**Supplementary Files**

**An Integrative Reverse Vaccinology, Immunoinformatic, Docking and Simulation Approaches Towards Designing of Multi-epitopes Based Vaccine Against Monkeypox Virus**

Asad Ullah1, Farah Shahid2, Mahboob Ul Haq1, 3, Muhammad Tahir ul Qamar2, Muhammad Irfan4, Bilal Shaker5.Sajjad Ahmad1, \*, Faris Alrumaihi 6, Khaled S. Allemailem 6, Ahmad Almatroudi 6

1Department of Health and Biological Sciences, Abasyn University, Peshawar 25000, Pakistan

[asad.ullah@abasyn.edu.pk](mailto:asad.ullah@abasyn.edu.pk), [mahboob.haq@abasyn.edu.pk](mailto:mahboob.haq@abasyn.edu.pk). [sajjad.ahmad@abasyn.edu.pk](mailto:sajjad.ahmad@abasyn.edu.pk)

2Department of Bioinformatics and Biotechnology, Government College University Faisalabad, Faisalabad 38000, Pakistan; [farah.shahid.209@gmail.com](mailto:farah.shahid.209@gmail.com) (F.S.); [tahirulqamar@gcuf.edu.pk](mailto:tahirulqamar@gcuf.edu.pk) (M.T.Q.)

3Department of Pharmacy, Abasyn University, Peshawar 25000, Pakistan.

4Department of Oral Biology, College of Dentistry, University of Florida, Gainesville, FL 32611, USA.[irfanmuhammad@ufl.edu](mailto:irfanmuhammad@ufl.edu).

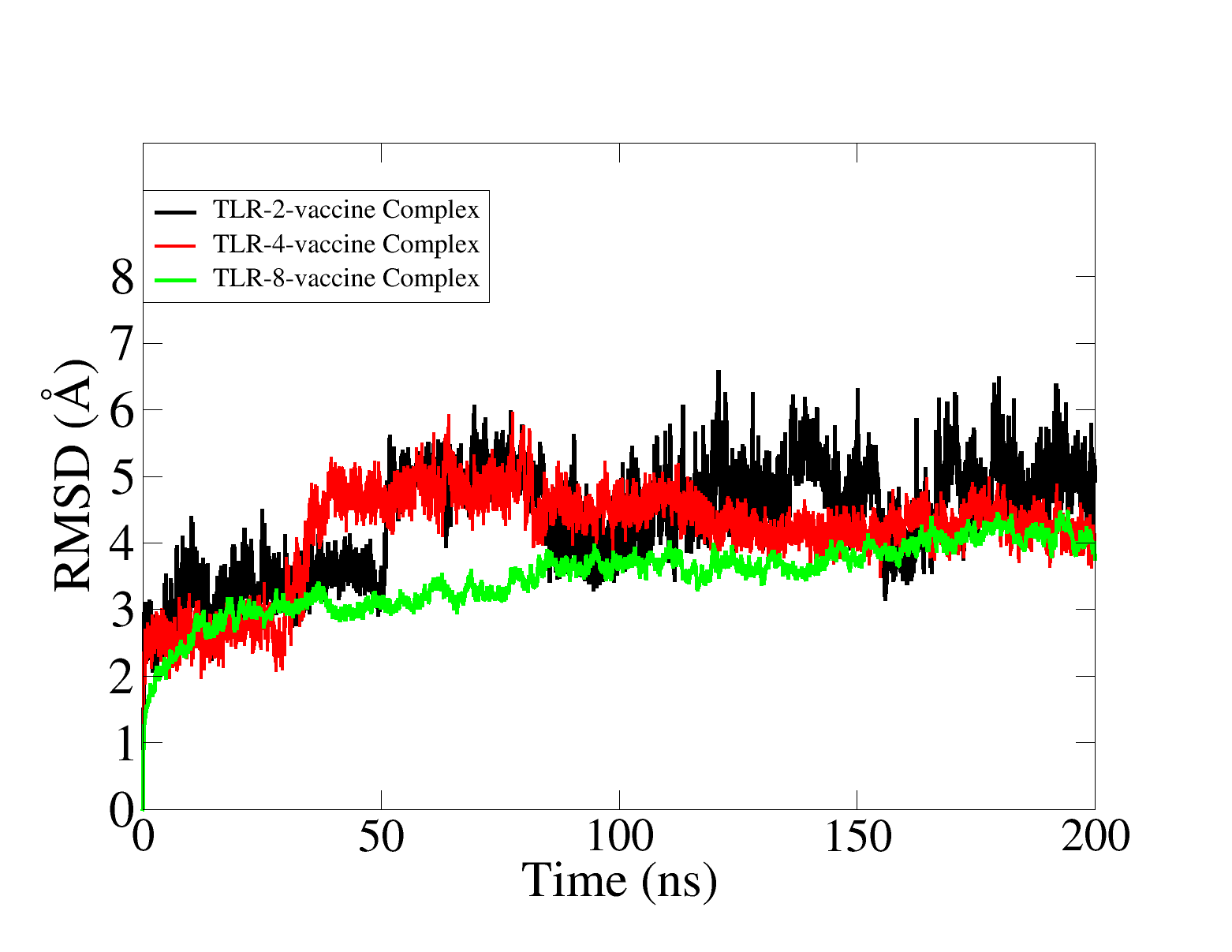
5Department of biomedical engineering, Chung-Ang University, Seoul, South Korea. [Ch.bilal321@outlook.com](mailto:Ch.bilal321@outlook.com).

6 Department of Medical Laboratories, College of Applied Medical Sciences, Qassim University, Buraydah 51452, Saudi Arabia; [f\_alrumaihi@qu.edu.sa](mailto:f_alrumaihi@qu.edu.sa) (F.A.); [k.allemailem@qu.edu.sa](mailto:k.allemailem@qu.edu.sa) (K.S.A.); [aamtrody@qu.edu.sa](mailto:aamtrody@qu.edu.sa) (A.A.)

\*Correspondence author: [sajjad.ahmad@abasyn.edu.pk](mailto:sajjad.ahmad@abasyn.edu.pk)

**Table S1.** Accession no of proteomes used in the study.

|  |  |
| --- | --- |
| **Serial number** | **Accession number** |
| 1 | ASM645832v1\_protein |
| 2 | ASM645838v1\_protein |
| 3 | ASM645866v1\_protein |
| 4 | ASM645886v1\_protein |
| 5 | ASM645888v1\_protein |
| 6 | ASM646512v1\_protein |
| 7 | ASM646514v1\_protein |
| 8 | ASM646516v1\_protein |
| 9 | ASM646526v1\_protein |
| 10 | ASM646528v1\_protein |
| 11 | ASM646530v1\_protein |
| 12 | ASM646536v1\_protein |
| 13 | ASM646542v1\_protein |
| 14 | ASM646570v1\_protein |
| 15 | ASM646572v1\_protein |
| 16 | ASM646574v1\_protein |
| 17 | ASM646582v1\_protein |
| 18 | ASM646584v1\_protein |
| 19 | ASM646590v1\_protein |
| 20 | ASM647196v1\_protein |
| 21 | ASM1433735v1\_protein |
| 22 | ASM1433736v1\_protein |
| 23 | ASM1433737v1\_protein |
| 24 | ASM1433738v1\_protein |
| 25 | ASM1433738v1\_protein |
| 26 | ASM1433739v1\_protein |
| 27 | ASM1433740v1\_protein |
| 28 | ASM1433741v1\_protein |
| 28 | ASM1433742v1\_protein |
| 30 | ASM1433743v1\_protein |
| 31 | ASM1433743v1\_protein |
| 32 | ASM1433744v1\_protein |
| 33 | ASM1462154v1\_protein |
| 34 | ASM1462155v1\_protein |
| 35 | ASM1462155v1\_protein |
| 36 | ASM1462157v1\_protein |
| 37 | ASM1462158v1\_protein |
| 38 | ASM1462159v1\_protein |
| 39 | ASM646592v1\_protein |



**S-Fig.1.** Duplicate simulation of complexes using different initial velocity.