

Supplementary Information

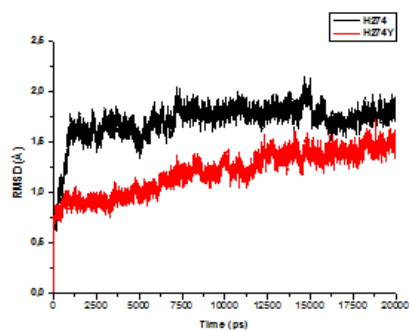
Understanding the Cross-resistance of oseltamivir to H1N1 and H5N1 Influenza A neuraminidase mutations using multi-dimensional computational analyses

Ashona Singh^a and Mahmoud E. Soliman^{a*}

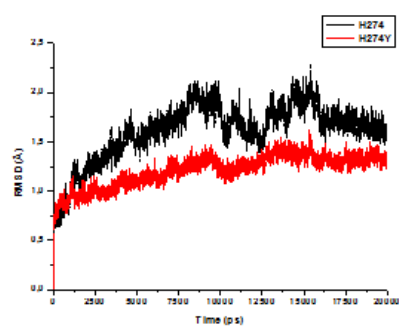
^a School of Health Sciences, University of KwaZulu-Natal, Westville, Durban 4000, South Africa

* Corresponding author: Mahmoud E. Soliman, email: soliman@ukzn.ac.za

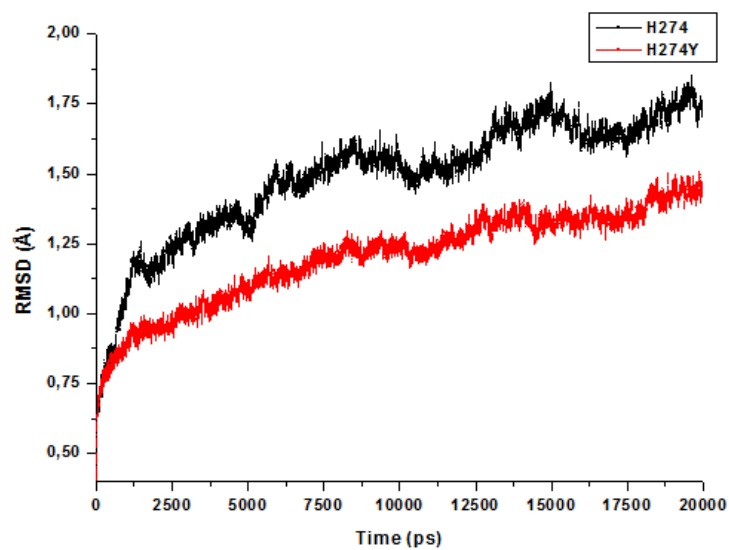
Telephone: +27 31 260 7413, Fax: +27 31 260 7413



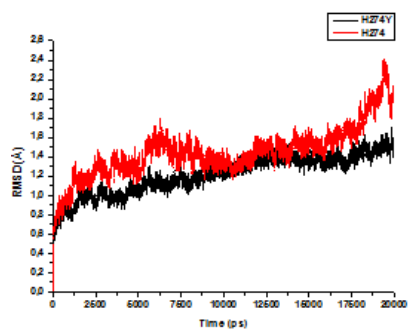
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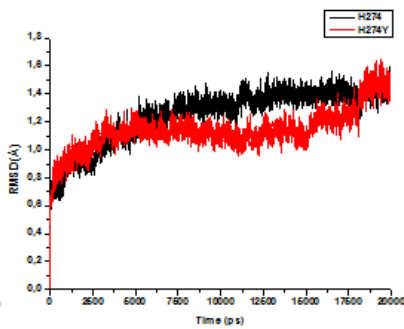
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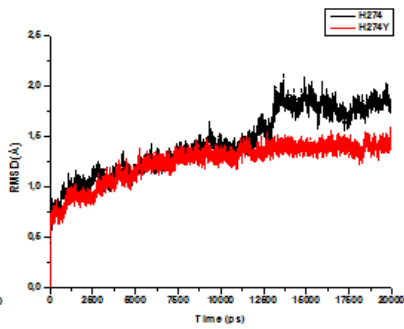
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T3

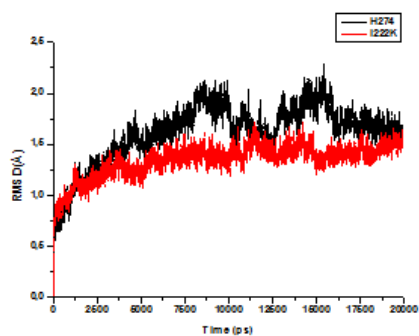


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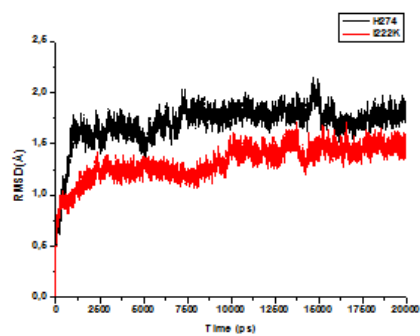


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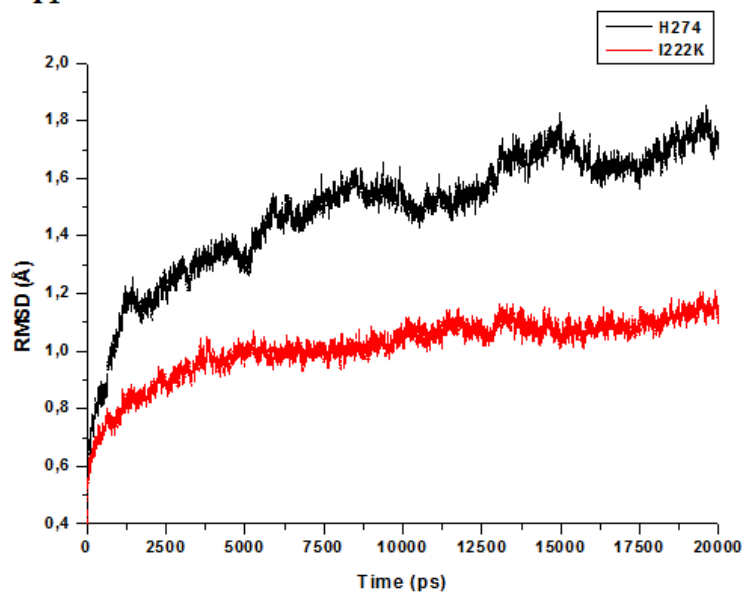
S1: RMSD of WT_{H5N1} and H274Y_{H5N1} over 20 ns



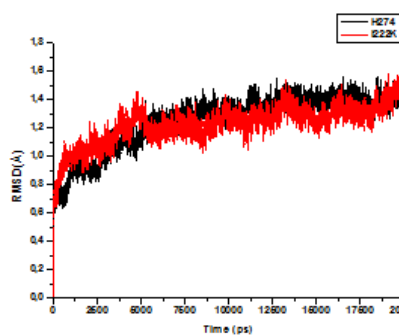
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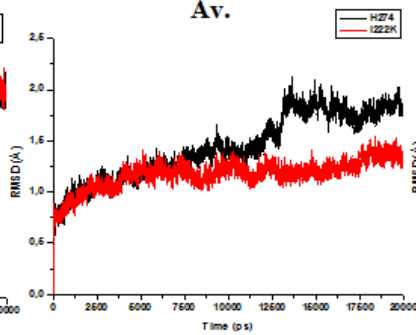
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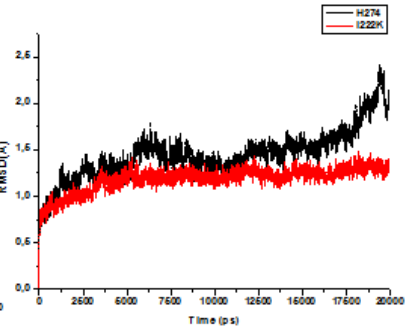
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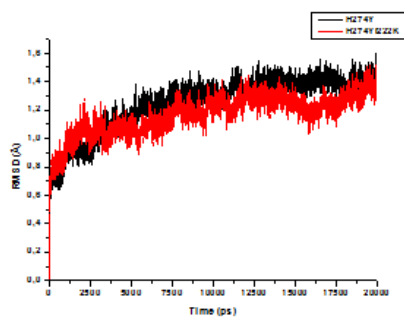


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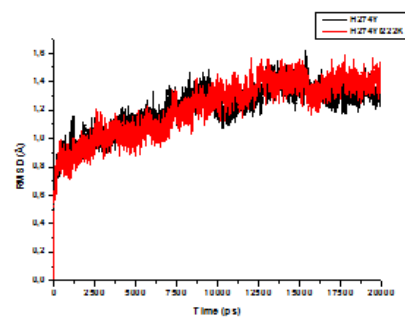


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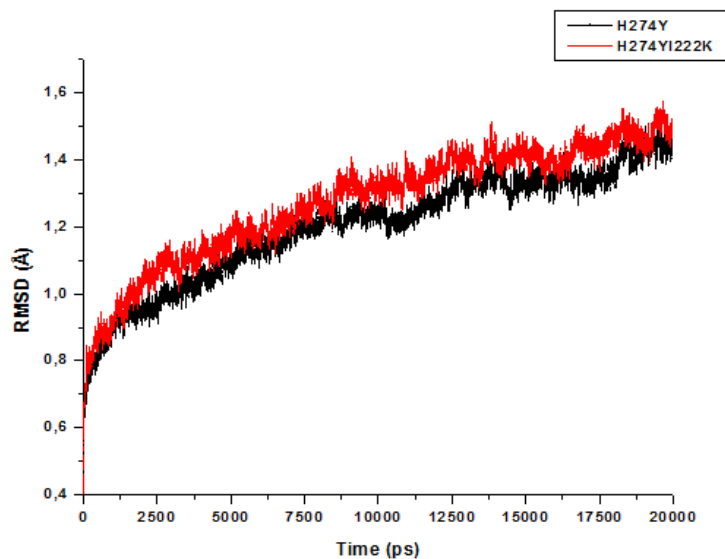
S2: RMSD of WT_{H5N1} and I222K_{H5N1} over 20 ns



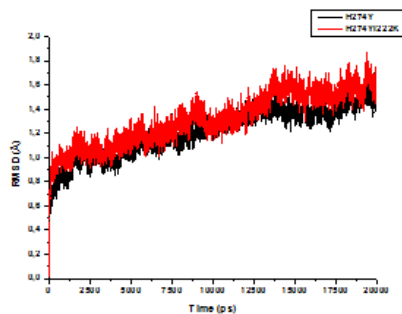
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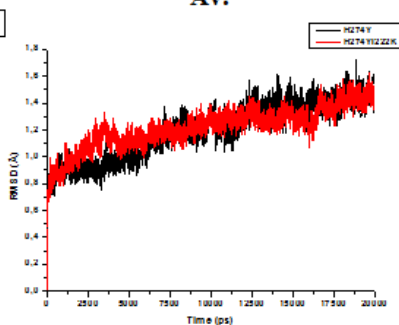
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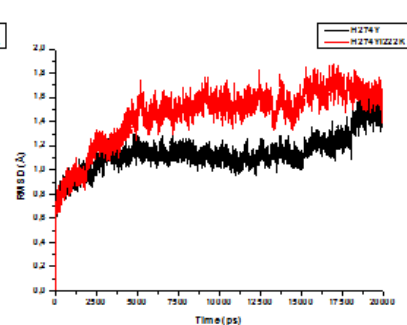
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T3

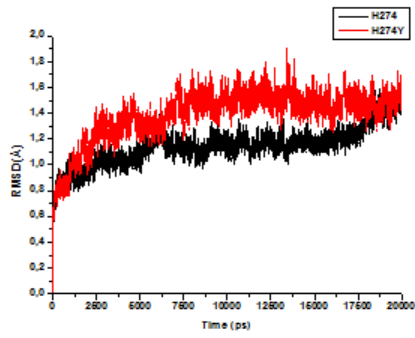


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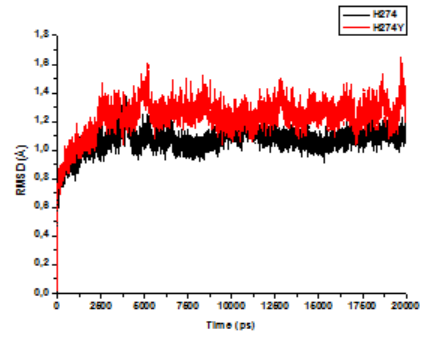


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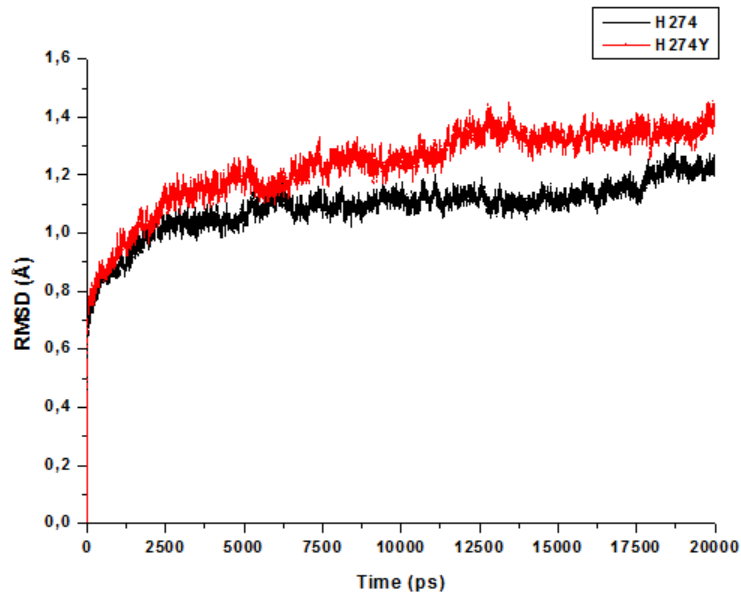
S3: RMSD of H274Y_{H5N1} and H274Y-I222K_{H5N1} over 20 ns



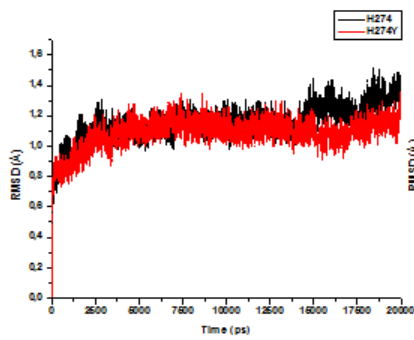
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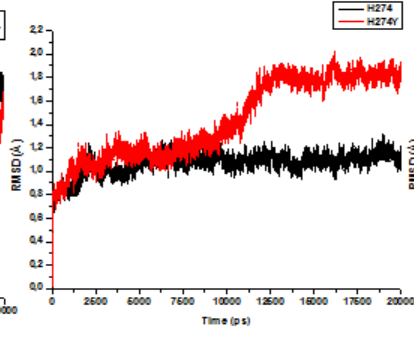
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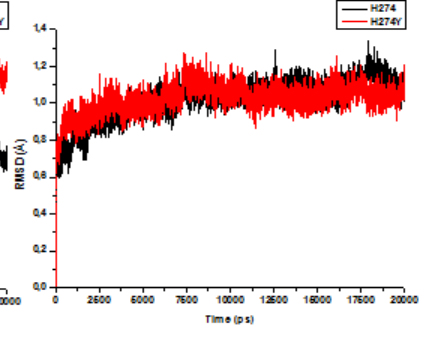
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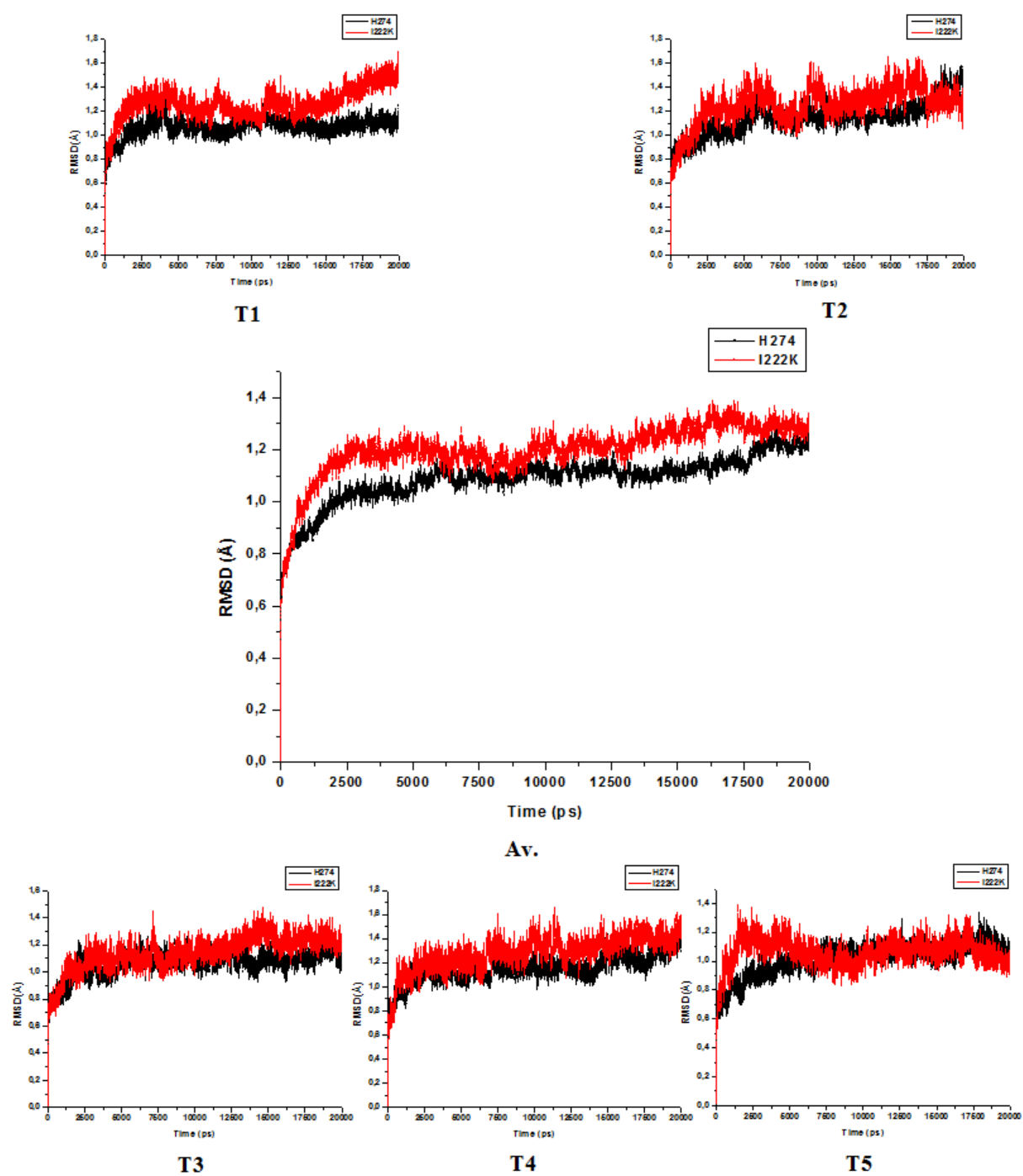


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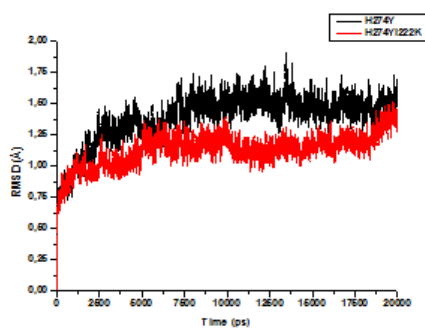


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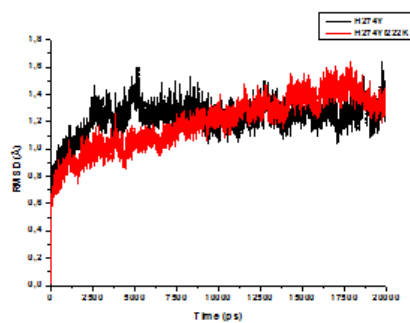
S4: RMSD of WT_{HINI} and H274Y_{HINI} over 20 ns



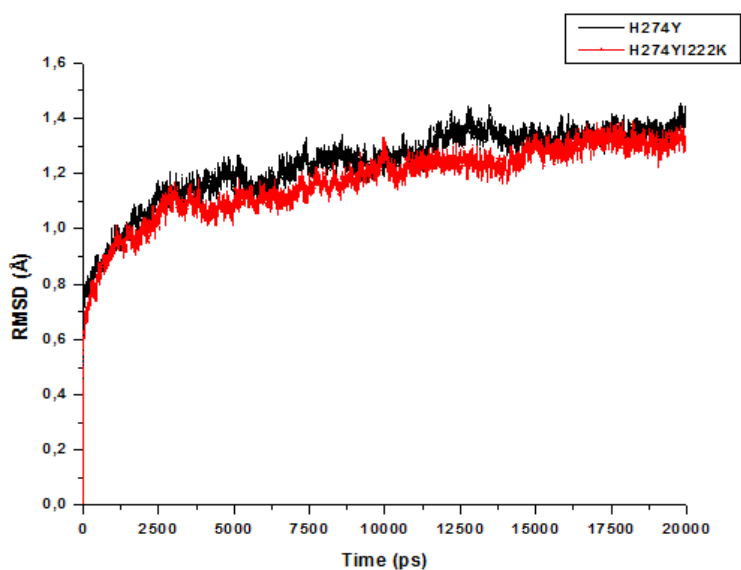
S5: RMSD of WT_{H1N1} and I222K_{H1N1} over 20 ns



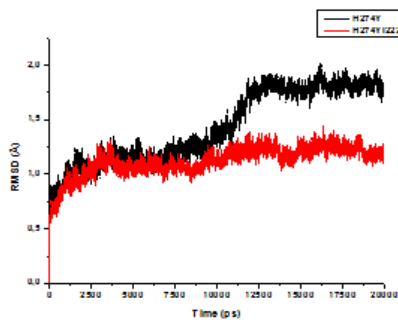
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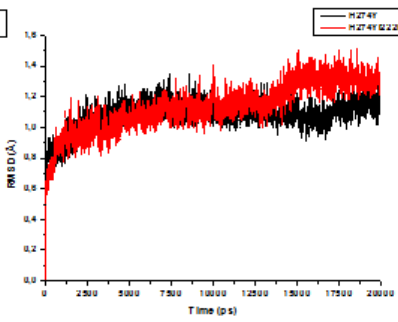
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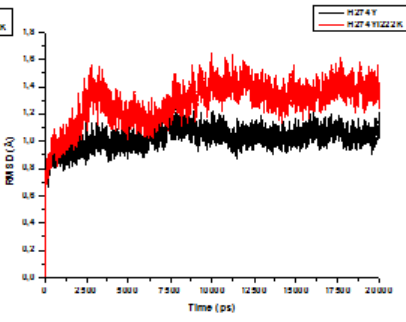
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T3

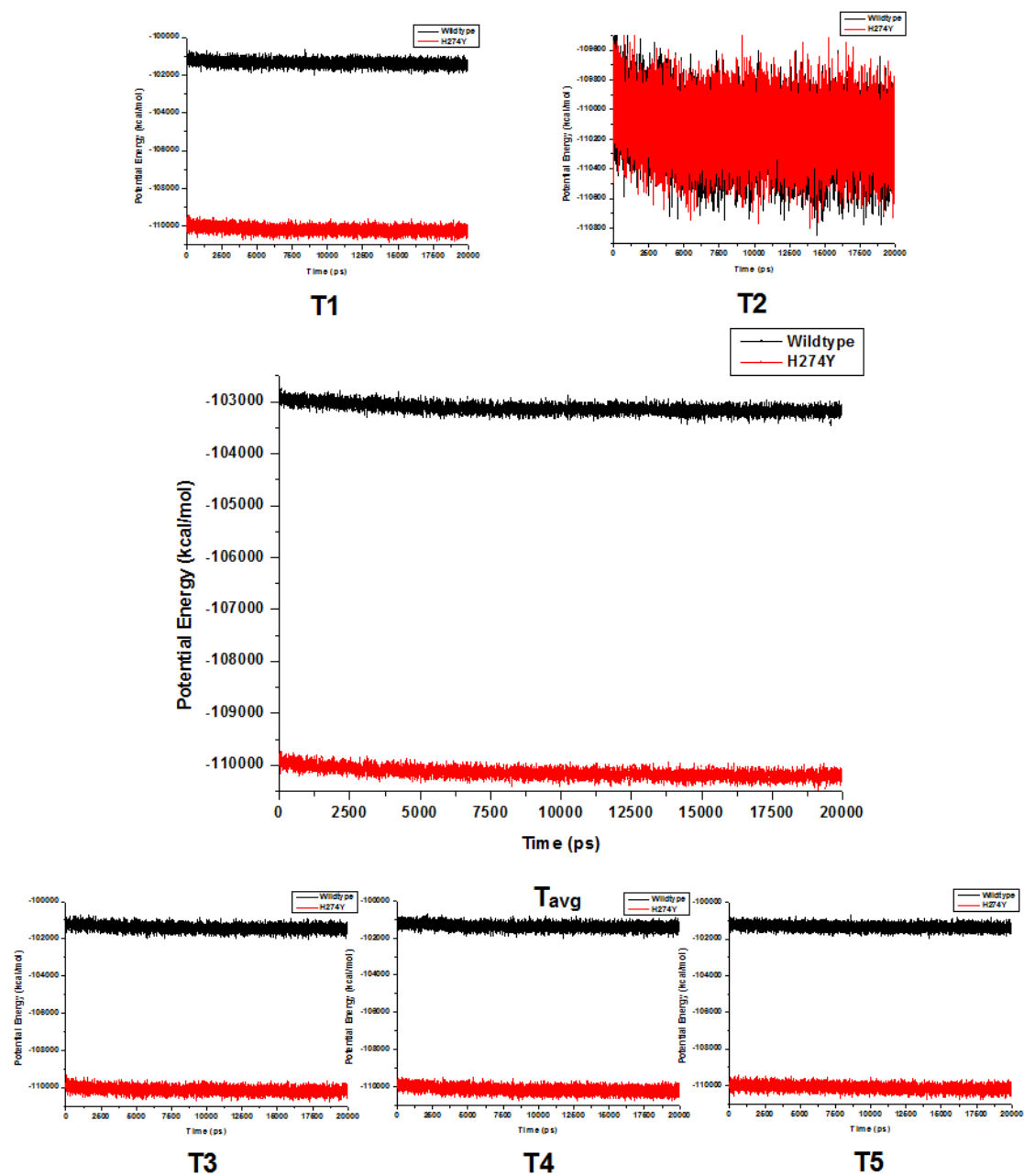


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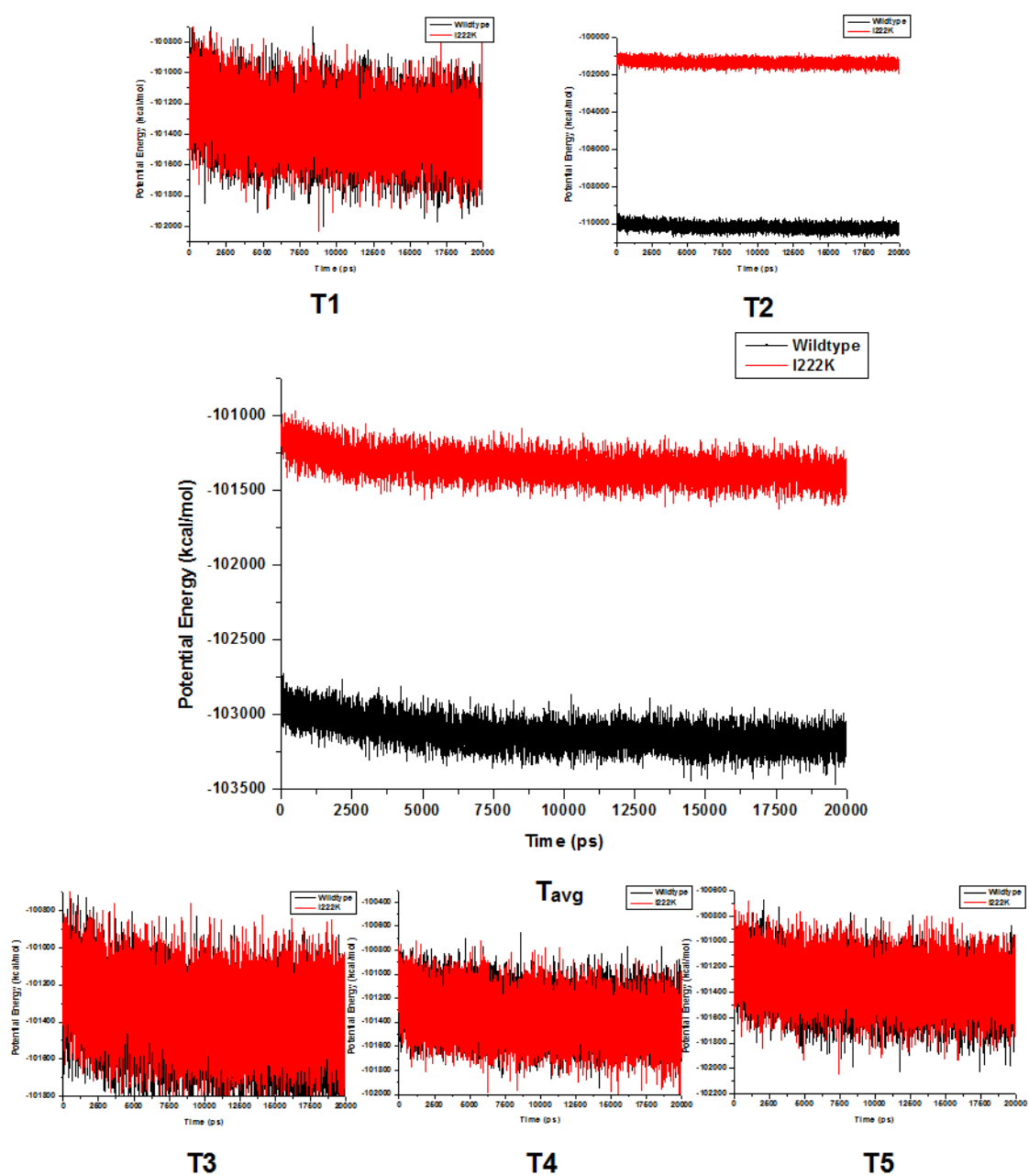


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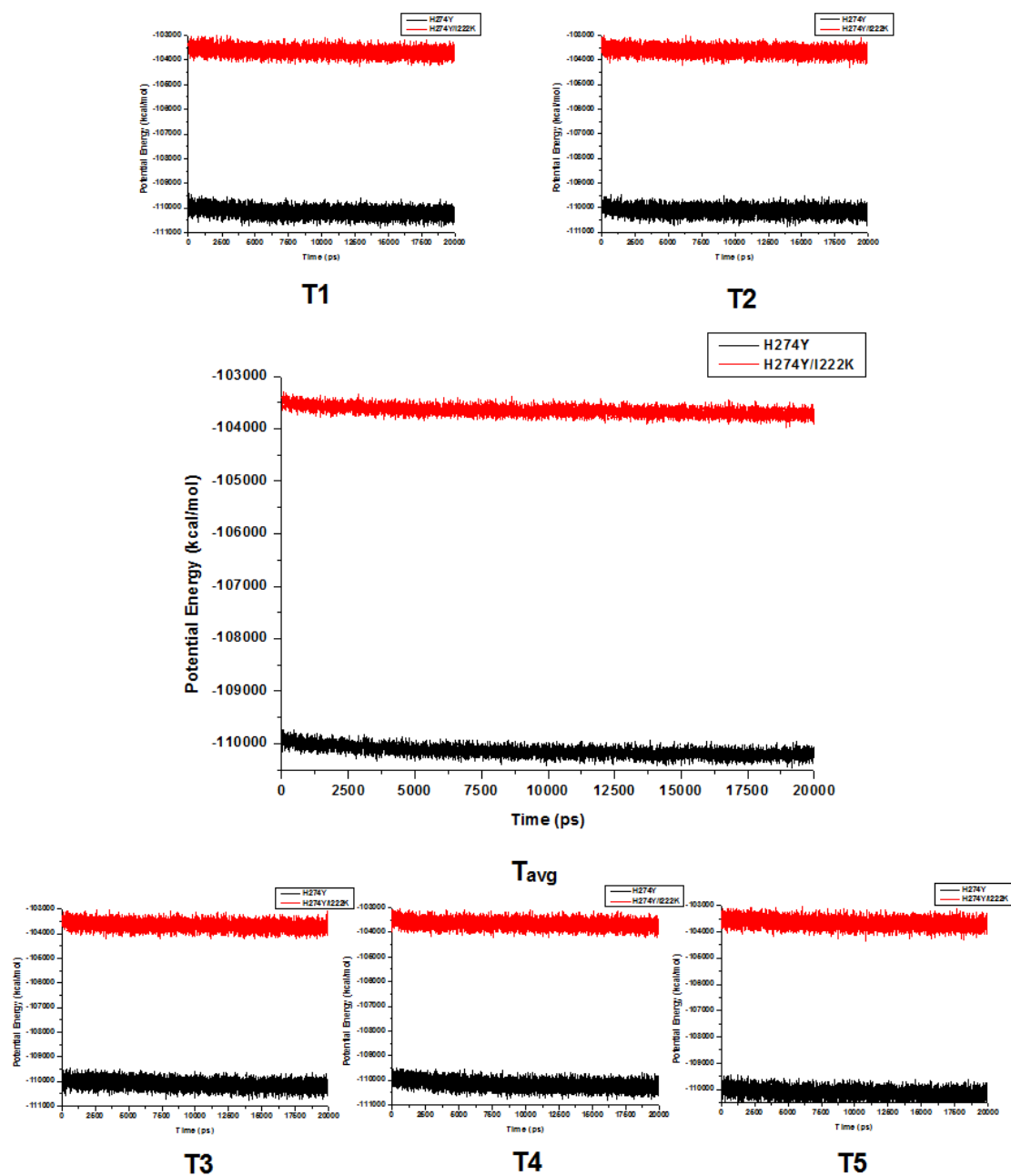
S6: RMSD of H274Y_{H1N1} and H274Y-I222K_{H1N1} over 20 ns



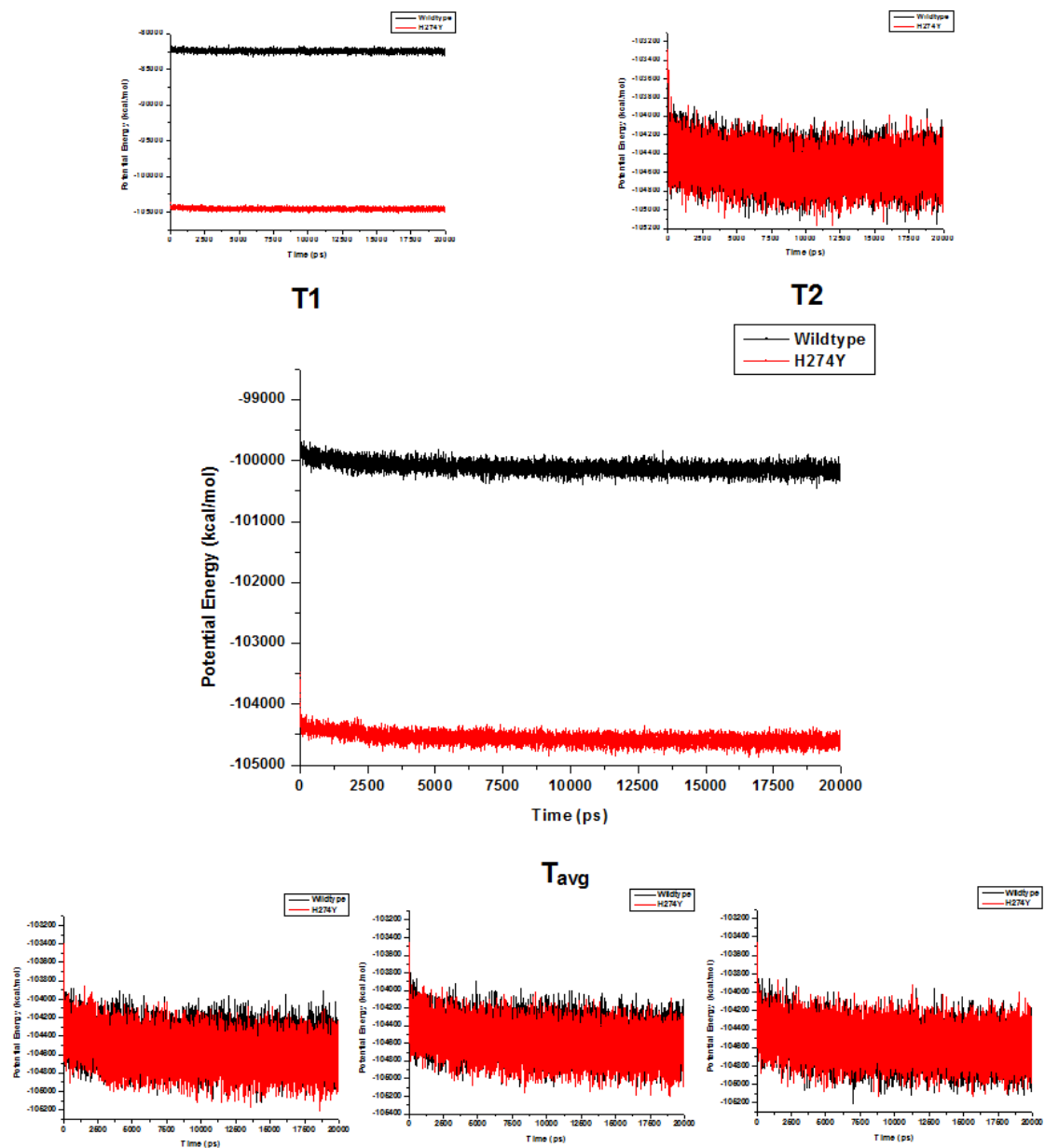
S7: Potential energy profile average of WT_{H5N1} and H274Y_{H5N1} over 20 ns



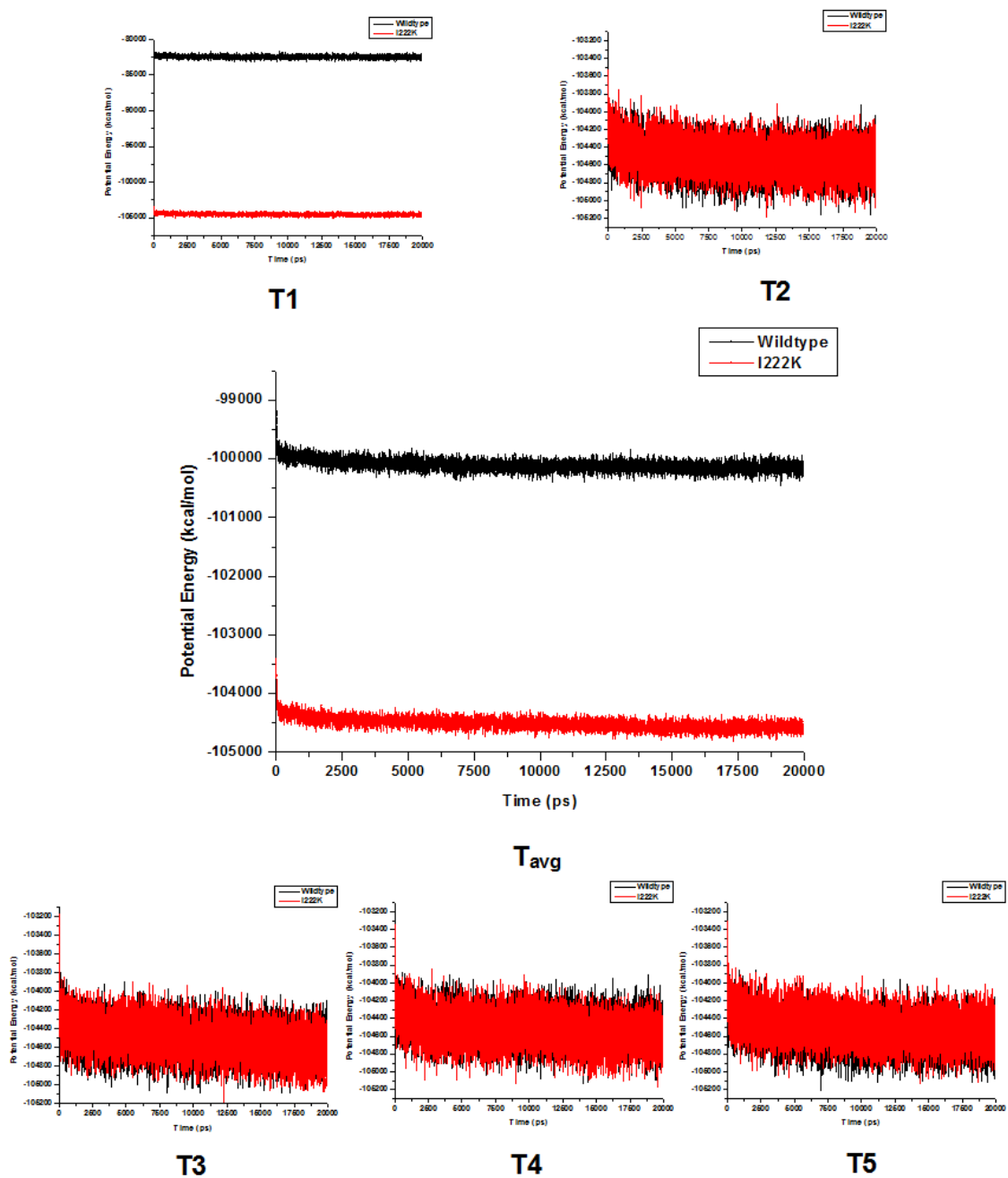
S8: Potential energy profile average of WT_{H5N1} and I222K_{H5N1} over 20 ns



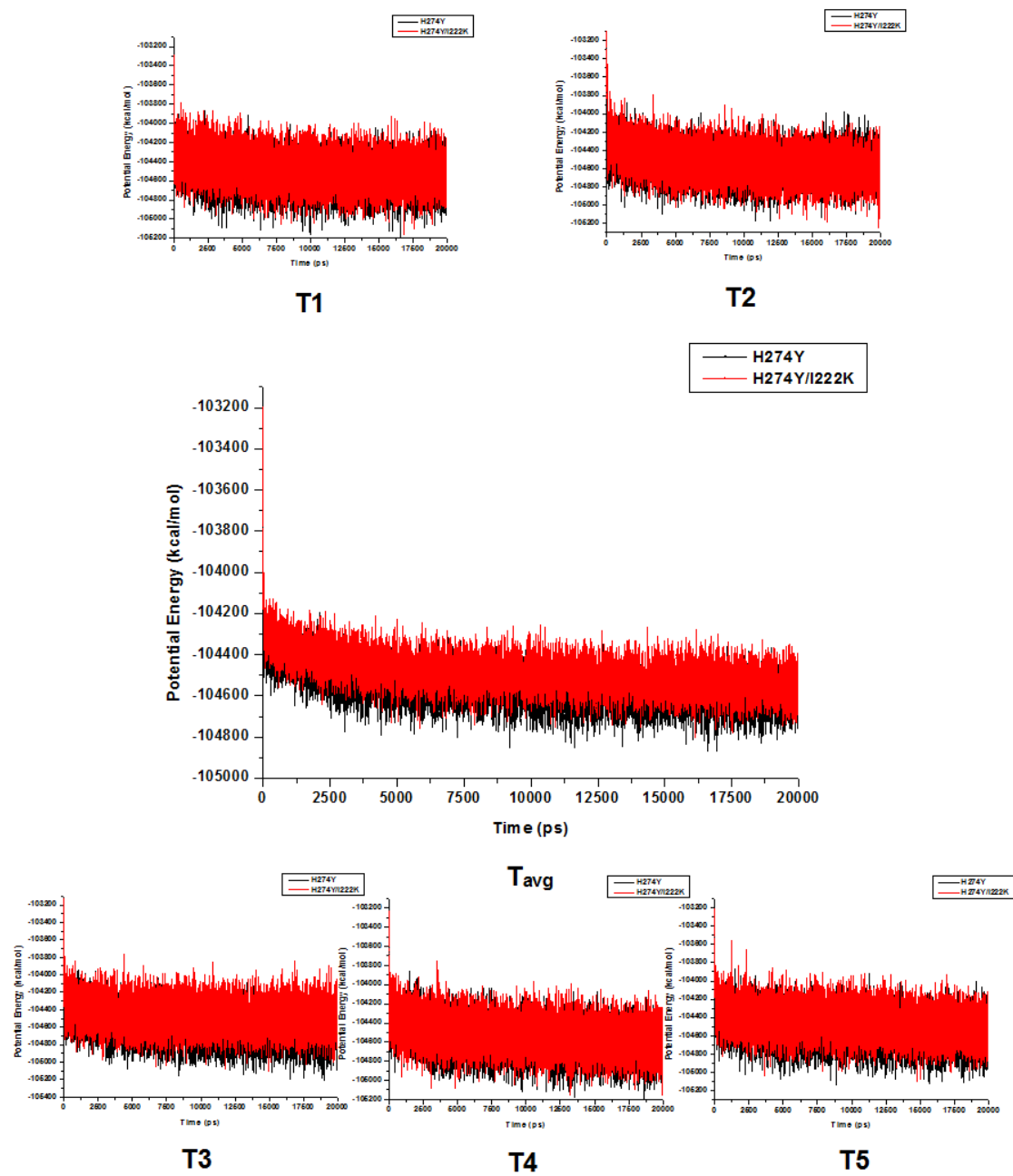
S9: Potential energy profile average of H274Y_{H5N1} and H274Y-I222K_{H5N1} over 20 ns



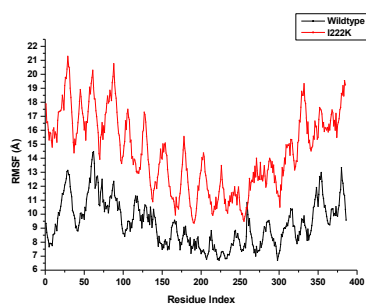
S10: Potential energy profile average of WT_{H1N1} and H274Y_{H1N1} over 20 ns



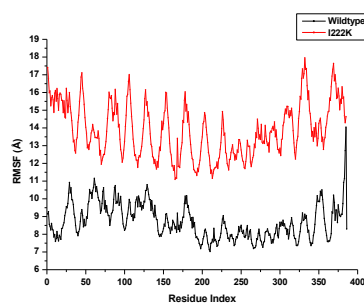
S11: Potential energy profile average of WT_{HIN1} and I222K_{HIN1} over 20 ns



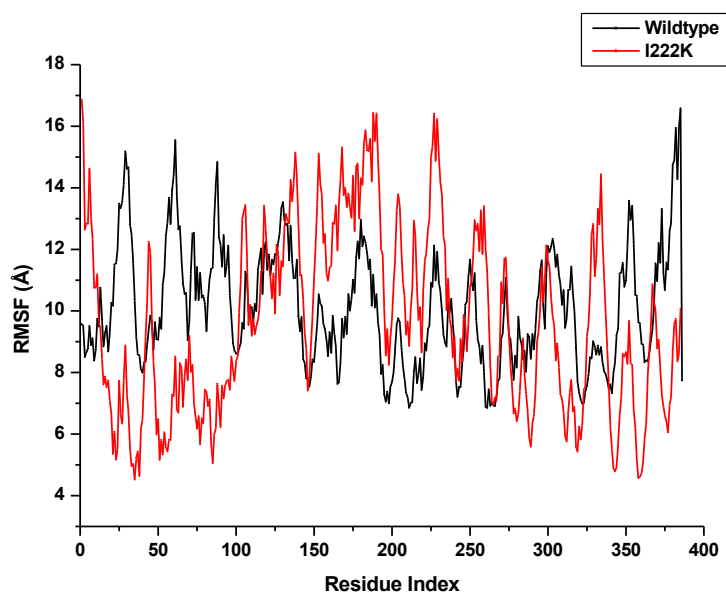
S12: Potential energy profile average of H274Y_{H1N1} and H274Y-I222K_{H1N1} over 20 ns



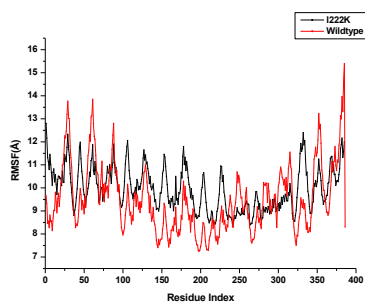
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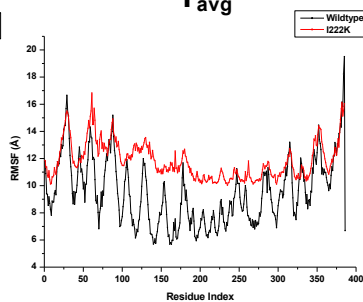
T2



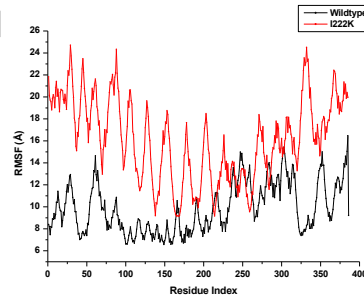
T_{avg}



T3

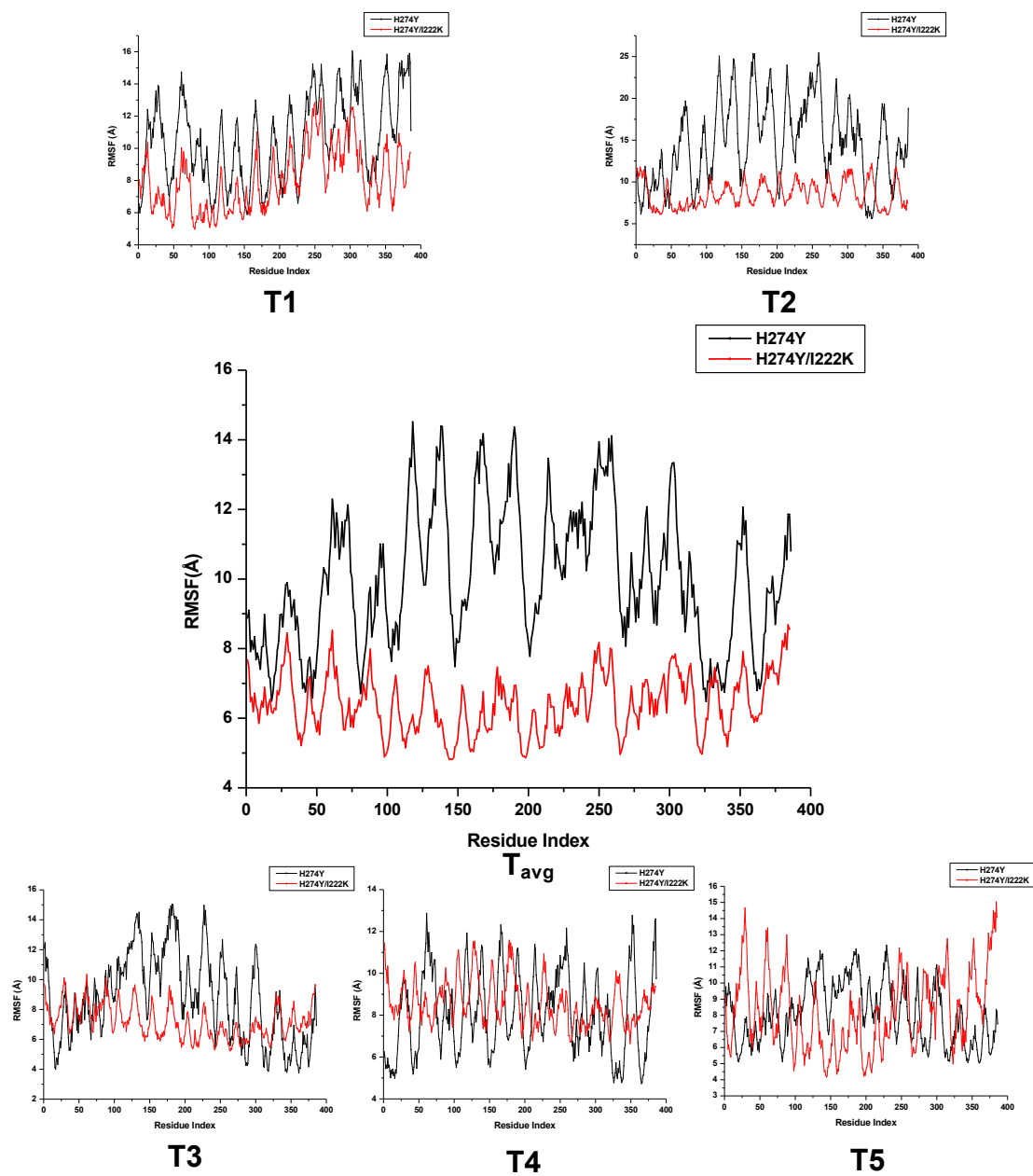


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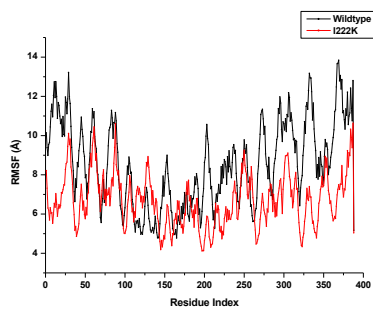


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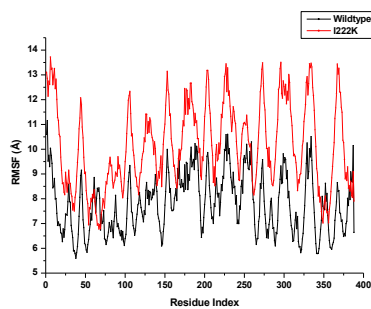
S13: RMSF of WT_{H5N1} and I222K_{H5N1} across 20 ns



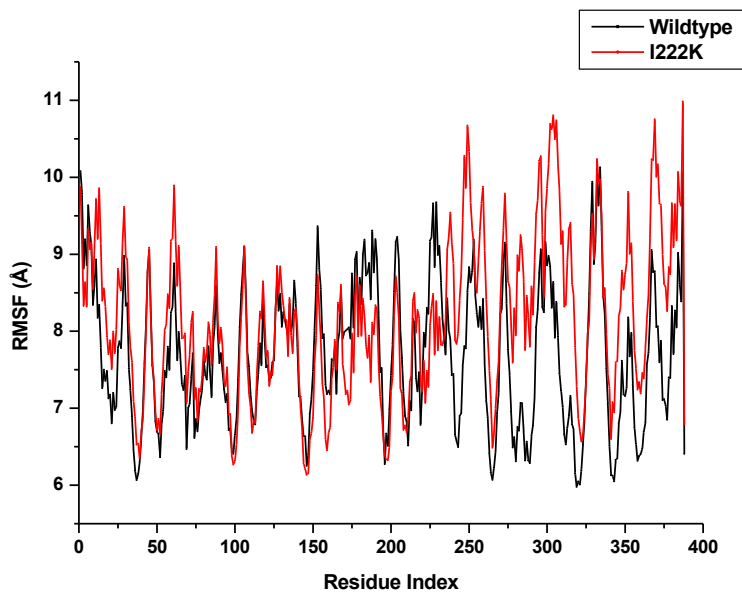
S14: RMSF of H274Y_{H5N1} and H274Y-I222K_{H5N1} across 20 ns



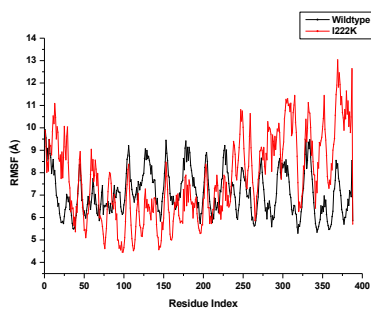
T1



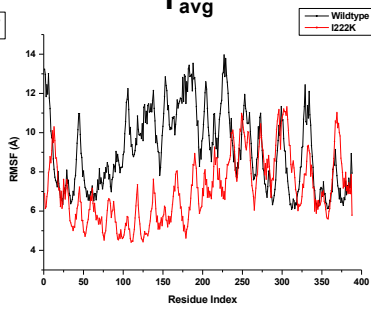
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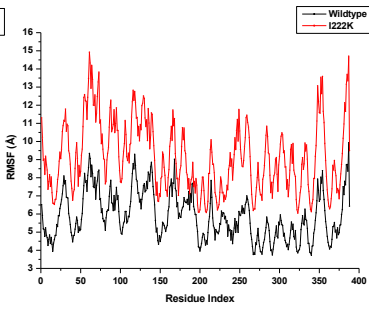
T_{avg}



T3

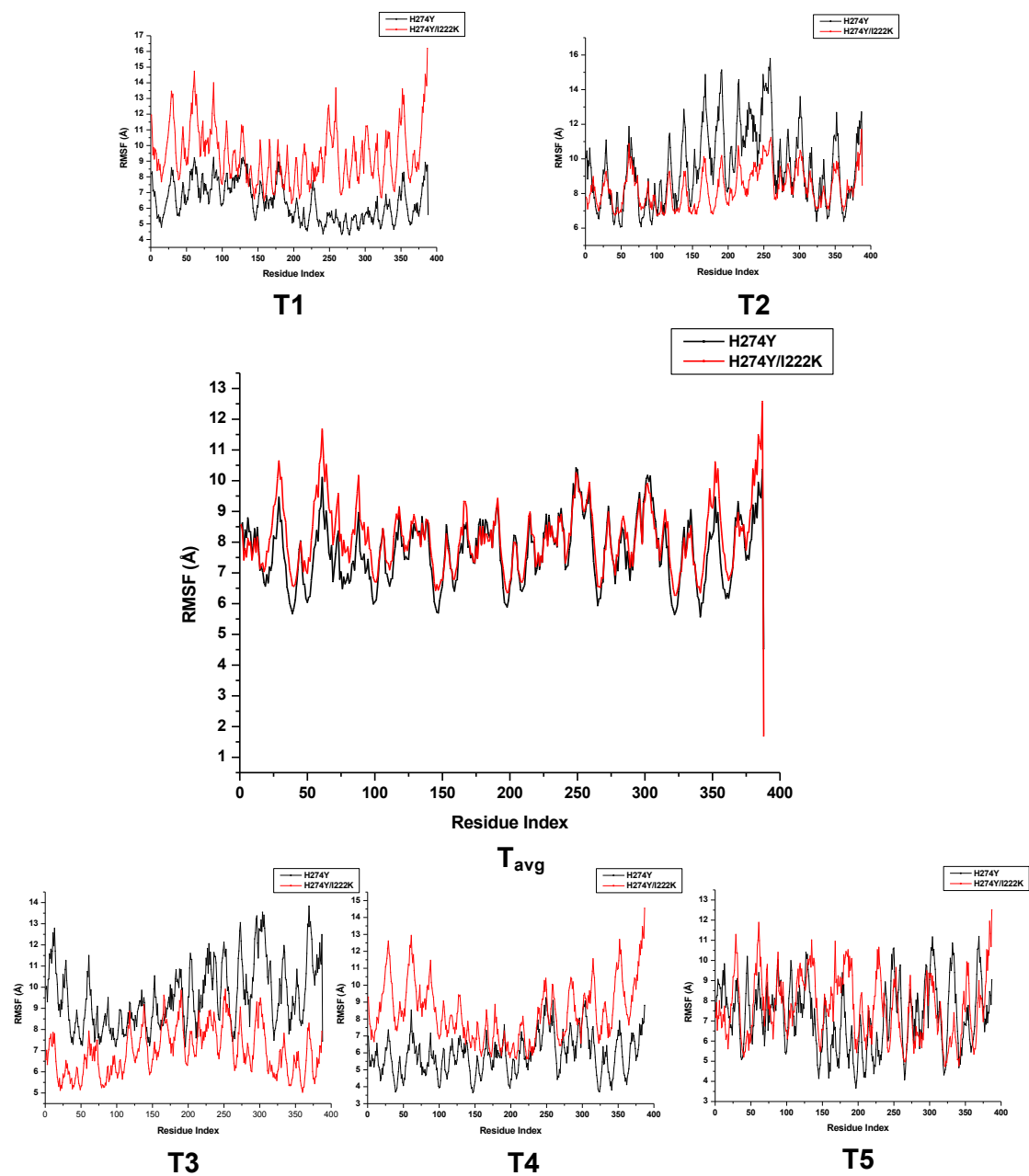


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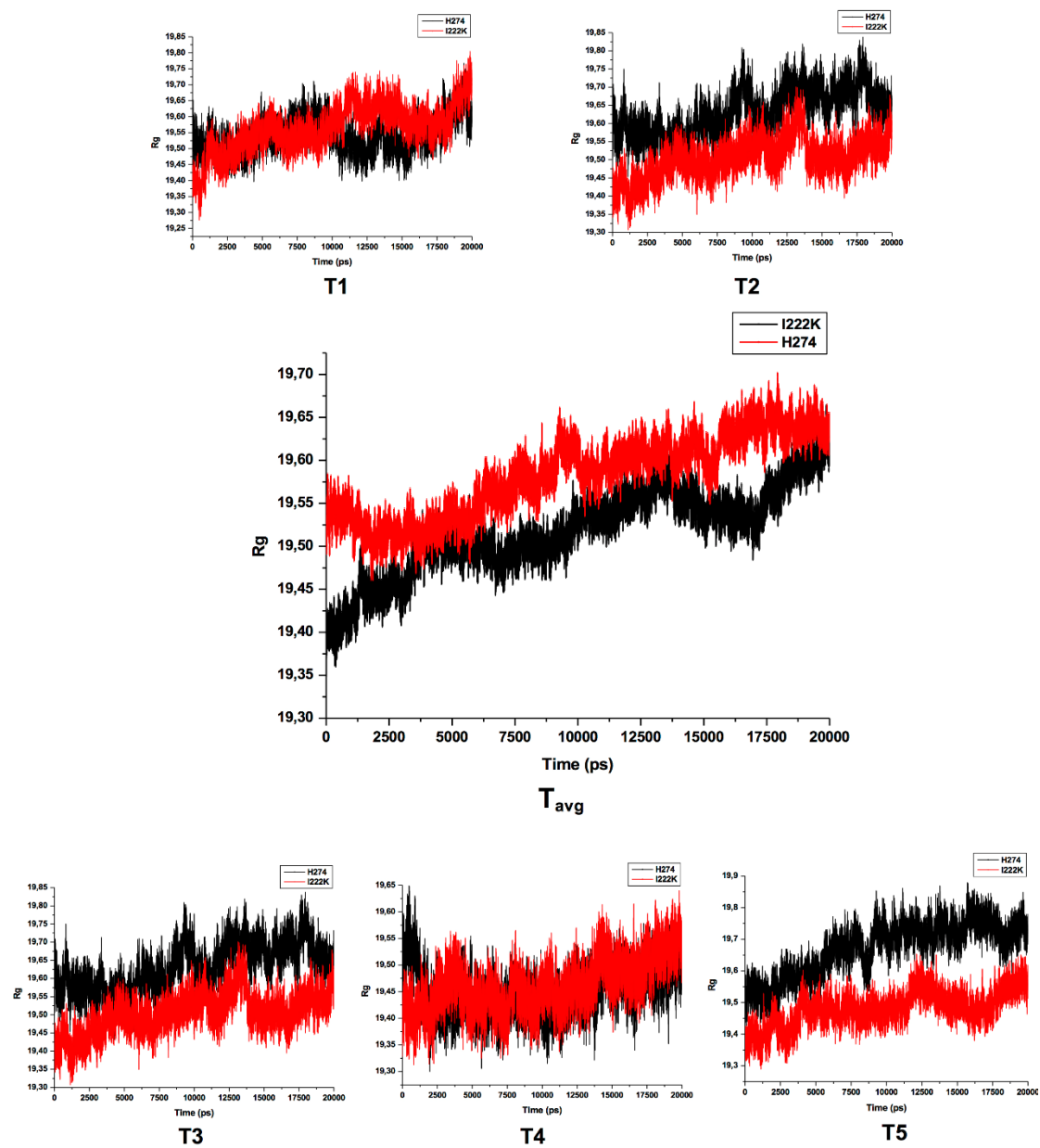


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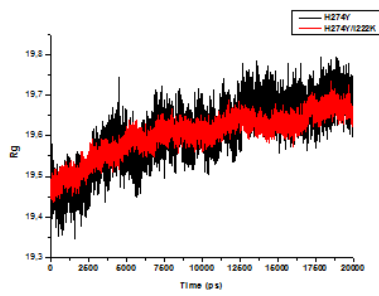
S15: RMSF of WT_{H1N1} and I222K_{H1N1} over 20 ns



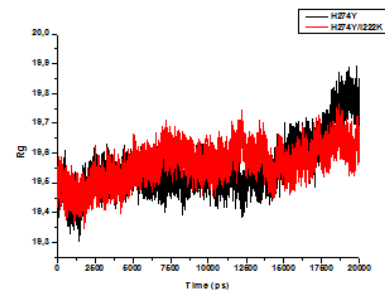
S16: RMSF of H274Y_{H1N1} and H274Y-I222K_{H1N1} over 20 ns



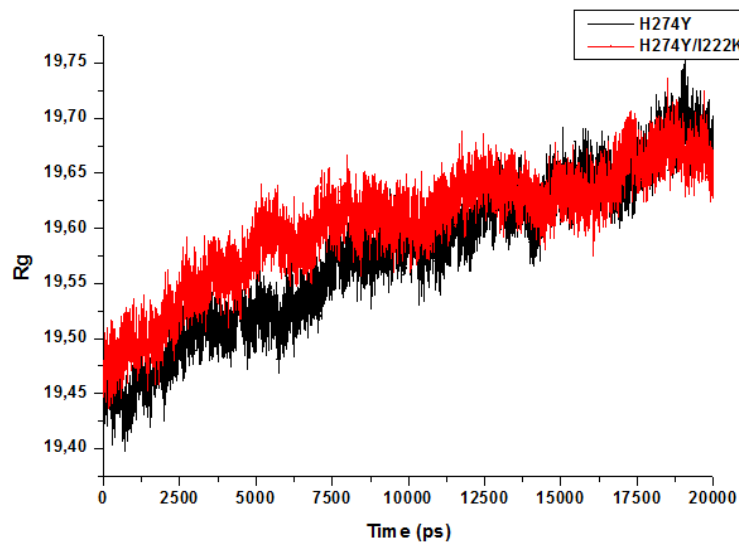
S17: Radius of gyration average of WT_{H5N1} and I222K_{H5N1} over 20 ns



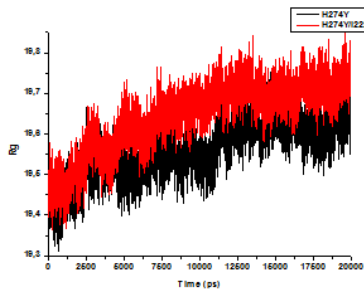
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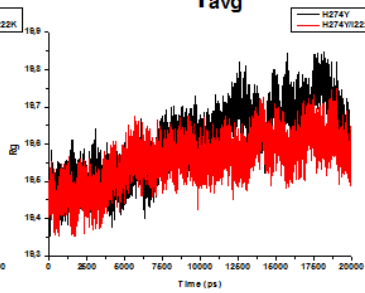
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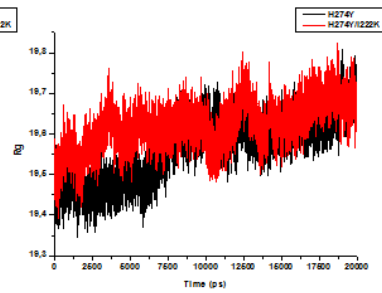
Tavg



T3

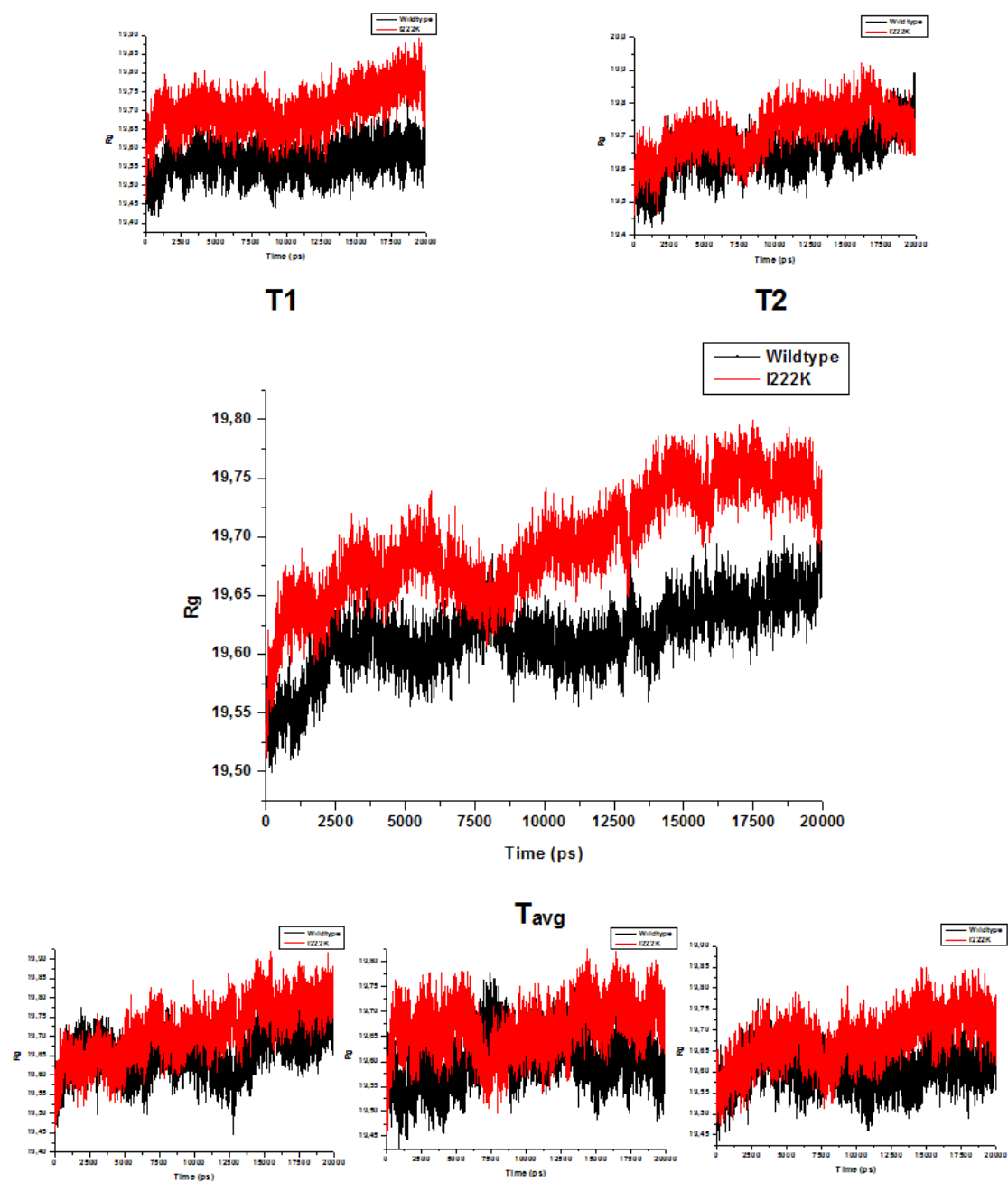


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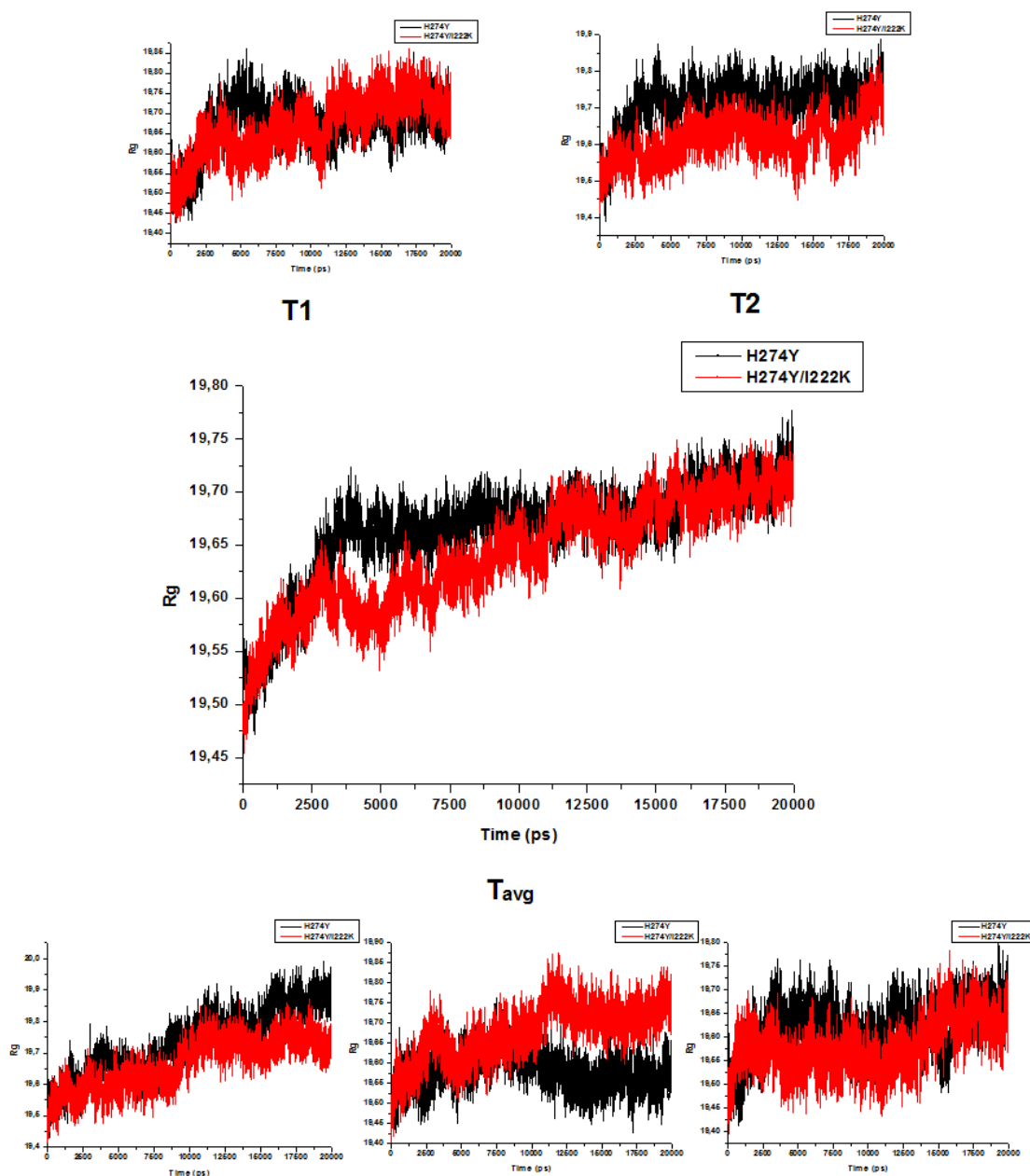


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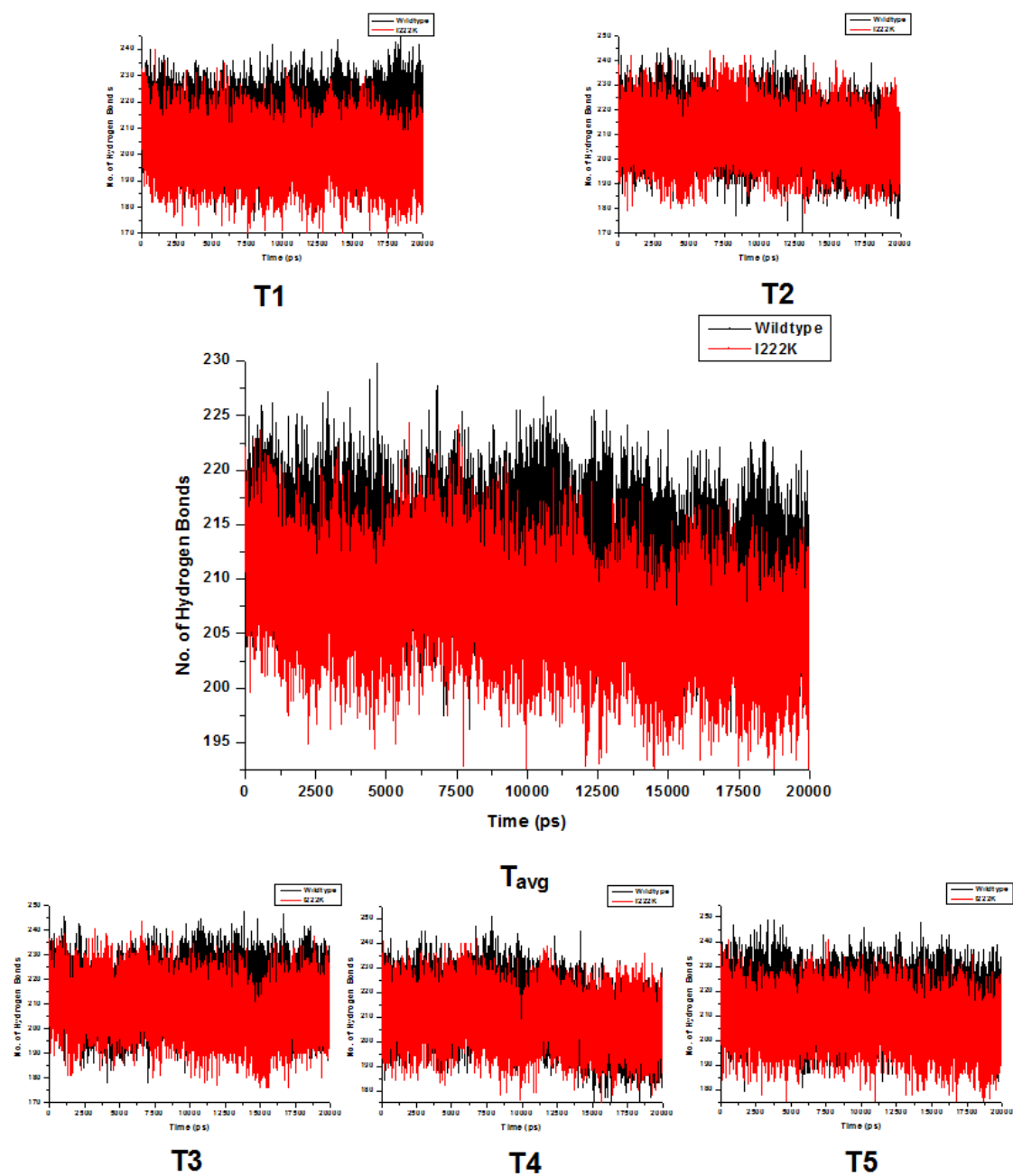
S18: Radius of gyration average of H274Y_{H5N1} and H274Y-I222K_{H5N1} over 20 ns



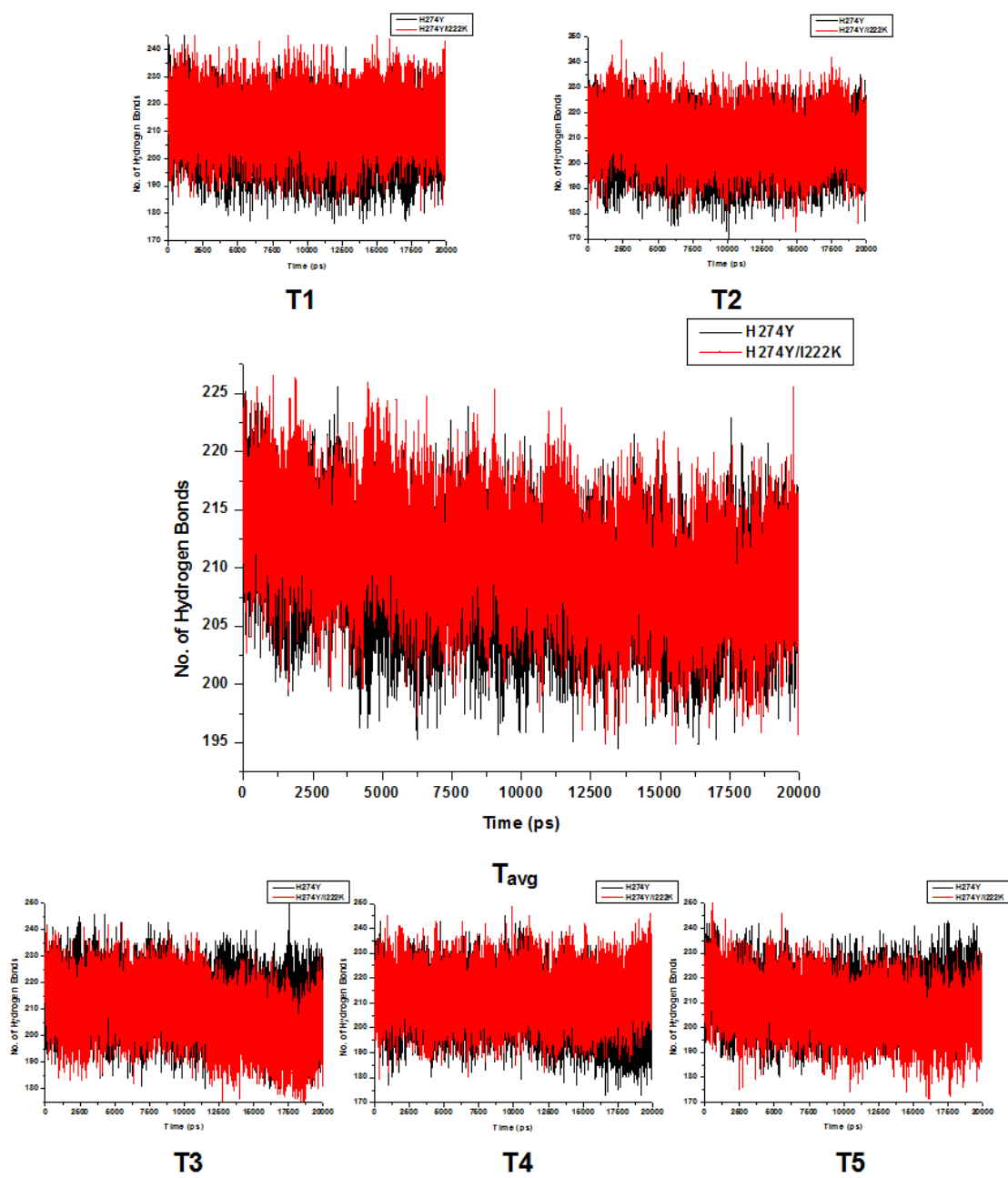
S19: Radius of gyration average of WT_{H1N1} and I222K_{H1N1} over 20 ns



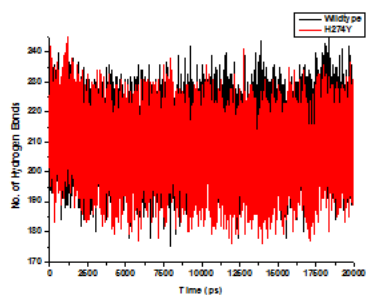
S20: Radius of gyration average of H274Y_{H1N1} and H274Y-I222K_{H1N1} over 20 ns



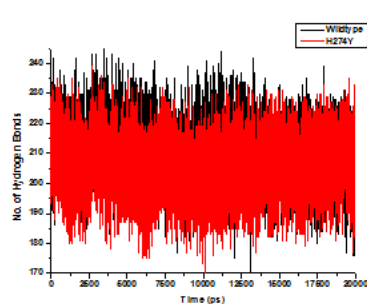
S21: No. of hydrogen bonds averaged over 20 ns for WT_{H5N1} and I222K_{H5N1}



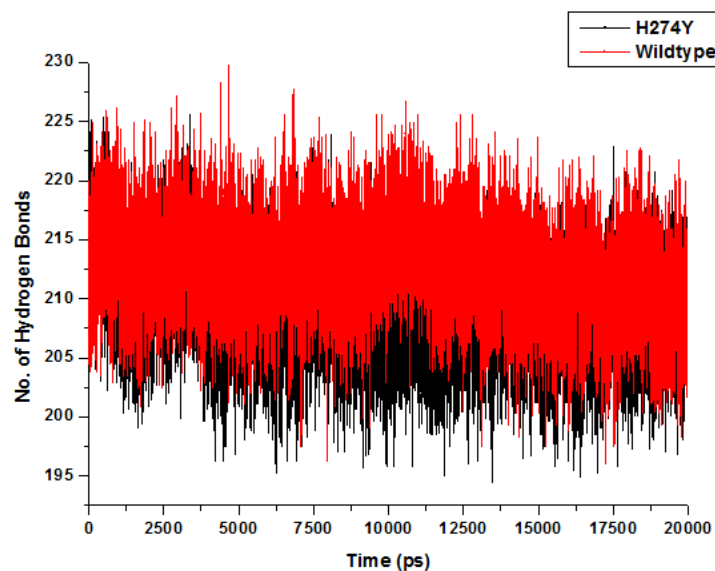
S22: No. of hydrogen bonds averaged over 20 ns for H274Y_{H5N1} and H274Y-I222K_{H5N1}



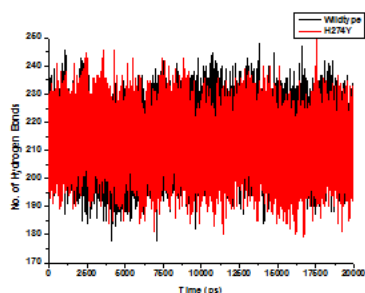
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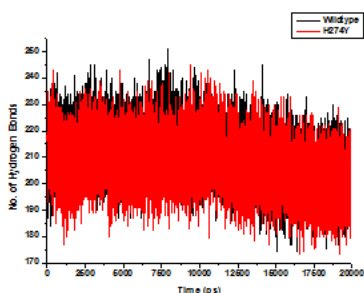
T2



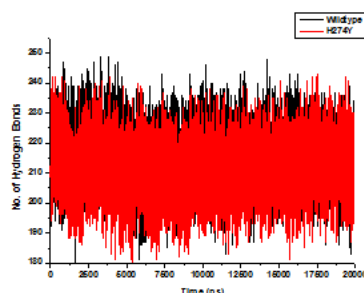
T_{avg}



T3

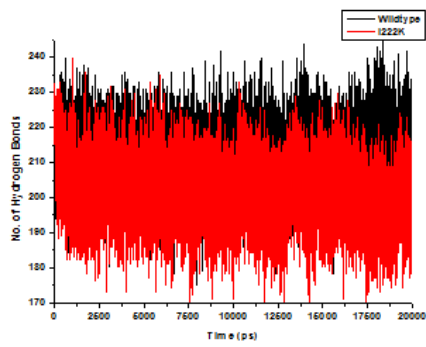


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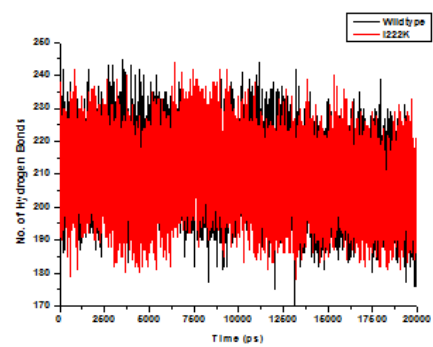


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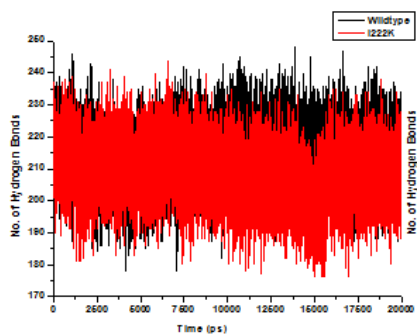
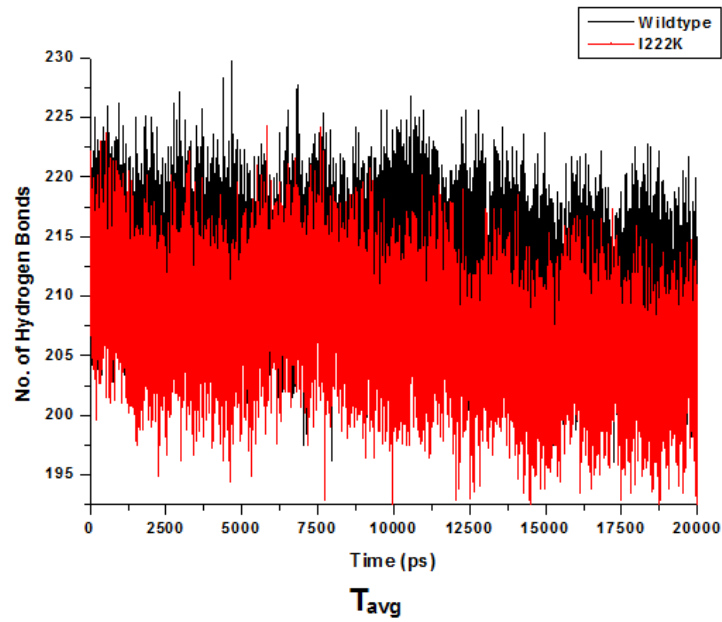
S23: No. of hydrogen bonds averaged over 20 ns for WT_{H1N1} and H274Y_{H1N1}



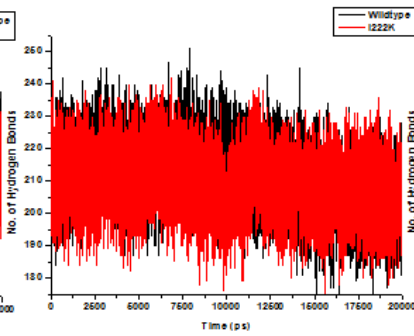
T1



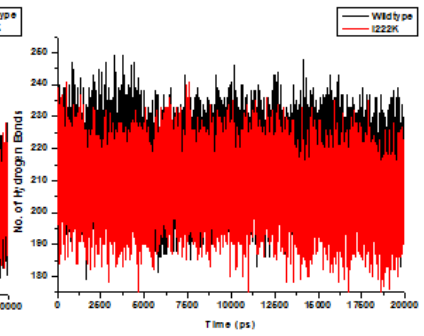
T2



T3

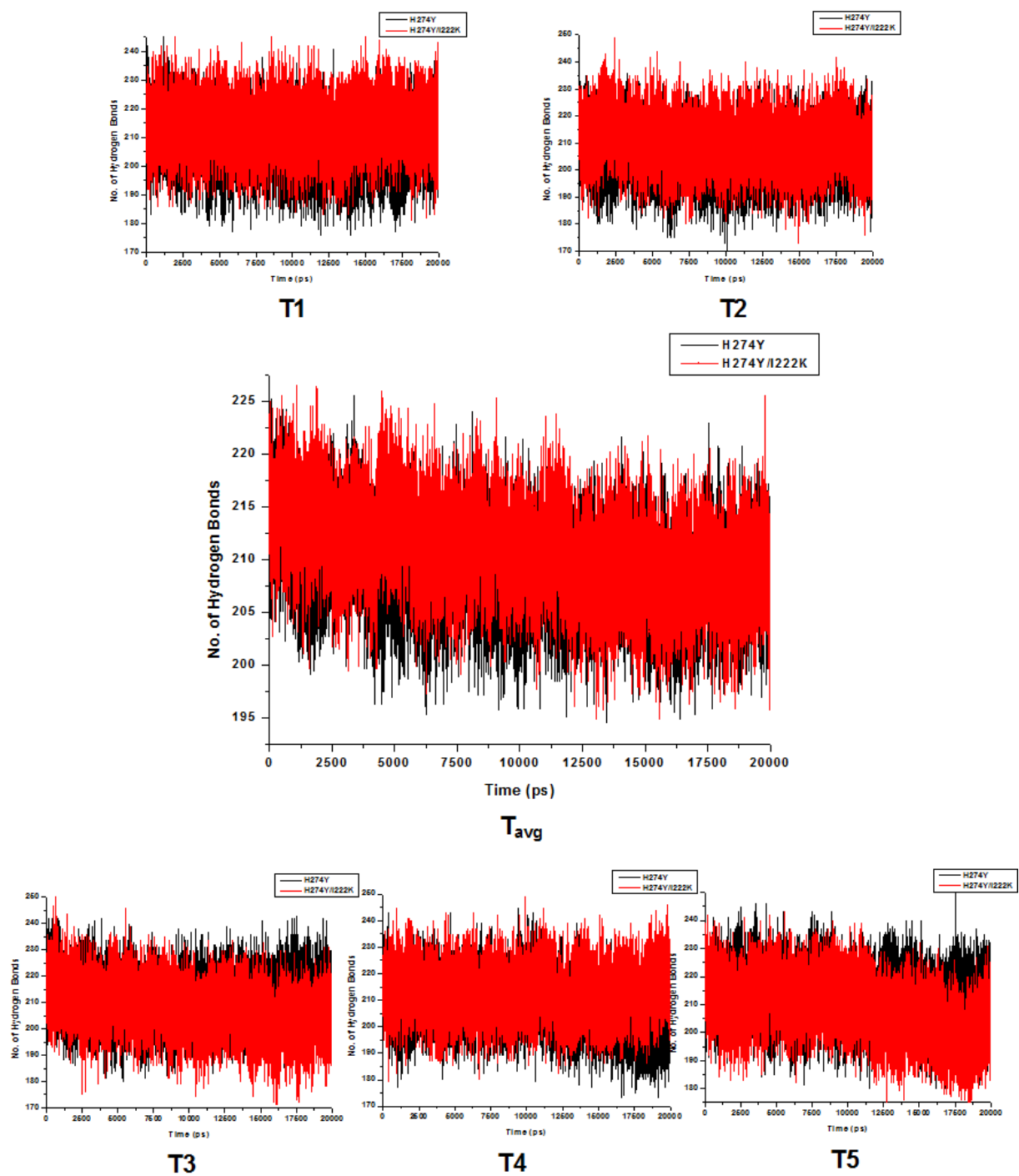


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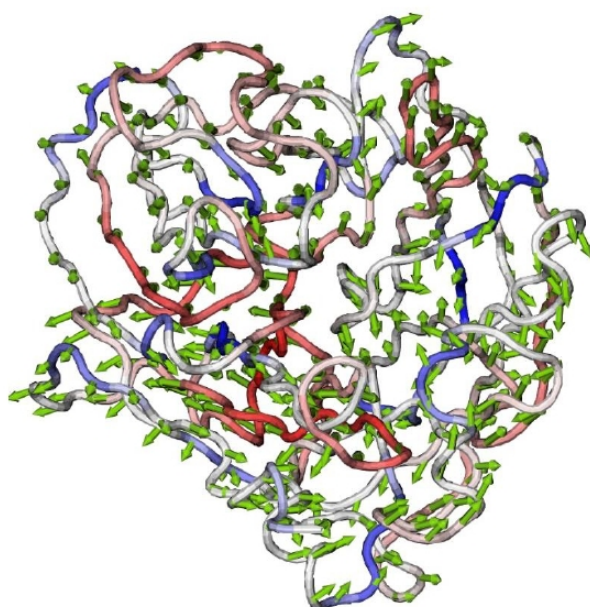


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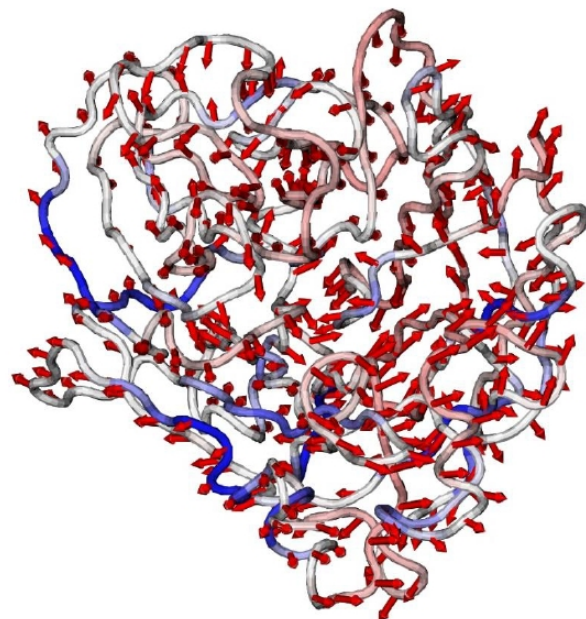
S24: No. of hydrogen bonds averaged over 20 ns for WT_{H1N1} and I222K_{H1N1}



S25: No. of hydrogen bonds averaged over 20 ns for H274Y_{H1N1} and H274Y-I222K_{H1N1}

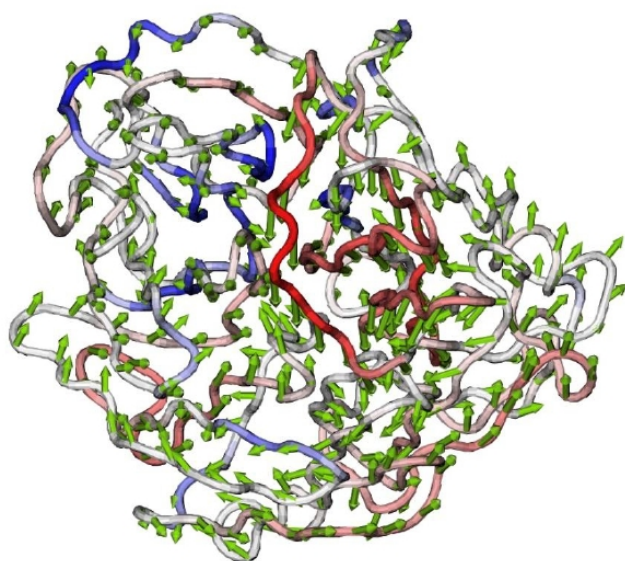


NM1

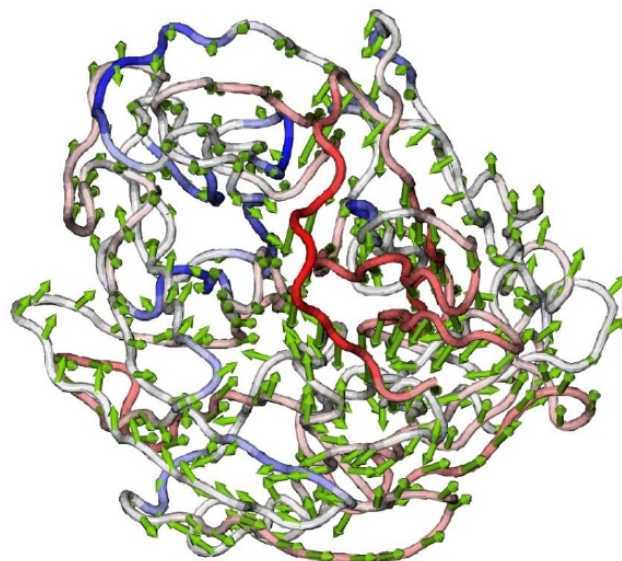


NM2

S26: Porcupine derivatives of eigenvectors of normal modes 1 and 2 of WT_{H5N1}

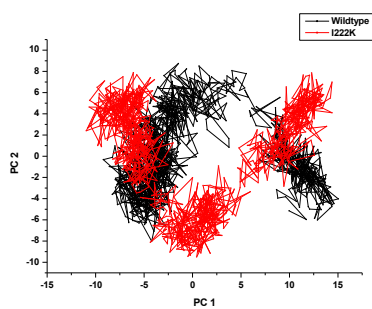


NM1

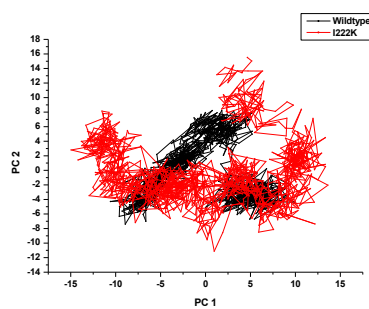


NM2

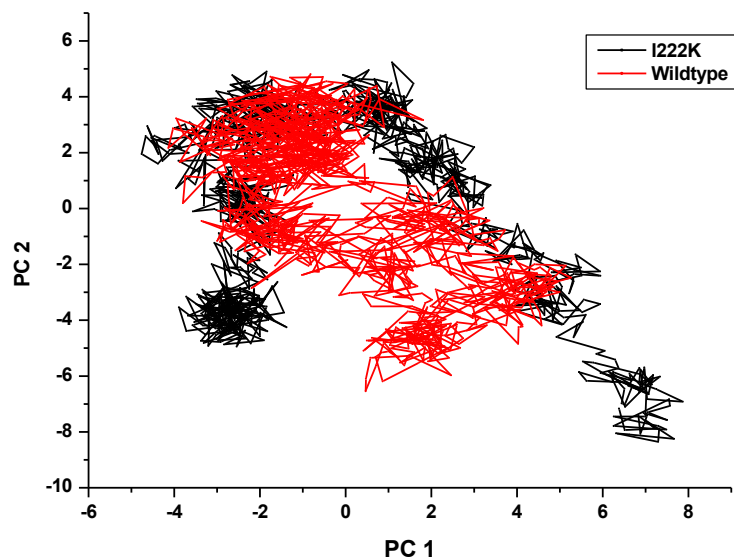
S27: Porcupine derivatives of eigenvectors of normal modes 1 and 2 of H274Y_{H5N1}



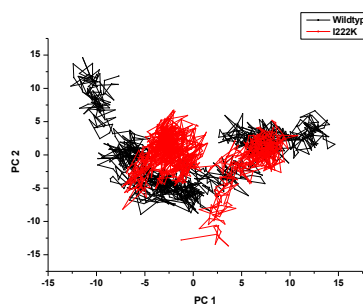
T1



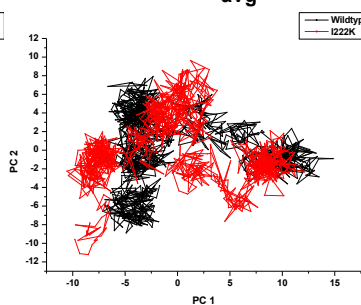
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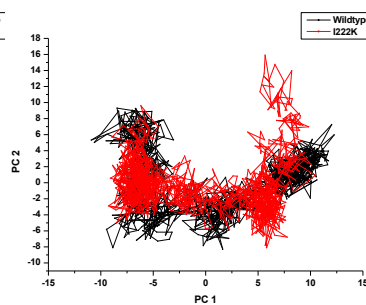
T_{avg}



T3

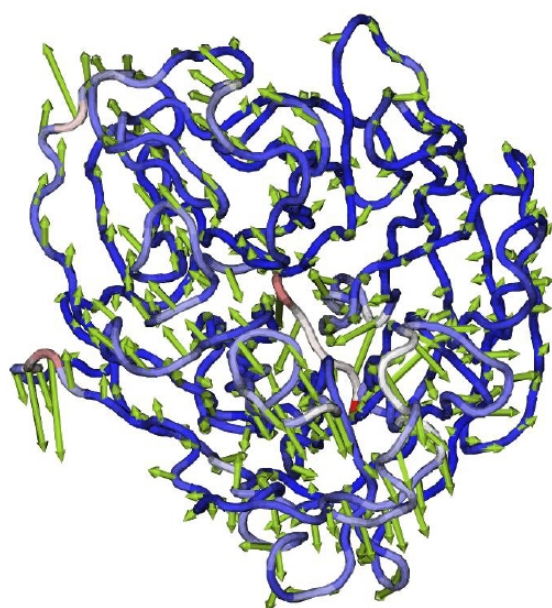


T4



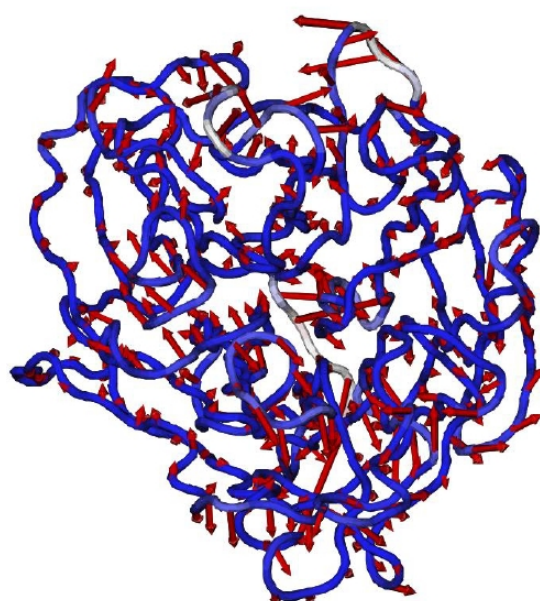
T5

S28: PCA of WT_{H5N1} and I222K_{H5N1} over 20 ns



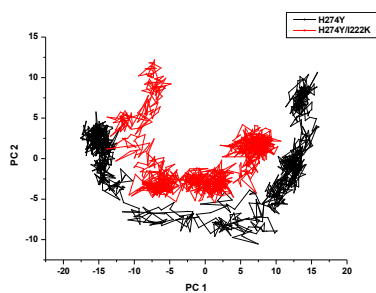
NM1

Natural
mutation

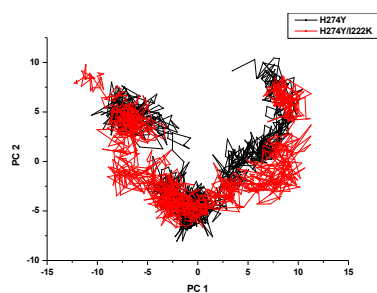


NM2

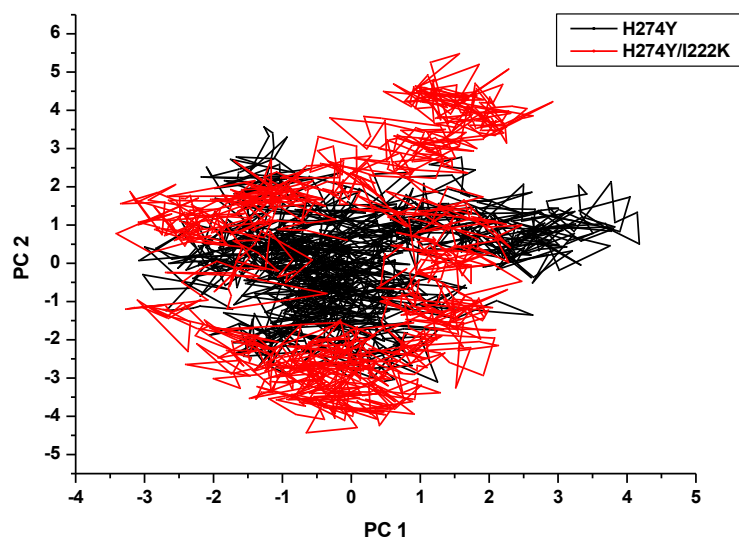
S29: Porcupine derivatives of eigenvectors of normal modes 1 and 2 of I222K_{H5N1}



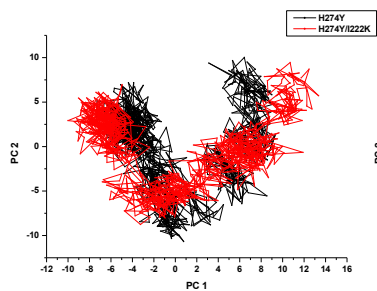
T1



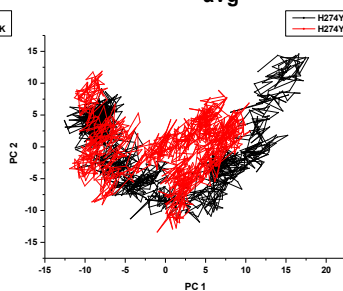
T2



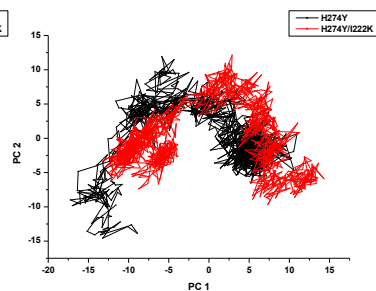
T_{avg}



T3

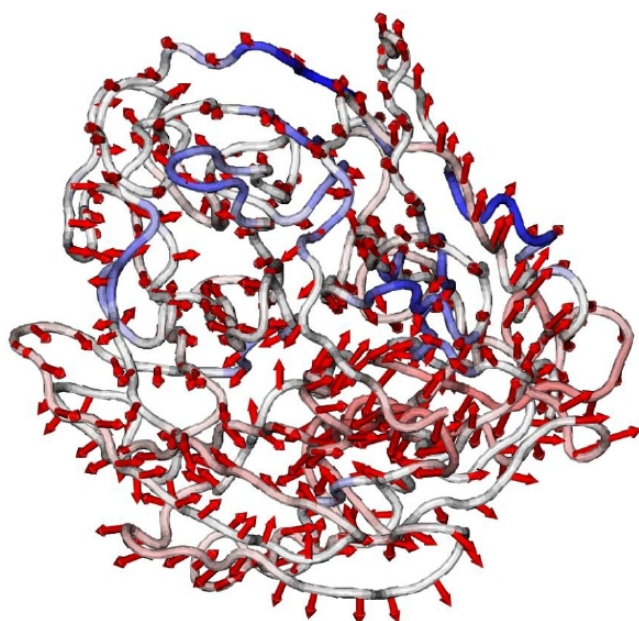


T4

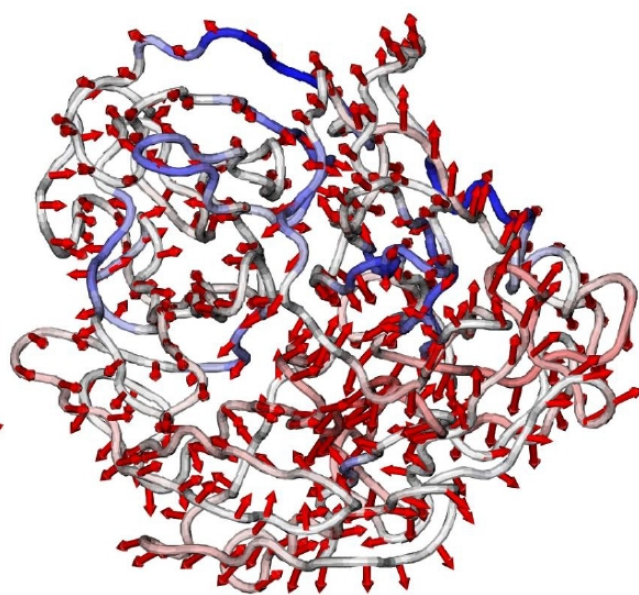


T5

S30: PCA of H274Y_{H5N1} and H274Y-I222K_{H5N1} over 20 ns

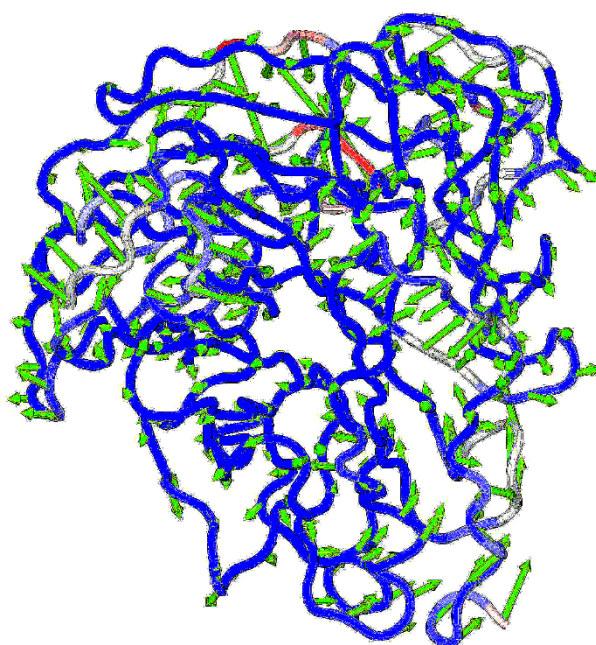


NM1

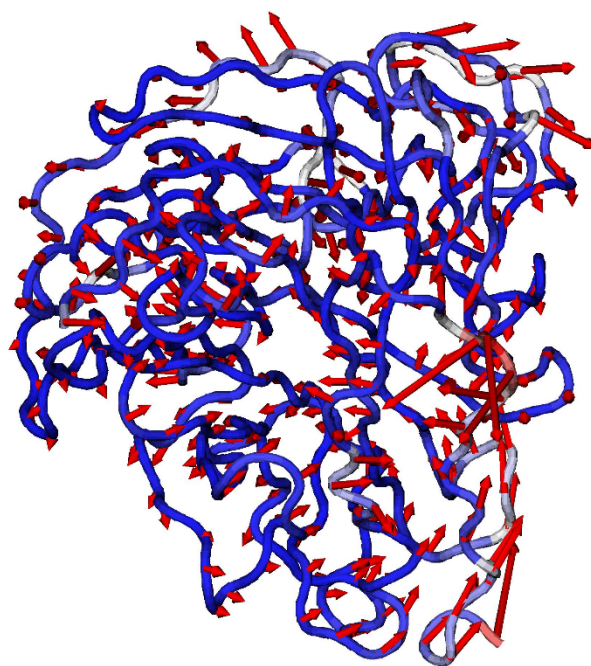


NM2

S31: Porcupine derivatives of eigenvectors of normal modes 1 and 2 of H274Y-I222K_{H5N1}

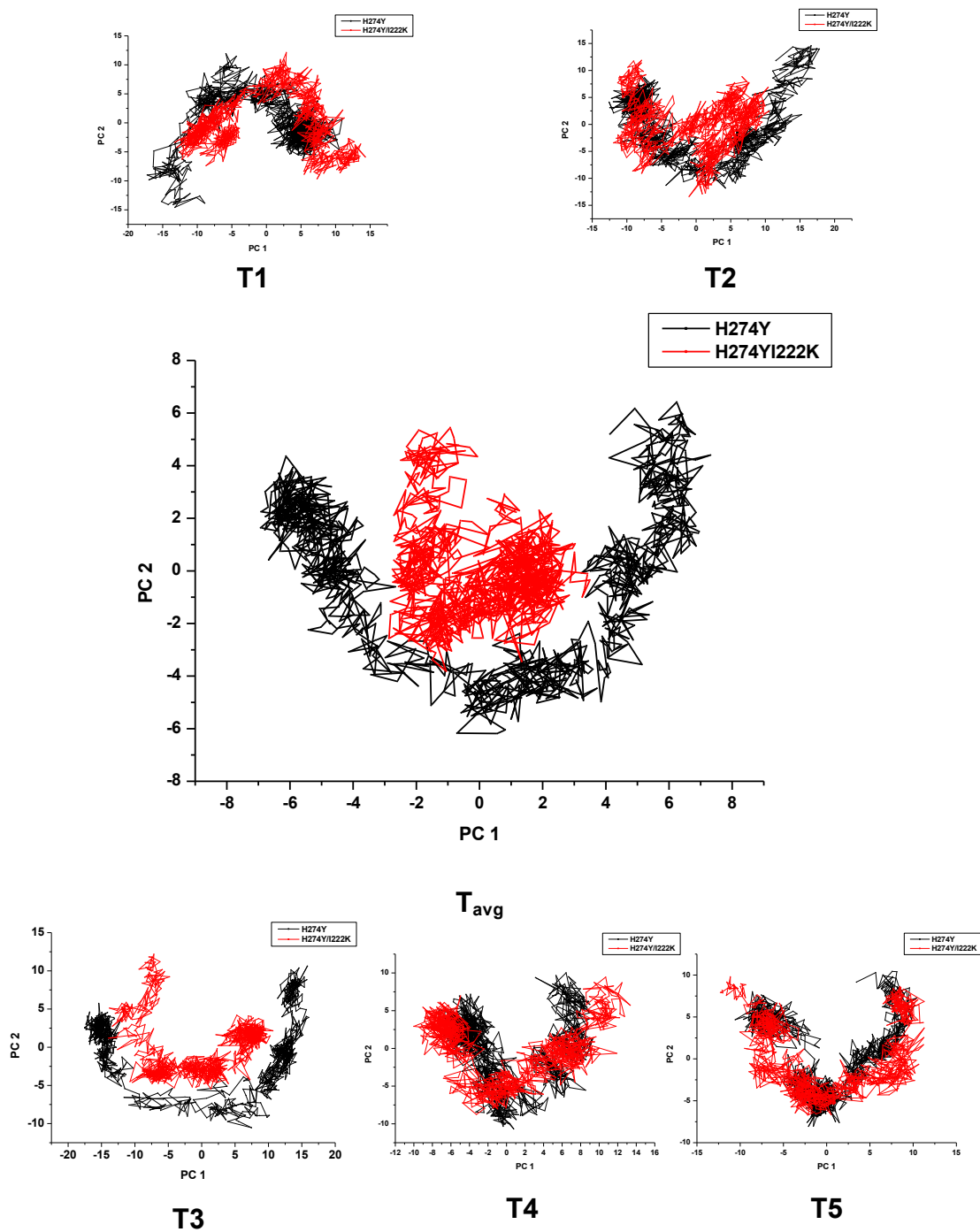


NM1

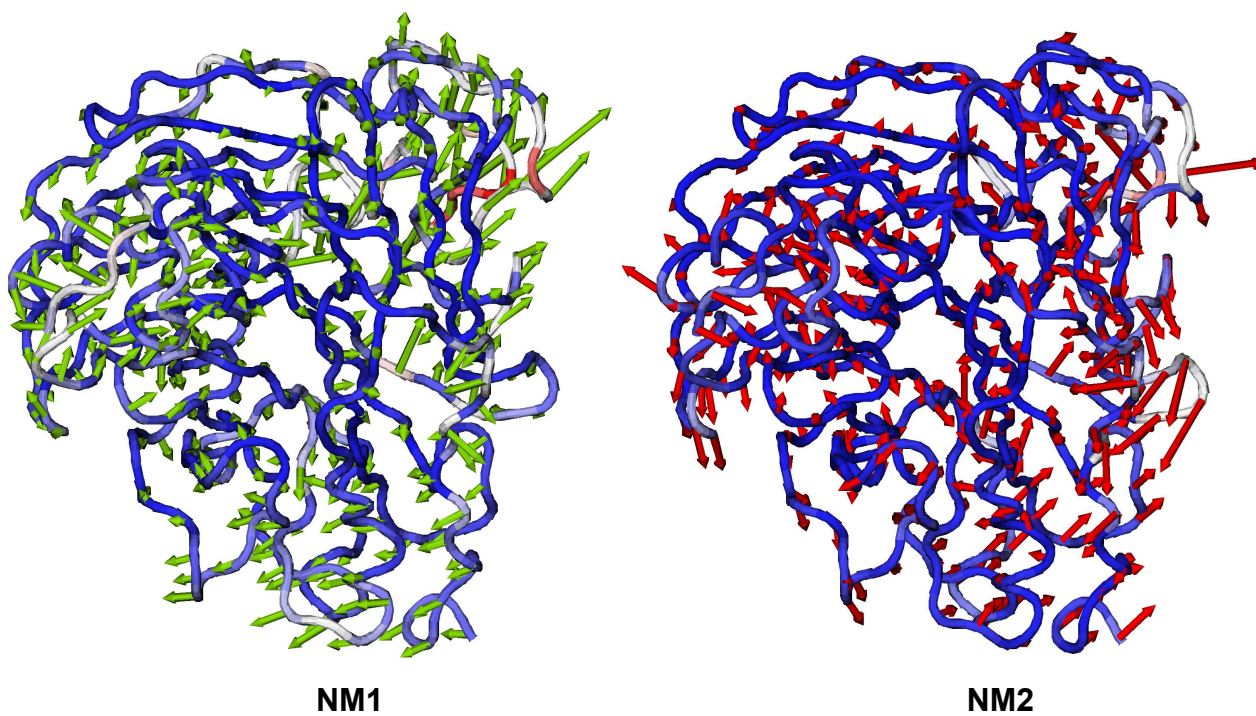


NM2

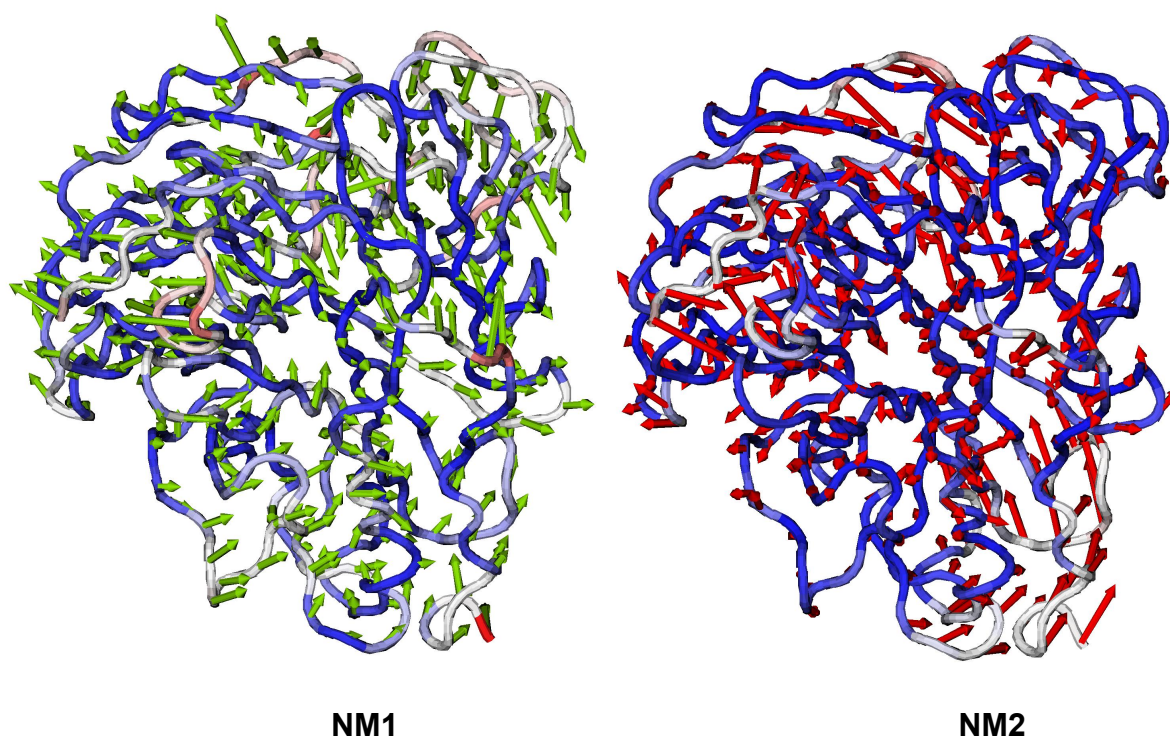
S32: Porcupine derivatives of eigenvectors of normal modes 1 and 2 of WT_{H1N1}



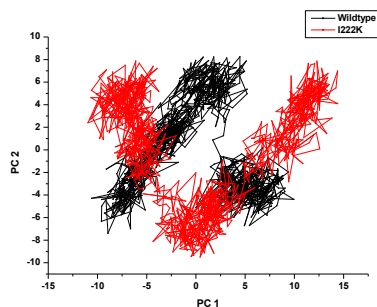
S33: PCA of H274Y_{H1N1} and H274Y-I222K_{H1N1} over 20 ns



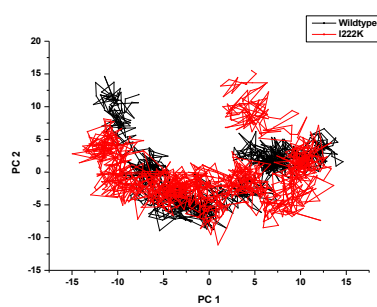
S34: Porcupine derivatives of eigenvectors of normal modes 1 and 2 of H274Y-I222K_{H1N1}



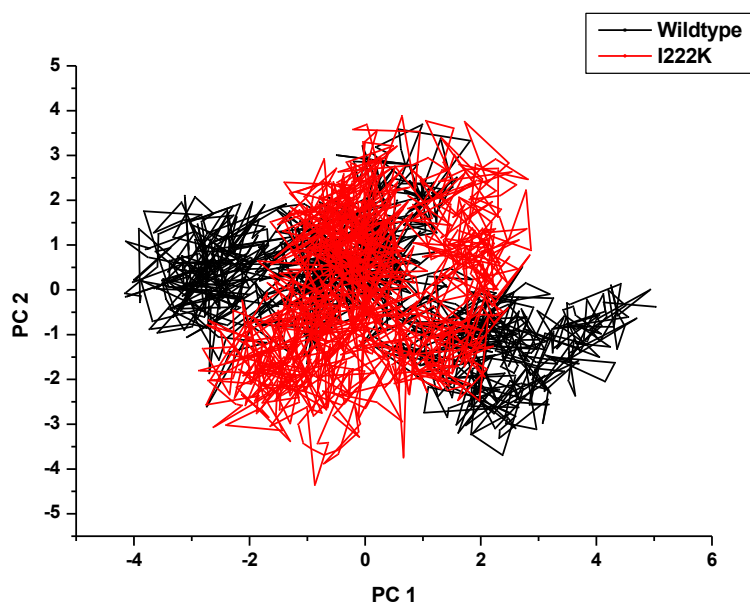
S35: Porcupine derivatives of eigenvectors of normal modes 1 and 2 of H274Y_{H1N1}



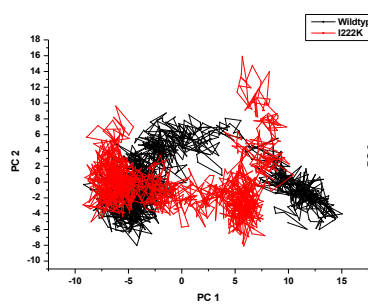
T1



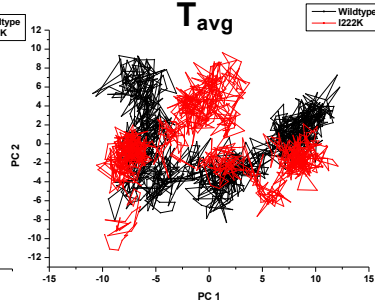
T2



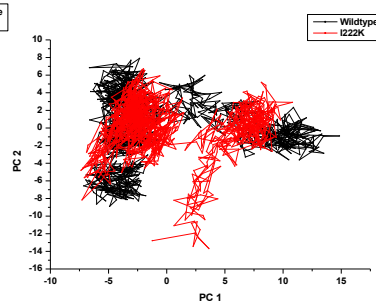
T_{avg}



T3

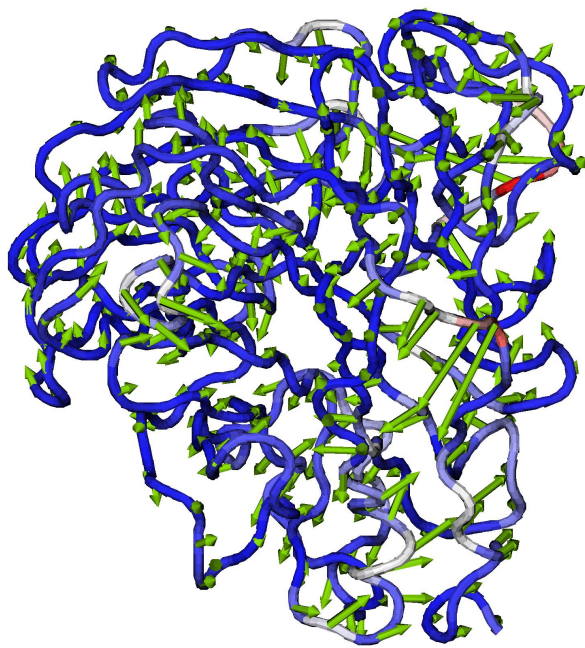


T4

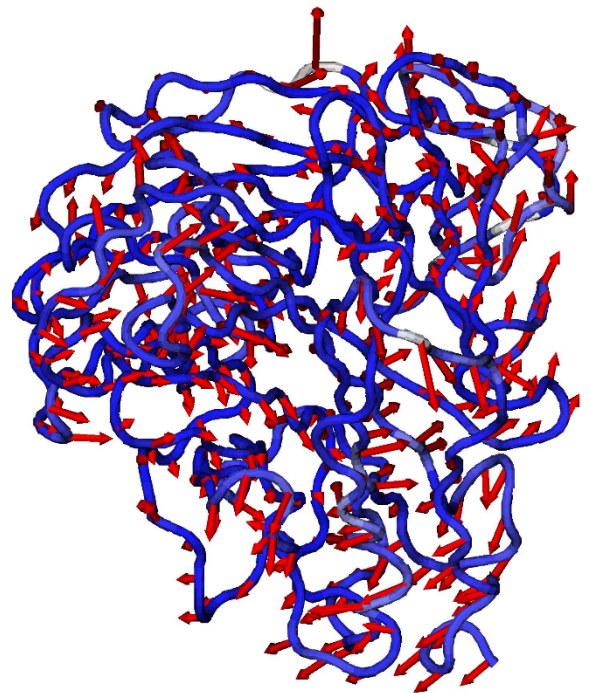


T5

S36: PCA of WT_{H1N1} and I222K_{H1N1} over 20 ns

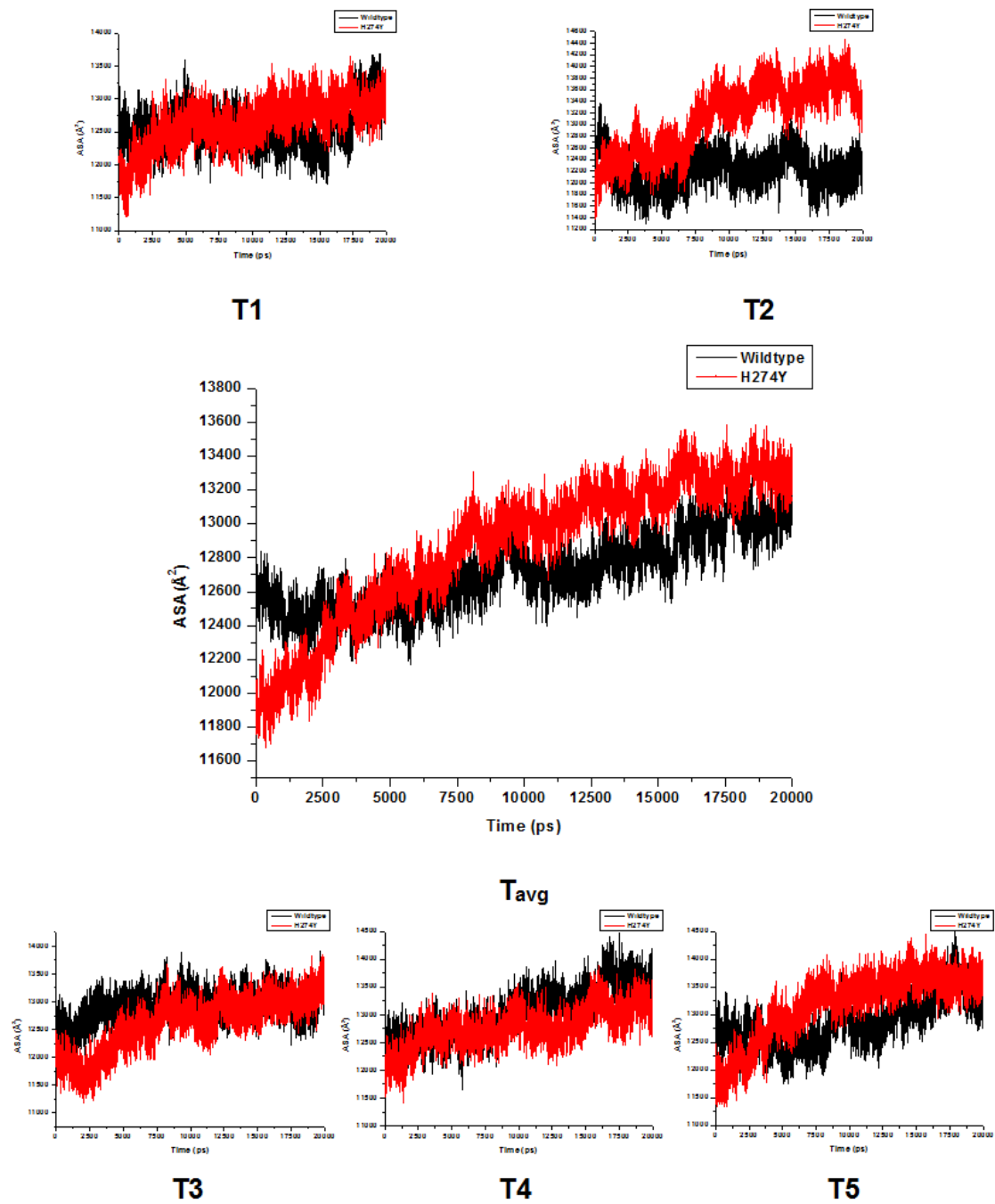


NM1

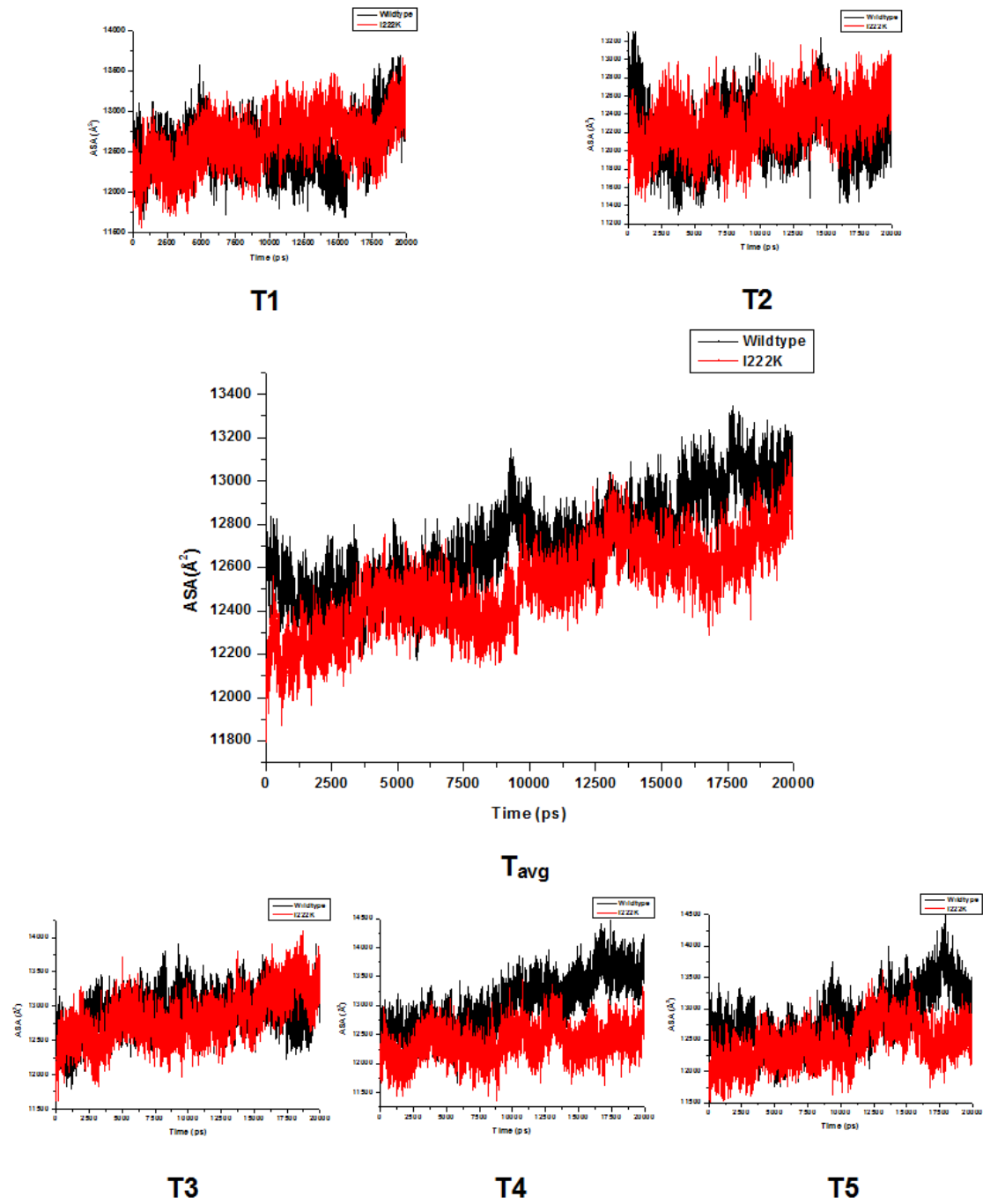


NM2

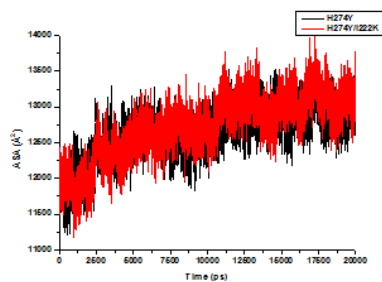
S37: Porcupine derivatives of eigenvectors of normal modes 1 and 2 of I222K_{H1N1}



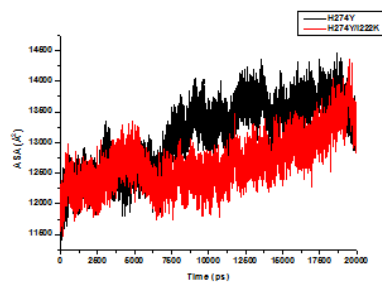
S38: SASA average of WT_{H5N1} and H274Y_{H5N1} over 20 ns



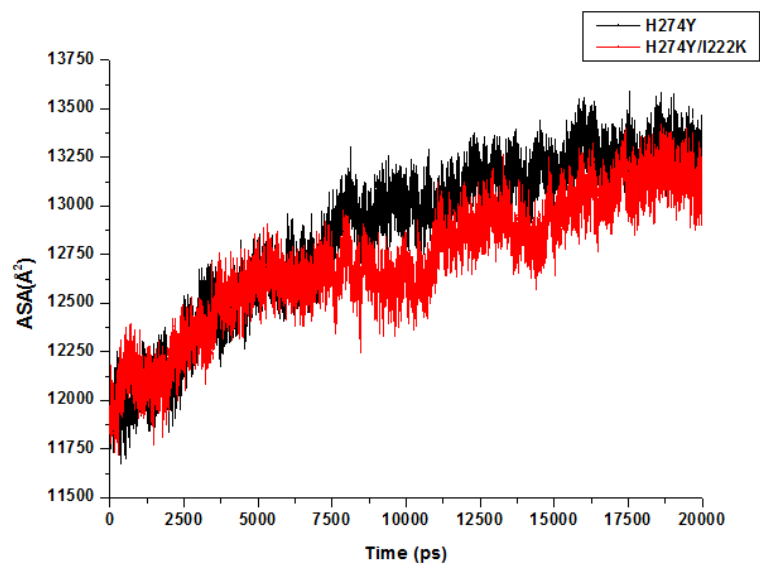
S39: SASA average of WT_{H5N1} and I222K_{H5N1} over 20 ns



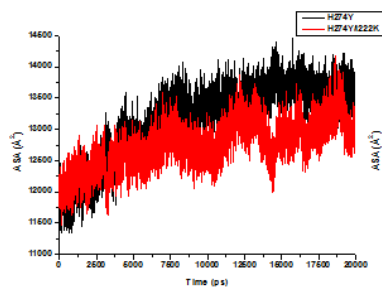
T1



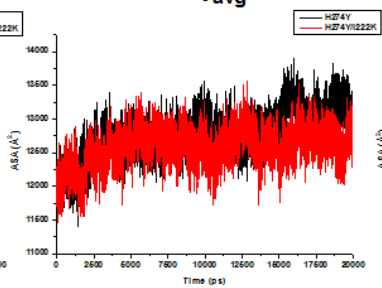
T2



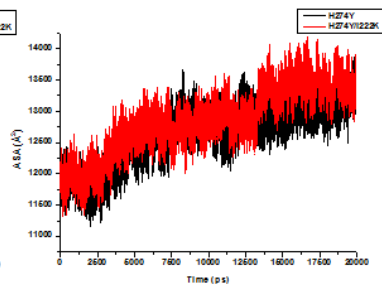
Tavg



T3

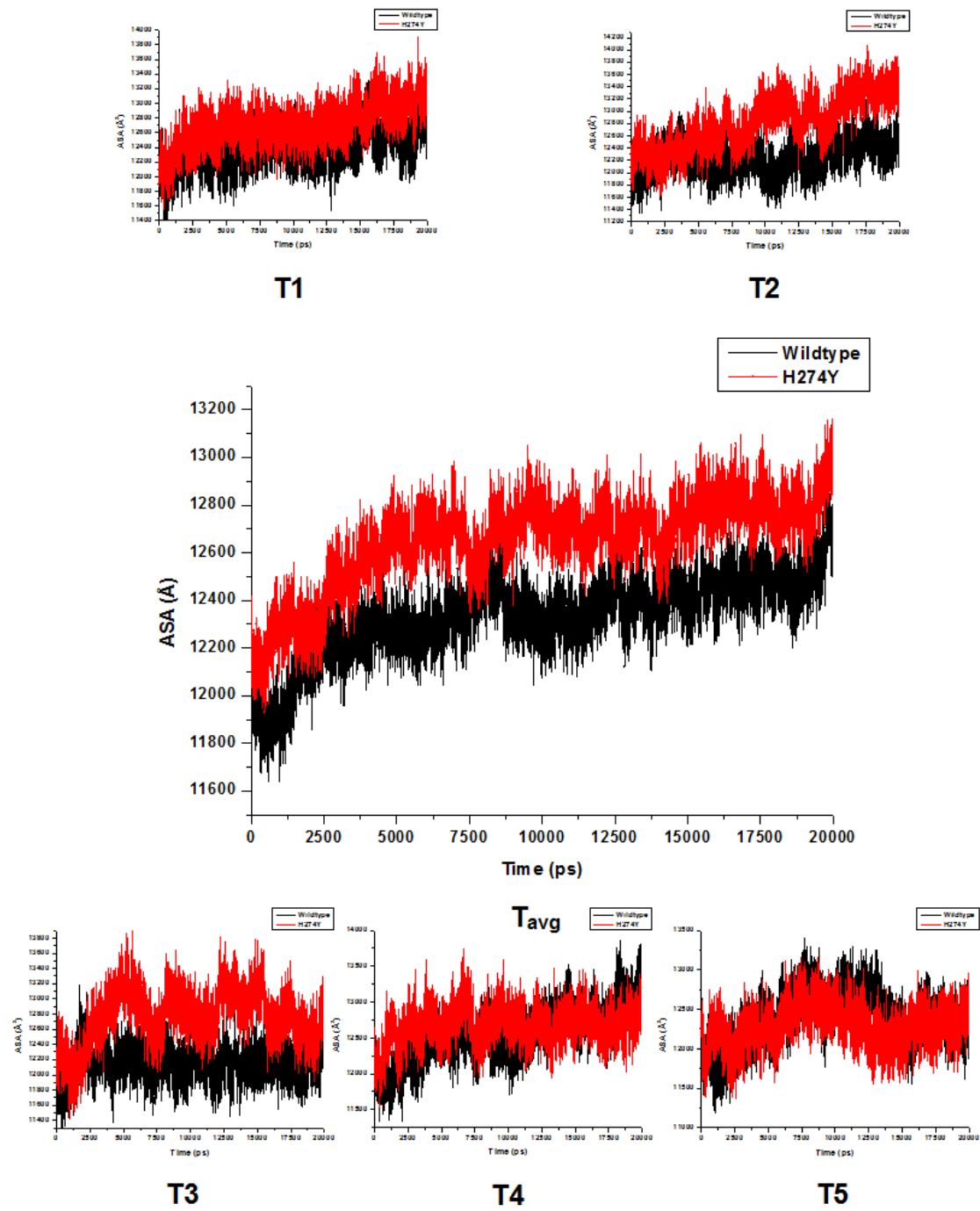


T4

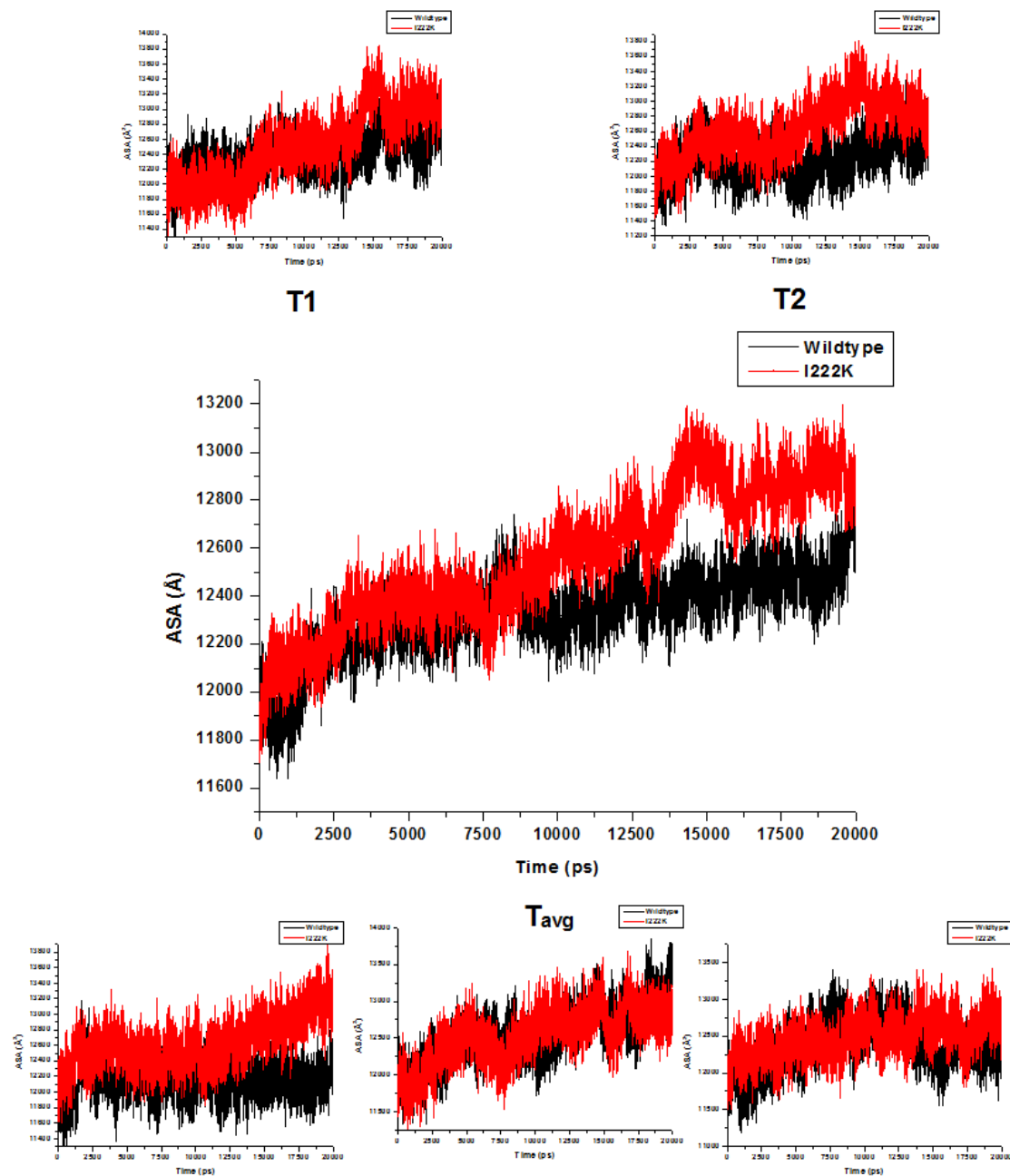


T5

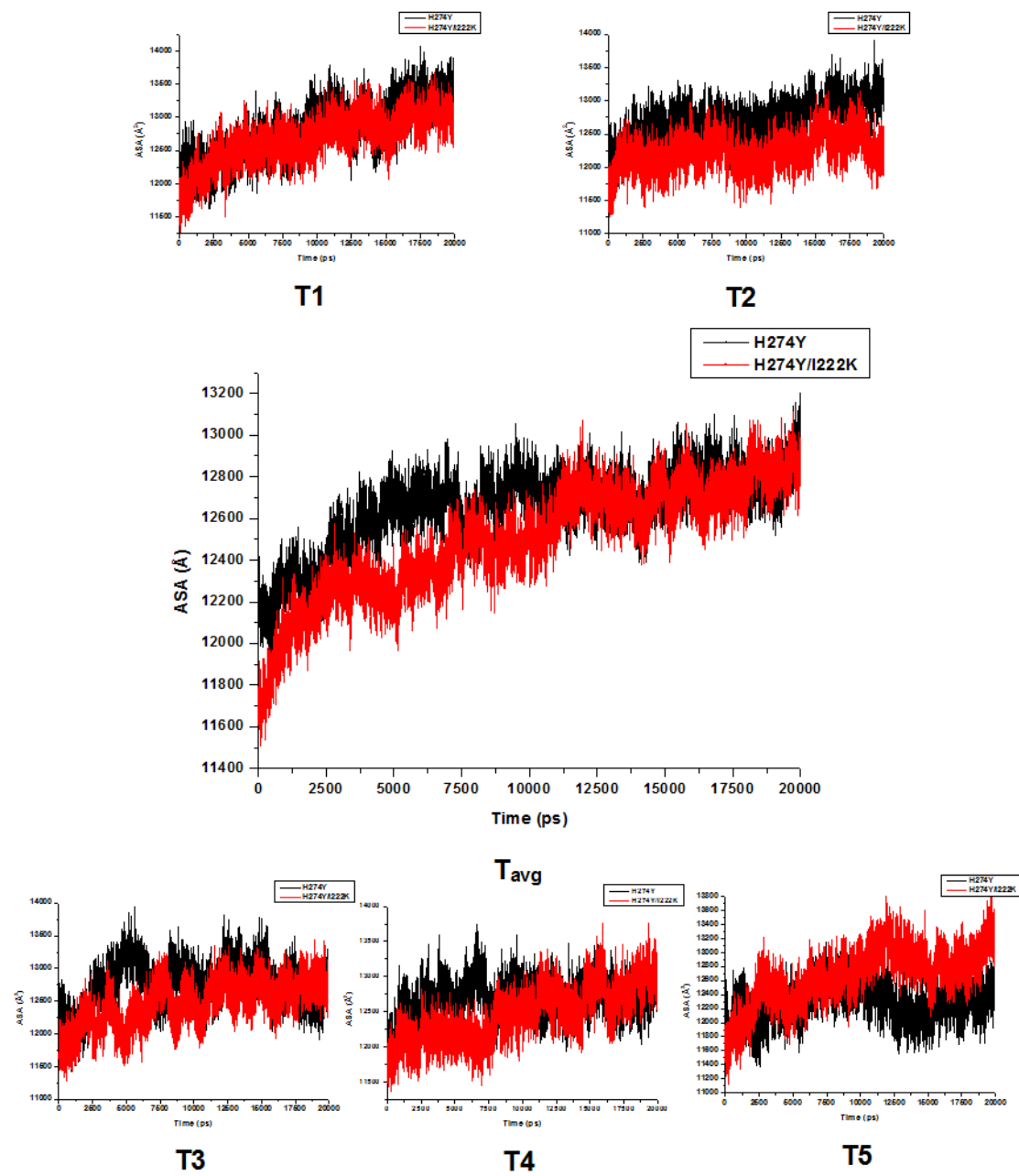
S40: SASA average of H274Y_{H5N1} and H274Y-I222K_{H5N1} over 20 ns



S41: SASA average of WT_{H1N1} and H274Y_{H1N1} over 20 ns



S42: SASA average of WT_{H1N1} and I222K_{H1N1} over 20 ns



S43: SASA average of H274Y_{H1N1} and H274Y-I222K_{H1N1} over 20 ns