

Captions for the five movie/mpg files

1. HDAC2-SAHA-Ca-K.mpg

Title: The “Metal-dependent” regulatory effect for the $\text{Ca}^{2+} \rightarrow \text{K}^+$ mutant model.

Description: The remote “second metal site” dependent regulatory effect on the deprotonation of SAHA in HDAC2 after the $\text{Ca}^{2+} \rightarrow \text{K}^+$ mutation. The proton on the SAHA:O1 atom could rapidly transfer to the H145 residue after the $\text{Ca}^{2+} \rightarrow \text{K}^+$ mutation.

2. HDAC2-SAHA-Ca-K-Y308H.mpg

Title: The “Metal-dependent” regulatory effect for the $\text{Ca}^{2+} \rightarrow \text{K}^+/\text{Y308H}$ mutant model.

Description: The remote “second metal site” dependent regulatory effect on the deprotonation of SAHA in HDAC2 after the $\text{Ca}^{2+} \rightarrow \text{K}^+/\text{Y308H}$ mutation. The proton on the SAHA:O1 atom could rapidly transfer to the H145 residue after the $\text{Ca}^{2+} \rightarrow \text{K}^+/\text{Y308H}$ mutation.

3. HDAC2-SAHA-Ca-No.mpg

Title: The “Metal-dependent” regulatory effect for the $\text{Ca}^{2+} \rightarrow \text{No}$ mutant model.

Description: The remote “second metal site” dependent regulatory effect on the deprotonation of SAHA in HDAC2 after the $\text{Ca}^{2+} \rightarrow \text{No}$ mutation. The proton on the SAHA:O1 atom could rapidly transfer to the H145 residue after the $\text{Ca}^{2+} \rightarrow \text{No}$ mutation.

4. HDAC2-SAHA-wild type.mpg

Title: The “Metal-dependent” regulatory effect for the wild type model.

Description: The remote “second metal site” dependent regulatory effect on the deprotonation of SAHA in the wild type HDAC2. The proton on the SAHA:O1 atom could hardly transfer to the H145 residue in the wild type HDAC2.

5. HDAC2-SAHA-Y308H.mpg

Title: The “Metal-dependent” regulatory effect for the Y308H mutant model.

Description: The remote “second metal site” dependent regulatory effect on the deprotonation of SAHA in HDAC2 after the Y308H mutation. The proton on the SAHA:O1 atom could hardly transfer to the H145 residue after the Y308H mutation.