**Compressed folder name:** MSM\_python\_notebooks.zip

**Folder structure:**

**MSM\_python\_notebooks**

|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Dataset-I-Feature-Selection.ipynb

|Python script for selection of features (16 Cα-Cα distances) for the apo-p53 |simulations at 300 K and 310 K (Dataset-I).

|

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|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_Dataset-II-Feature-Selection.ipynb

|Python script for selection of features (32 Cα-Cα distances) for the |DNA-bound p53 simulations at 300 K and 310 K (Dataset-I).

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|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_LowTemp-Dataset-I-MSM.ipynb

|Python script for MSM calculations performed on apo-p53 simulations at |300 K (LowTemp-Dataset-I) using the 16 Cα-Cα distances as feature set.

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|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_HighTemp-Dataset-I-MSM.ipynb

|Python script for MSM calculations performed on apo-p53 simulations at |310 K (HighTemp-Dataset-I) using the 16 Cα-Cα distances as feature set.

|

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|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_LowTemp-Dataset-II-MSM.ipynb

|Python script for MSM calculations performed on DNA-bound p53 |simulations at 300 K (LowTemp-Dataset-II) using the 32 Cα-Cα distances as |feature set.

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|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_HighTemp-Dataset-II-MSM.ipynb

|Python script for MSM calculations performed on DNA-bound p53 |simulations at 310 K (HighTemp-Dataset-II) using the 32 Cα-Cα distances |as feature set.

|

|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ WT\_ZAFF.pdb

Topology file used for MSM calculations

**Compressed folder name: MD\_inputs.zip**

**Folder structure:**

**MD\_inputs**

|\_\_\_\_\_\_LowTemp-Dataset-I

| |

| |

| |\_\_\_\_\_\_\_ apo-p53.prmtop (Parameter/topology file for apo-p53)

| |

| |

| |\_\_\_\_\_\_\_ apo-p53.minrst (Minimized co-ordinated for apo-p53)

| |

| |

| |\_\_\_\_\_\_\_ heat\_solv\_300K.in (Input file for heating solvent at 300K)

| |

| |

| |\_\_\_\_\_\_\_ heat\_all\_300K.in (Input file for heating the system at 300K)

| |

| |

| |\_\_\_\_\_\_\_ equi\_300K.in (Input file for equilibration at 300K)

| |

| |

| |\_\_\_\_\_\_\_ prod\_300K.in (Input file for production run at 300K for 1μs)

|

|

|

|\_\_\_\_\_\_HighTemp-Dataset-I

| |

| |

| |\_\_\_\_\_\_\_ apo-p53.prmtop (Parameter/topology file for apo-p53)

| |

| |

| |\_\_\_\_\_\_\_ apo-p53.minrst (Minimized co-ordinated for apo-p53)

| |

| |

| |\_\_\_\_\_\_\_ heat\_solv\_310K.in (Input file for heating solvent at 310K)

| |

| |

| |\_\_\_\_\_\_\_ heat\_all\_310K.in (Input file for heating the system at 310K)

| |

| |

| |\_\_\_\_\_\_\_ equi\_310K.in (Input file for equilibration at 310K)

| |

| |

| |\_\_\_\_\_\_\_ prod\_310K.in (Input file for production run at 310K for 1μs)

|

|

|

|\_\_\_\_\_\_LowTemp-Dataset-II

| |

| |

| |\_\_\_\_\_\_\_ DNA\_bound\_p53.prmtop (Parameter/topology file for | | DNA-bound-p53)

| |

| |\_\_\_\_\_\_\_ DNA\_bound\_p53.minrst (Minimized co-ordinate file for | | DNA-bound-p53)

| |

| |\_\_\_\_\_\_\_ heat\_solv\_300K.in (Input file for heating solvent at 300K)

| |

| |

| |\_\_\_\_\_\_\_ heat\_all\_300K.in (Input file for heating the system at 300K)

| |

| |

| |\_\_\_\_\_\_\_ equi\_300K.in (Input file for equilibration at 300K)

| |

| |

| |\_\_\_\_\_\_\_ prod\_300K.in (Input file for production run at 300K for 1μs)

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|\_\_\_\_\_\_HighTemp-Dataset-II

|

|

|\_\_\_\_\_\_\_ DNA\_bound\_p53.prmtop (Parameter/topology file for | DNA-bound-p53)

|

|\_\_\_\_\_\_\_ DNA\_bound\_p53.minrst (Minimized co-ordinate file for | DNA-bound-p53)

|

|\_\_\_\_\_\_\_ heat\_solv\_310K.in (Input file for heating solvent at 310K)

|

|

|\_\_\_\_\_\_\_ heat\_all\_310K.in (Input file for heating the system at 310K)

|

|

|\_\_\_\_\_\_\_ equi\_310K.in (Input file for equilibration at 310K)

|

|

|\_\_\_\_\_\_\_ prod\_310K.in (Input file for production run at 310K for 1μs)