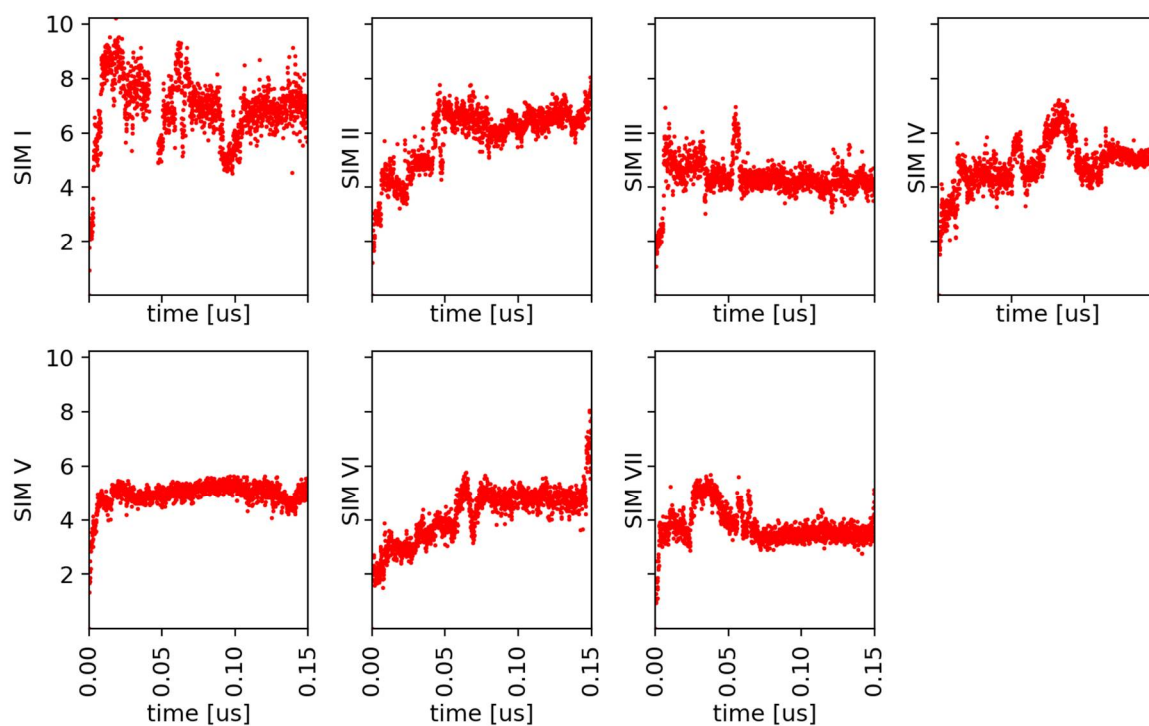
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*RMSD is given in Angstroms.*



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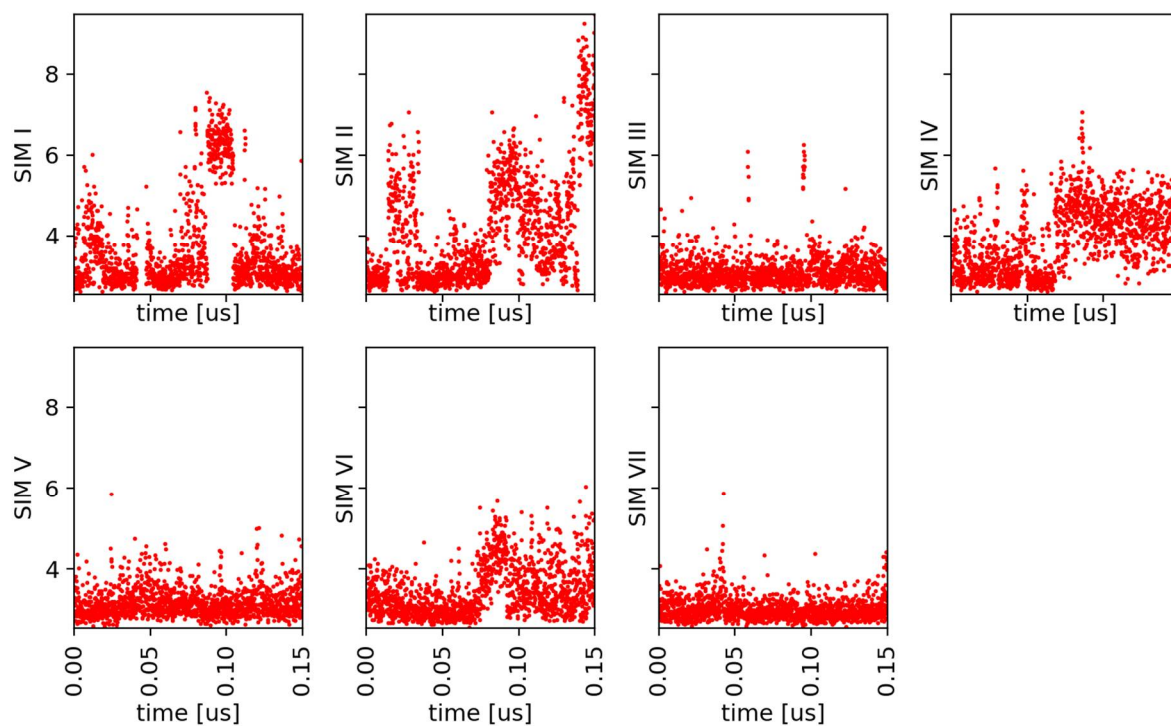
*RMSD is given in Angstroms.*



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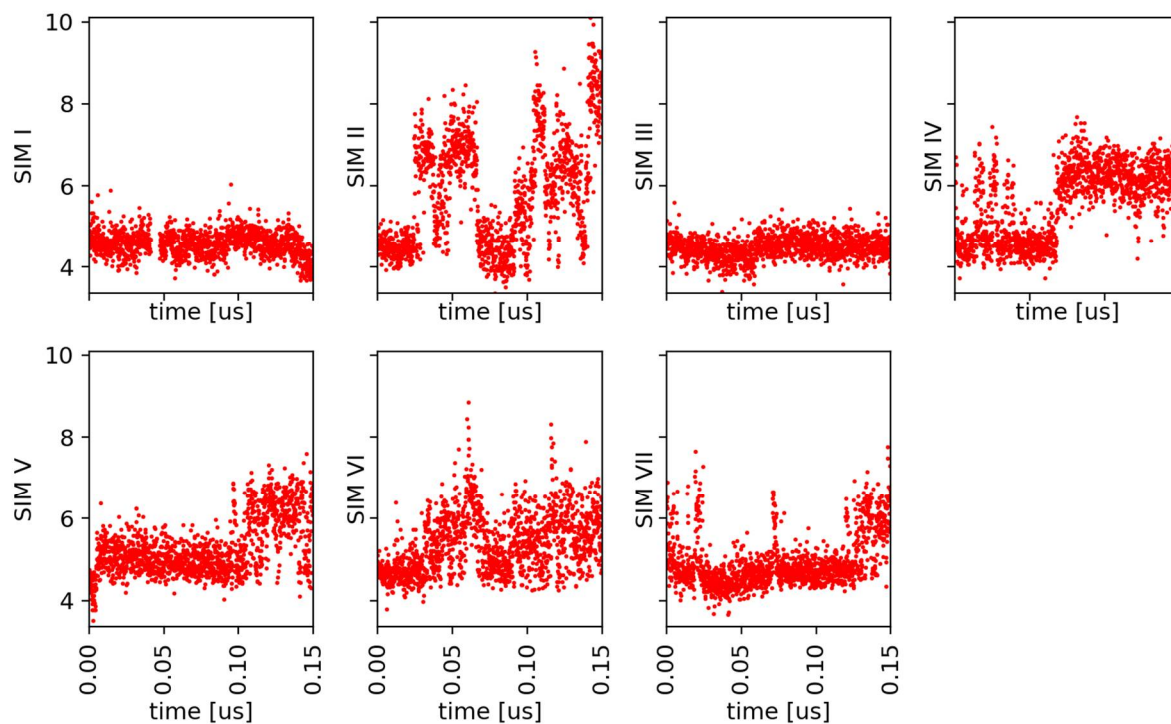
*RMSD is given in Angstroms.*





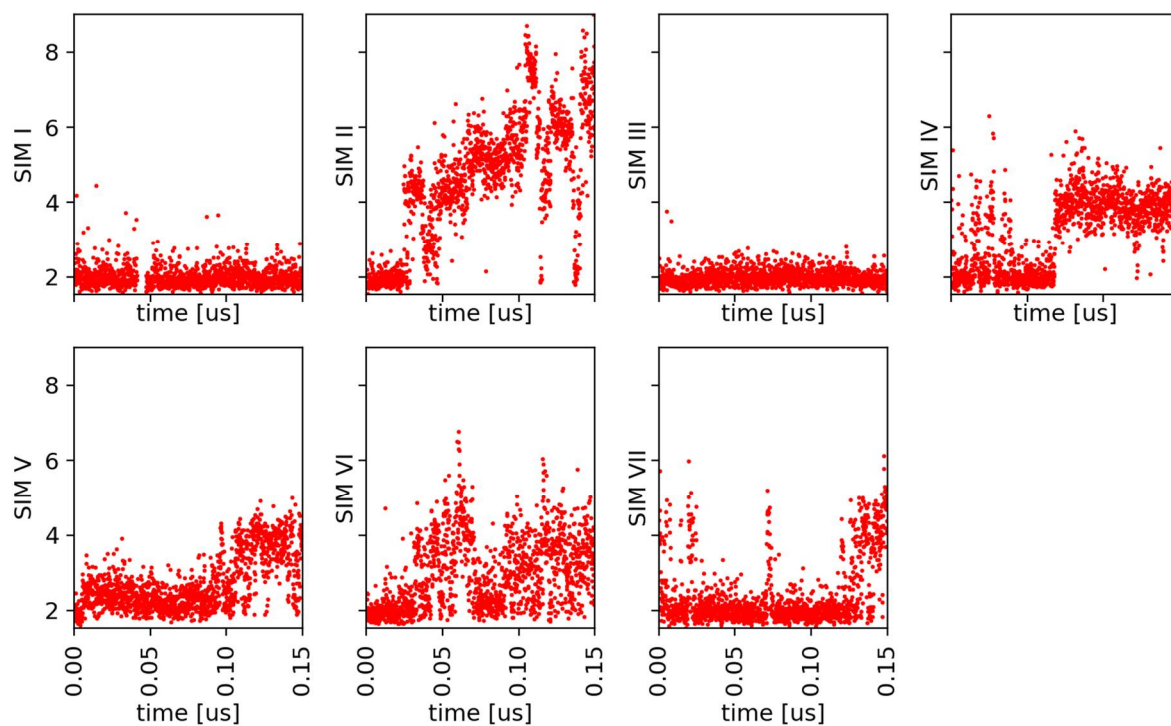
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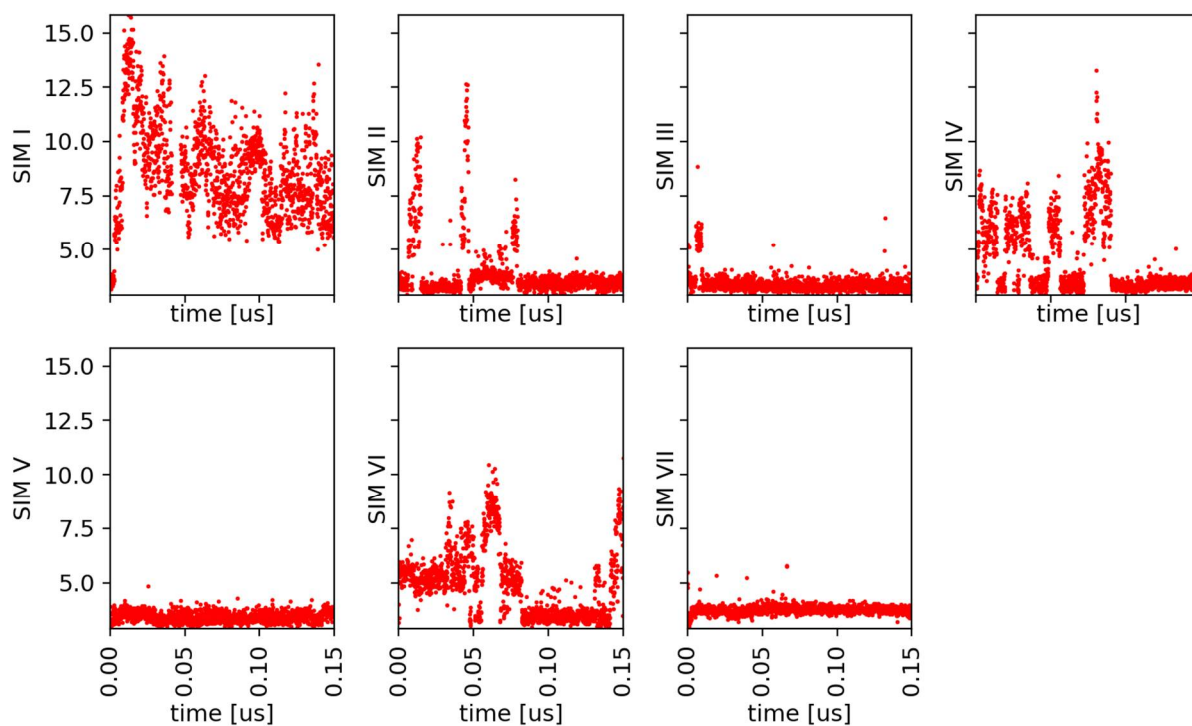
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*Distance is given in Angstroms.*



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*Distance is given in Angstroms.*



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*Distance is given in Angstroms.*