**File Description: created on 20.05.2020. updated on ---**

**This folder has five sub-folders.**

1. MD\_Simulations\_GSTs\_ASK1

This folder has MD simulation outputs of seven isoforms of GSTs with ASK1 (MAP3K5) in 7 sub folders named after the GST isoform type i.e. A1, M1, T1, P1, M3, and M5. The output of each isoform’s complex is present is separate directory. This is output generated from Gromacs package.

For example Folder **“A1” has the following files**

--- Essential Dynamics results of GSTA1

---RMSD data of GSTA1 from 0 to 20 ns

--Potential energy details of GSTA1 from 0 to 20 ns

--Radius of Gyration data of GSTA1 from 0 to 20 ns

**Similarly the sub folders of each isoform has the above mentioned files obtained for simulations of specific isoforms labelled accordingly representing that specific isoform.**

1. MD\_Simulations\_GSTs\_MAPK8

This folder has MD simulation outputs of seven isoforms of GSTs with MAPK8 in 7 sub folders named after the GST isoform type i.e. A1, M1, T1, P1, M3, and M5. The output of each isoform’s complex is present is separate directory. This is output generated from Gromacs package.

 --Essential Dynamics results of GSTA1

-- Potential energy details of GSTA1 from 0 to 20 ns

-- RMSD data of GSTA1 from 0 to 20 ns

-- Radius of Gyration data of GSTA1 from 0 to 20 ns

**Similarly, the sub folders of each isoform have the above-mentioned files obtained for simulations of specific isoforms.**

1. **Prediction\_of\_Hotspots**

This folder has output of interface residues, hotspot residues of each isoform complexed with MAPK8 and ASK1. This is the output generated from DrugScorePPI.

This folder has following PDF files, each file has the information about the interface residues and hot spot residues of each isoform in complex with ASK1 or MAPK8. User can understand output of each complex based on the file name.







1. **Protein\_Protein\_Docking\_GSTs\_ASK1:**

This folder has output of HADDOCK, protein-protein complex (GSTs with ASK1), details of intermolecular interactions (PDBSUM) and binding affinity parameters (PRODIGY). The output of each isoform’s is present is separate directory.

For example Folder **“GSTA1” has the following files**

Prodigy Folder – out put obtained form PRODIGY server such as binding affinity, interfacial residue details, etc.

--Protein-Protein complex generated from HADDOCK

--Output and Screenshot of HADDOCK easy interface server

 --This file has the output obtained from PDBSum server

**Similarly, the sub folders of each isoform have the above-mentioned files obtained for simulations of specific isoforms.**

1. **Protein\_Protein\_Docking\_GSTs\_MAPK8:**

This folder has output of HADDOCK, protein-protein complex (GSTs with ASK1), details of intermolecular interactions (PDBSUM) and binding affinity parameters (PRODIGY). The output of each isoform’s is present is separate directory.

For example, Folder **“GSTA1” has the following files**

Prodigy Folder – out put obtained from PRODIGY server such as binding affinity, interfacial residue details, etc.

--Protein-Protein complex generated from HADDOCK

--Output and Screenshot of HADDOCK easy interface server

 --This file has the output obtained from PDBSum server

**Similarly, the sub folders of each isoform have the above-mentioned files obtained for simulations of specific isoforms.**