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Electronic Supporting Information (ESI): In silico study of the inhibition of SARS-COV-2 viral cell entry by neem tree extracts

Daniel M Shadrack[2†*], Said A. H. Vuai[1], Isaac Onoka[1], Mtabazi G. Sahini[1]

[1]Department of Chemistry, College of Natural and Mathematical Sciences, University of Dodoma, P.O.Box 338 Dodoma, Tanzania.

[2] Department of Chemistry, Faculty of Natural and Applied Sciences, St. John's University of Tanzania, P.O.Box 47 Dodoma, Tanzania

*Correspondence: dmshadrack@gmail.com or mshadrack@sjut.ac.tz (DMS)

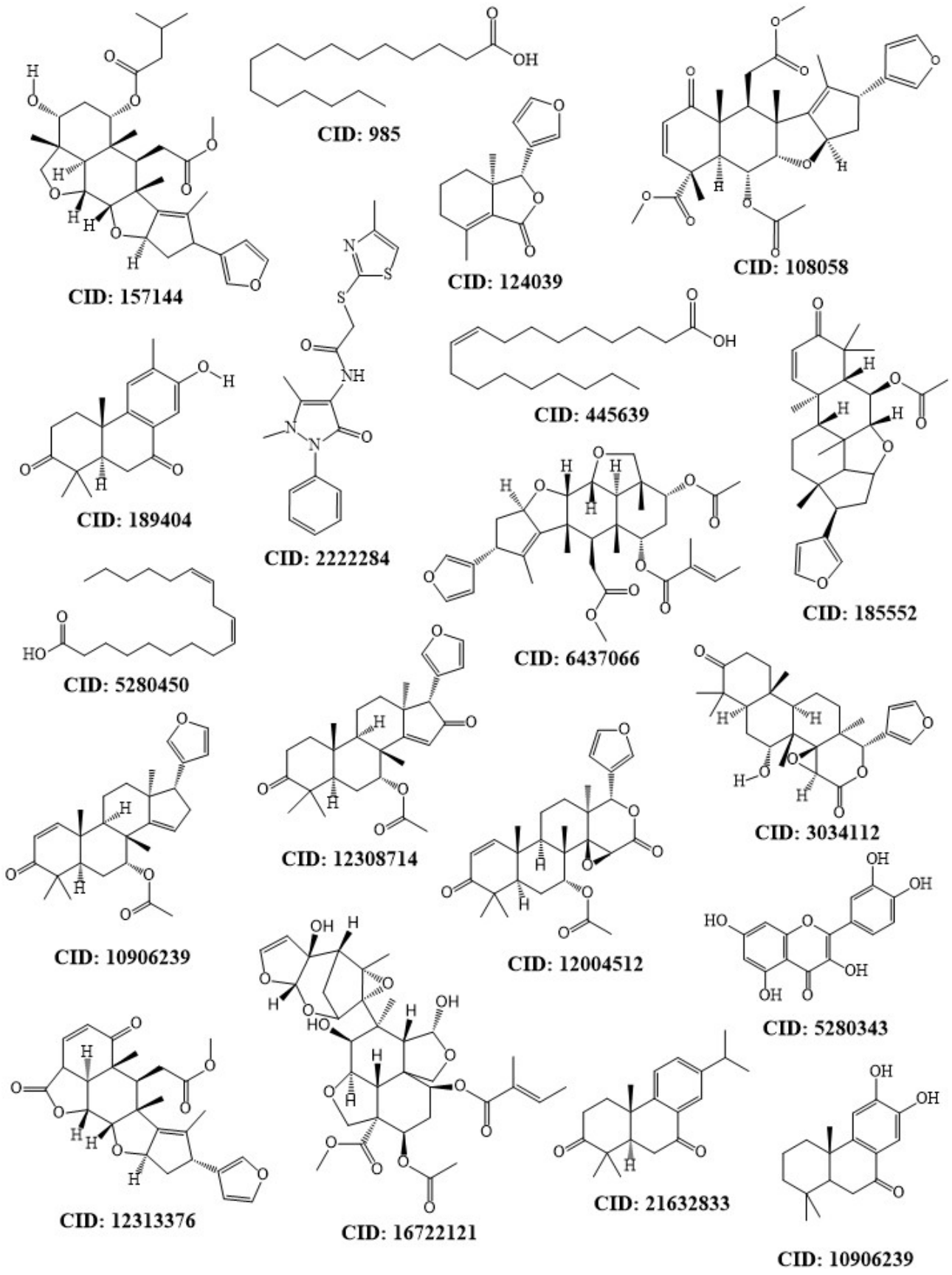
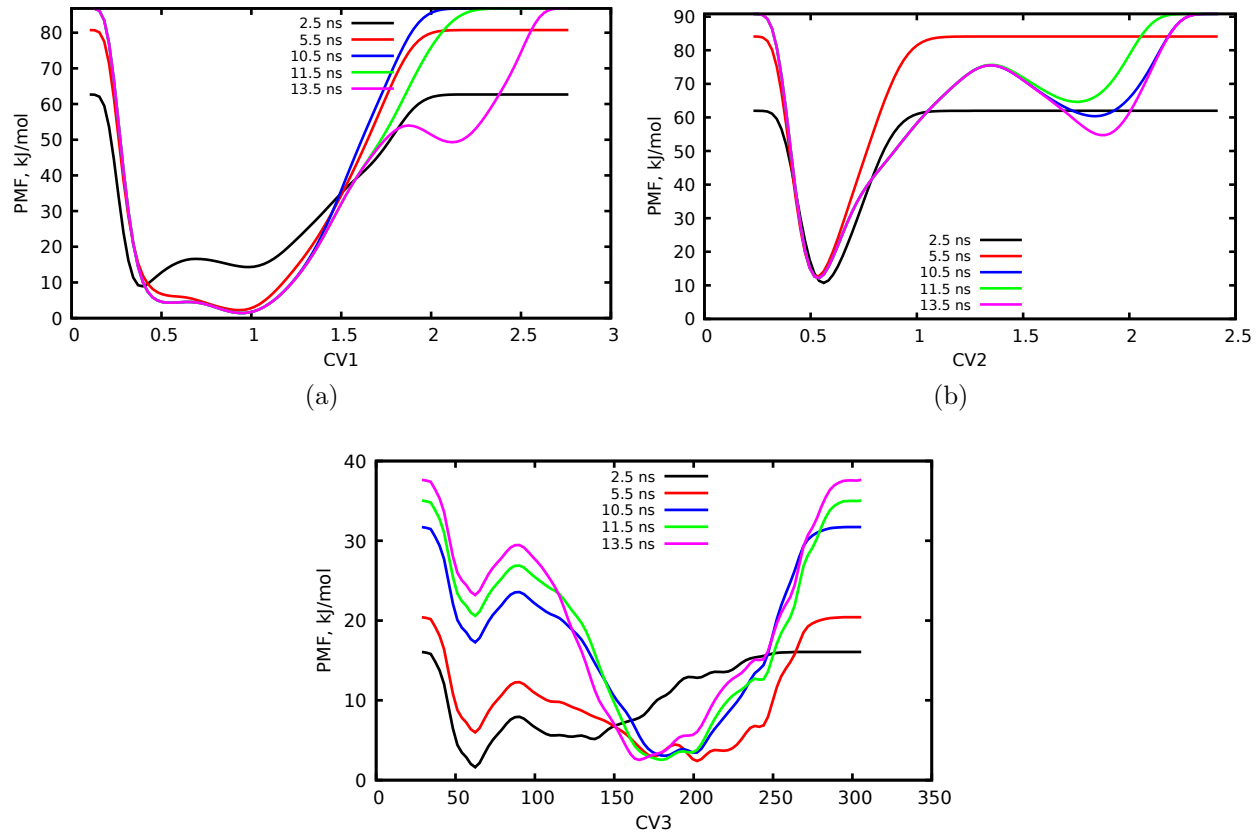
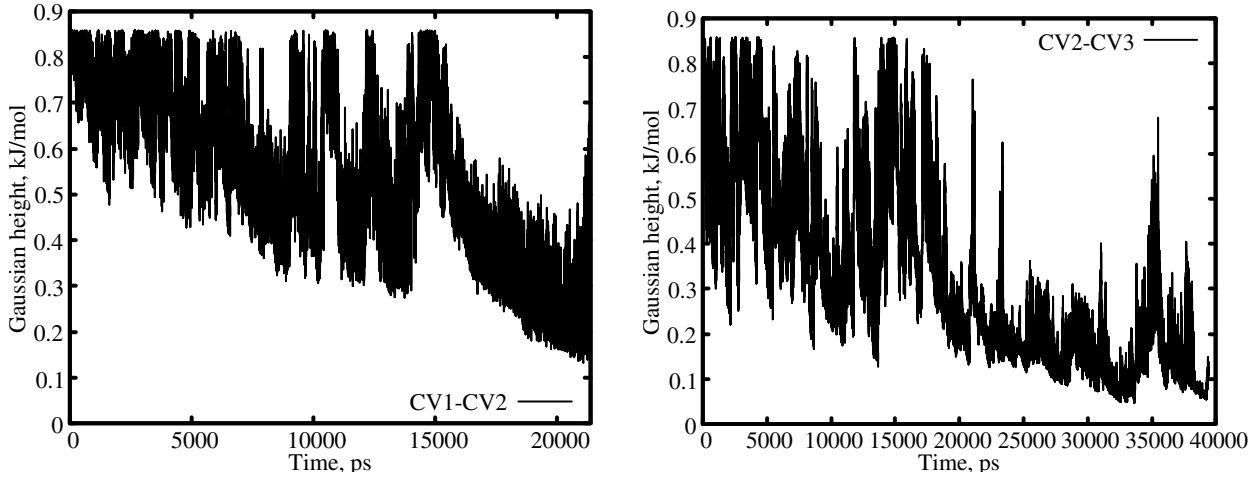


Figure S1: Chemical structure of 19 neem tree extracts used in this study.



(a) (b) (c)

Figure S2: Convergence free energies profiles for three CVs used in this study.



(a) (b)

Figure S3: Gaussian height evolution for CV1-CV2 and CV2-CV3. The systems started accumulating the bias at one local minimum, as the course of simulation time the bias added kept on growing and the Gaussian height progressively decreased. However, in the first 5 to 10 ns the systems escaped local minima and explored another phase spaces, which restored the Gaussian height to the initial value and started decreasing again. As the time progresses, the Gaussian height become smaller and the systems diffused with the entire CVs.

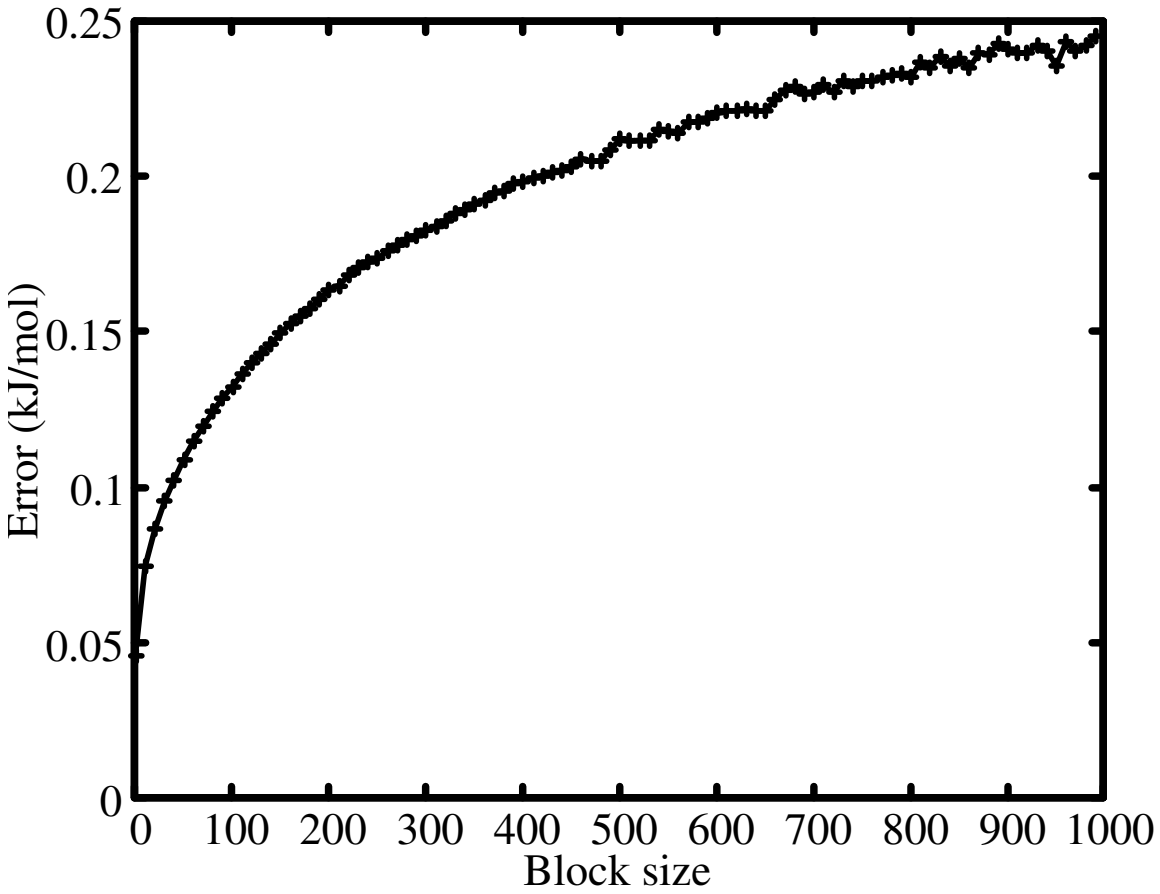


Figure S4: Block analysis of a metadynamics simulation using CV1.

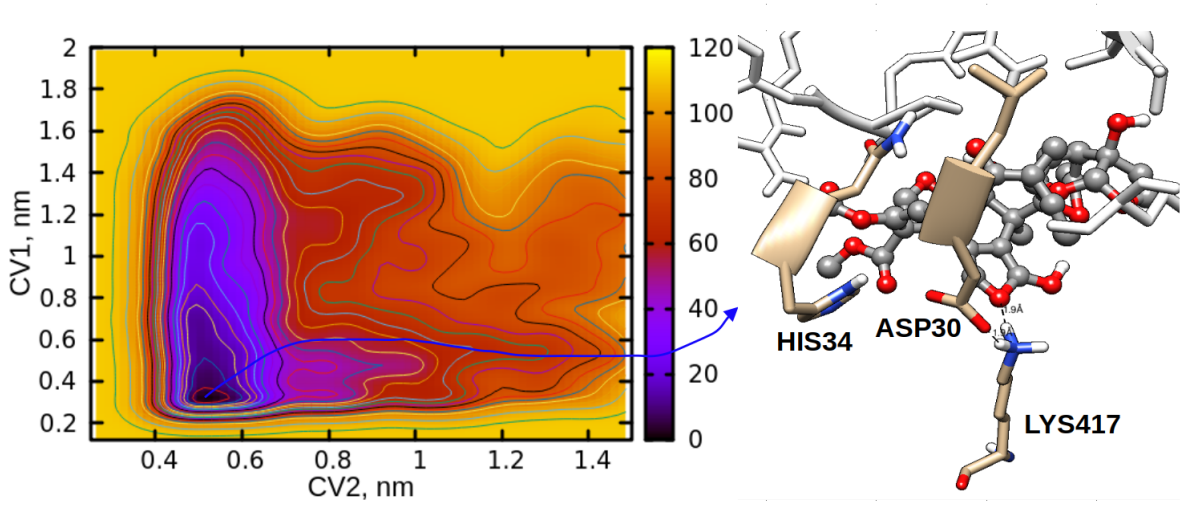


Figure S5: The interaction of azadirachtin H with residues at the spike RBD-ACE2 interface. Coordinates were taken at 0.503,0.32 for CV2 and CV1, respectively.