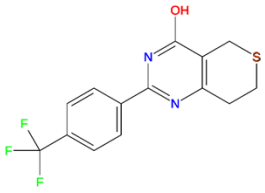
Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supplementary material



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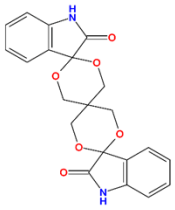

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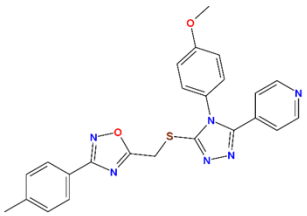

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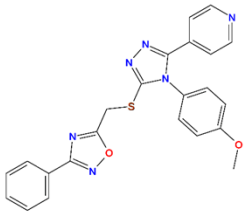

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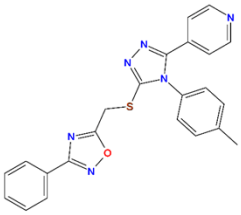

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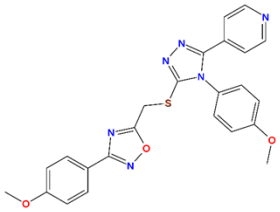

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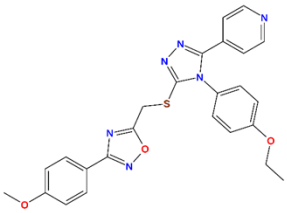

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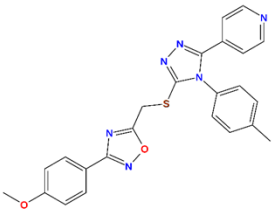

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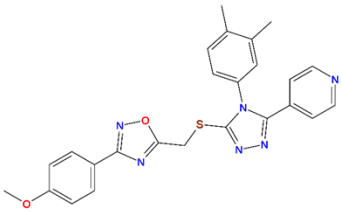

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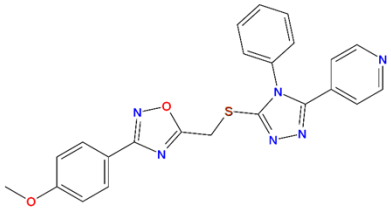

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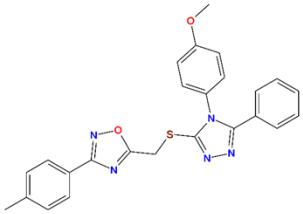

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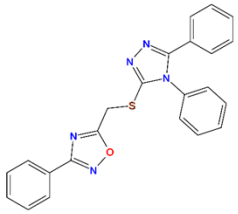

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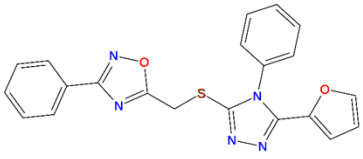

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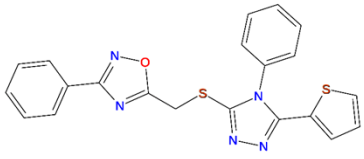

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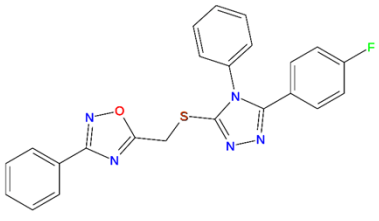

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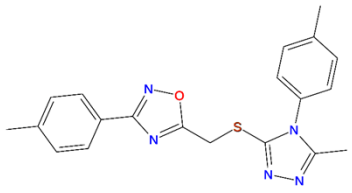

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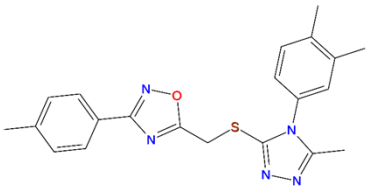

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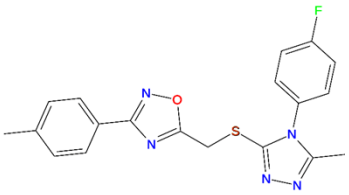

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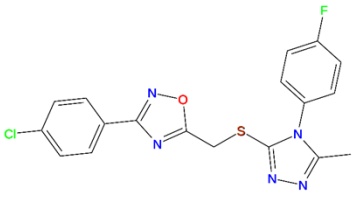

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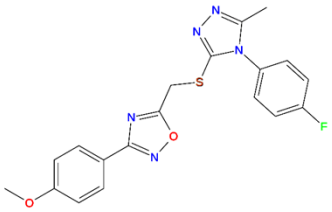

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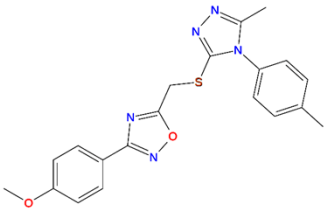

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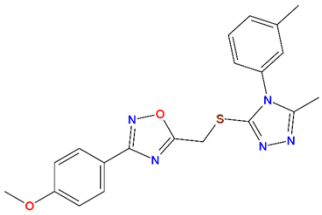

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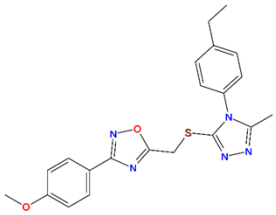

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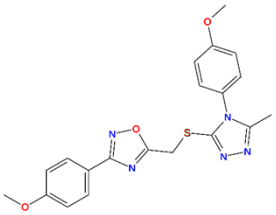

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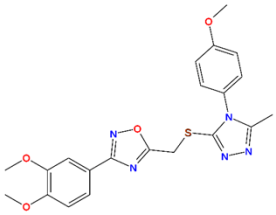

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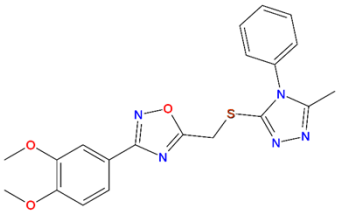

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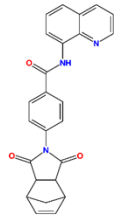
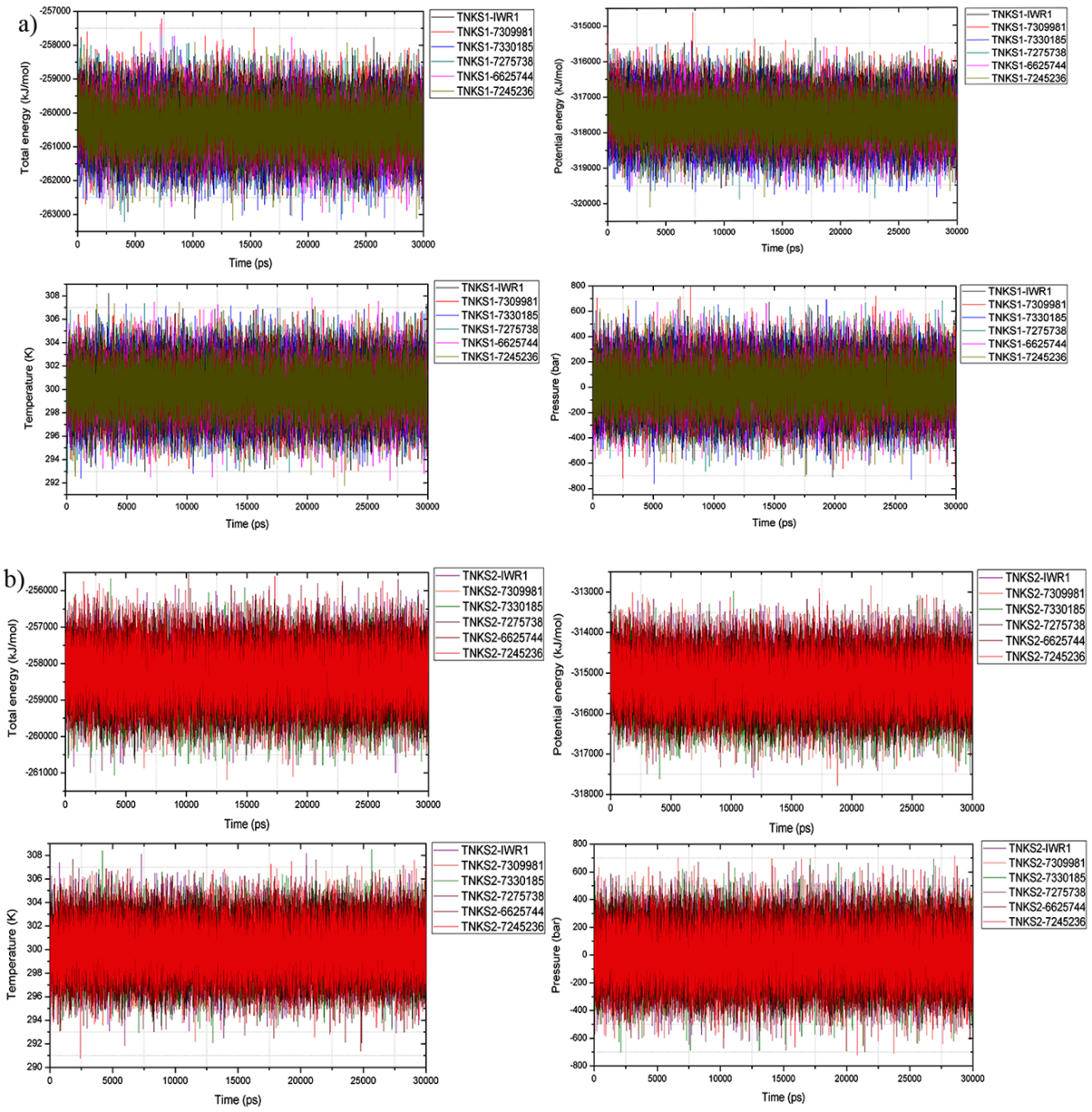
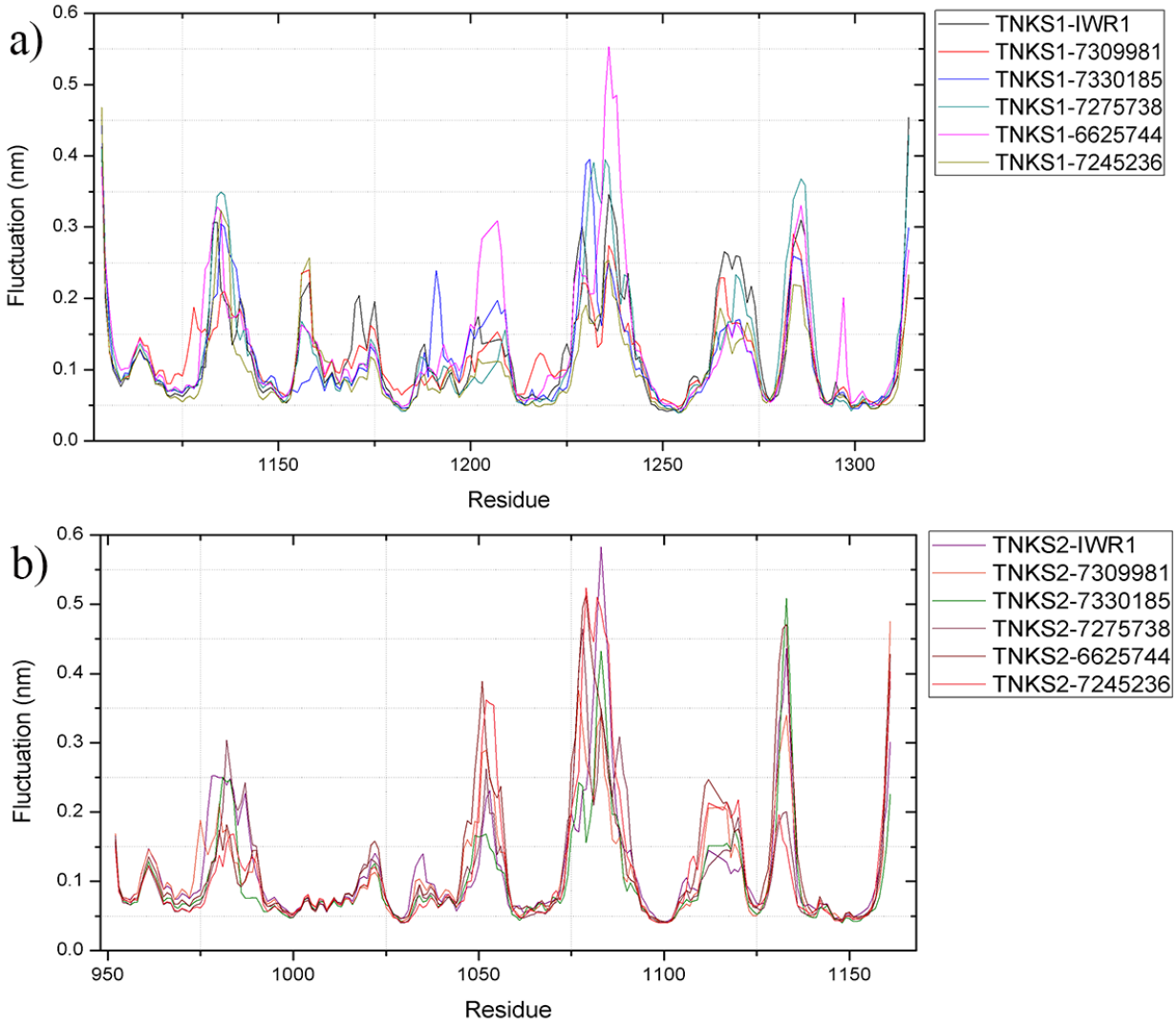


title: IWR-1

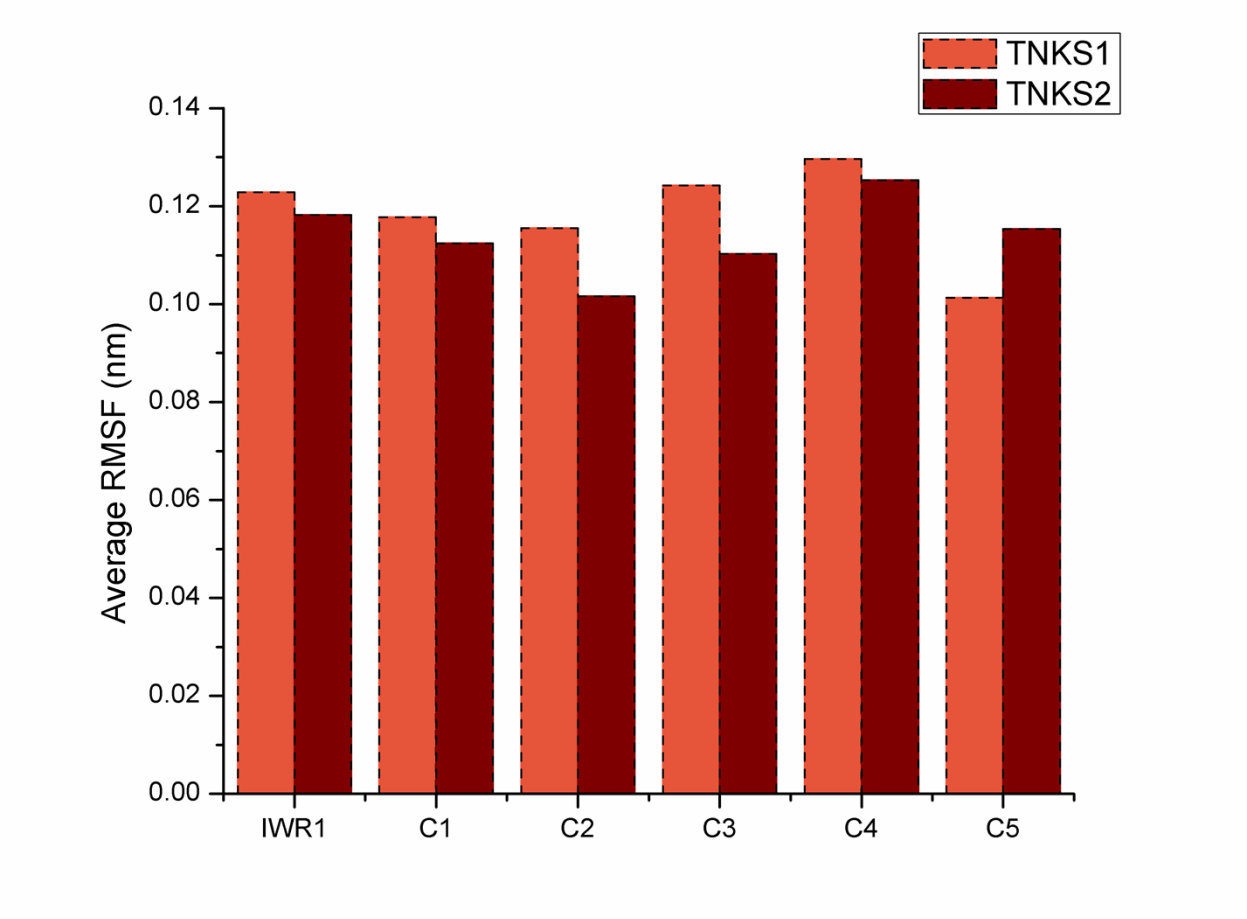
Supplementary Figure 1: Compounds reported to be dual inhibitors of TNKS1 and TNKS2 were selected as a training set for pharmacophore screening studies.



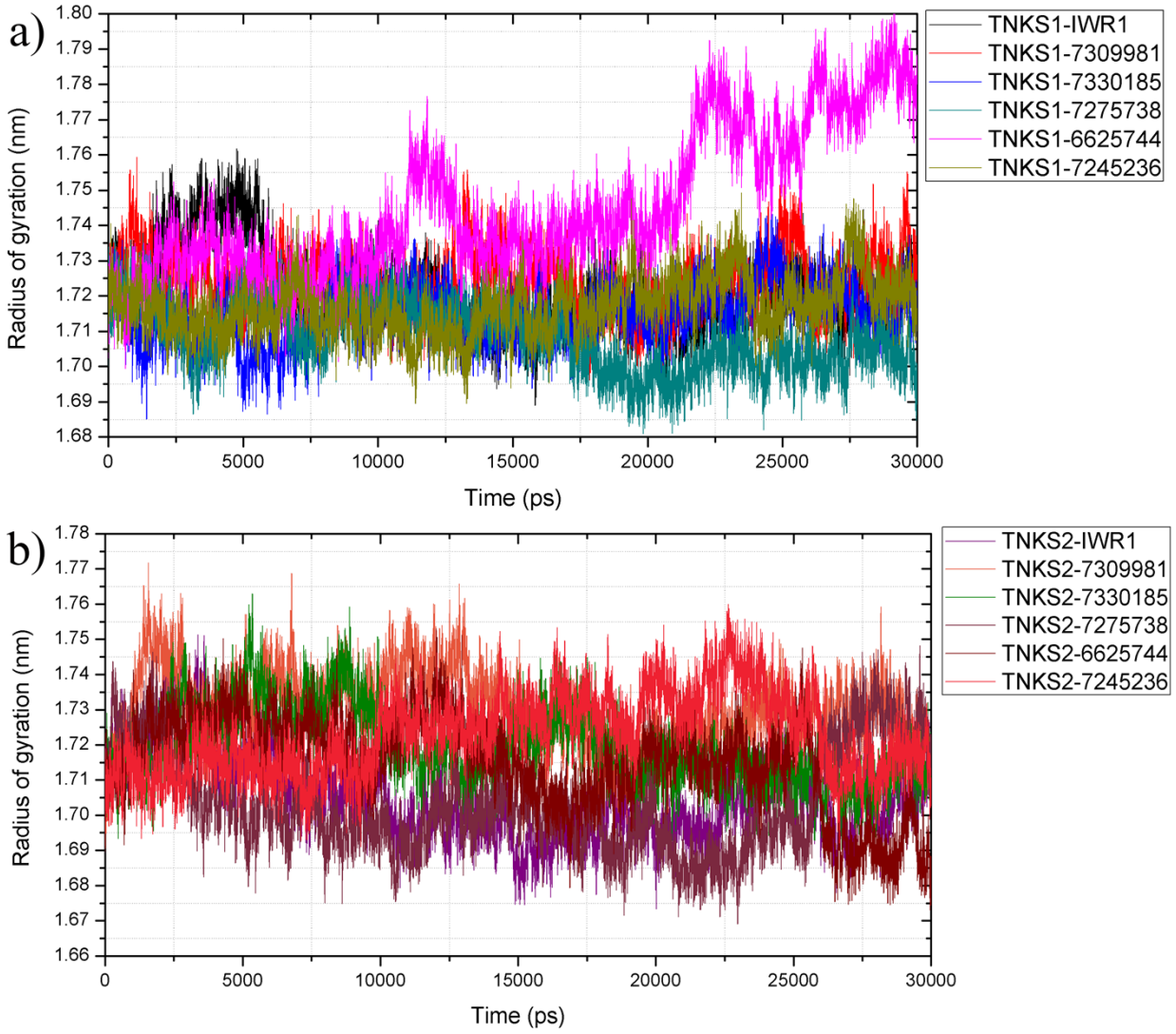
Supplementary Figure 2: a) Total energy, potential energy, temperature and pressure plots of MD simulation for TNKS1-IWR1, TNKS1-7309981, TNKS1-7330185, TNKS1-7275738, TNKS1-6625744 and TNKS1-7245236 complex in simulations of 30 ns. **b)** Total energy, potential energy, temperature and pressure plots of MD simulation for TNKS2-IWR1, TNKS2-7309981, TNKS2-7330185, TNKS2-7275738, TNKS2-6625744 and TNKS2-7245236 complex in simulations of 30 ns.



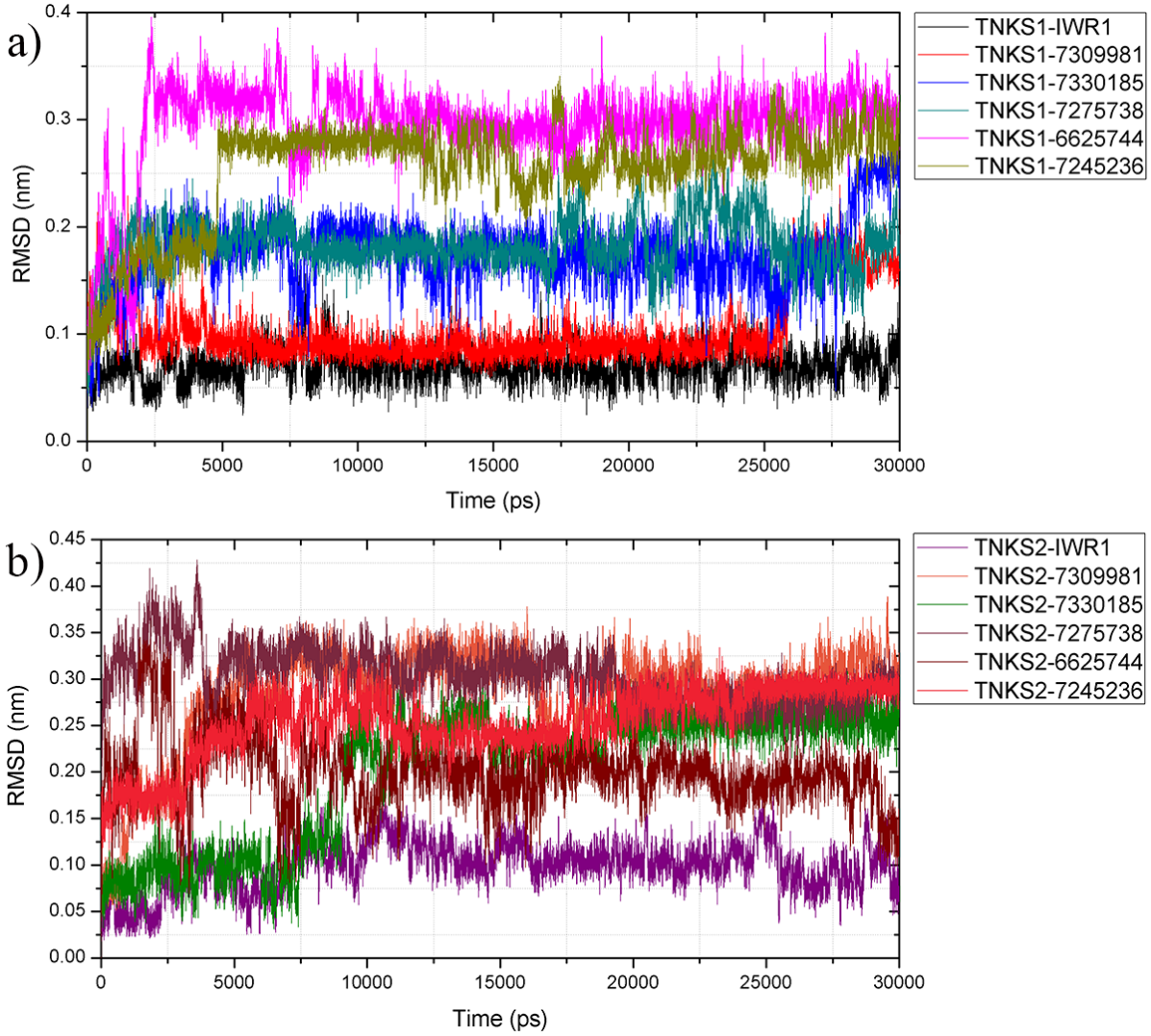
Supplementary Figure 3: Root mean square fluctuation of TNKS1 and TNKS2 in the presence of IWR1 and identified ligand molecules were depicted. a) TNKS1 b) TNKS2



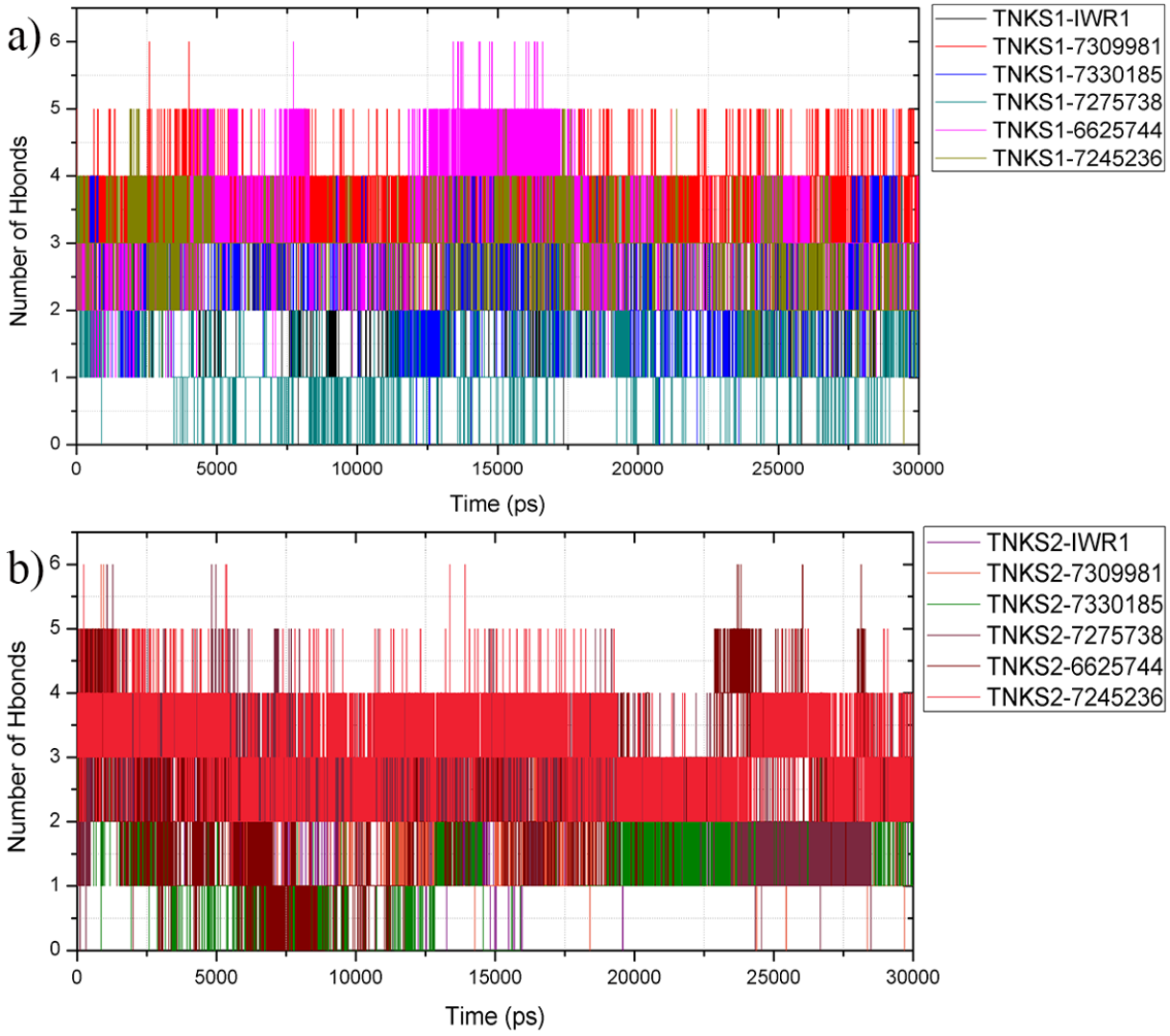
Supplementary Figure 4: The average means RMSF - using bars diagram was represented for the entire simulation time period against TNKS1 (orange) and TNKS2 (red) with all the compounds.



Supplementary Figure 5: The time evolution of the radius of gyration of TNKS1 and TNKS2 proteins the presence of IWR1 and identified ligand molecules were shows the compactness of structures with respect to time.



Supplementary Figure 6: RMSD of IWR1 and five ligand molecules in the active site residues of TNKS1 and TNKS2 during the 30 ns simulation time period. a) TNKS1 b) TNKS2



Supplementary Figure 7: Total number of intermolecular H bond interactions between IWR1 and five molecules in complex with TNKS1 and TNKS2 proteins. a) TNKS1 b) TNKS2