

***Homo sapiens* MDH1**

Uniprot ID: P40925

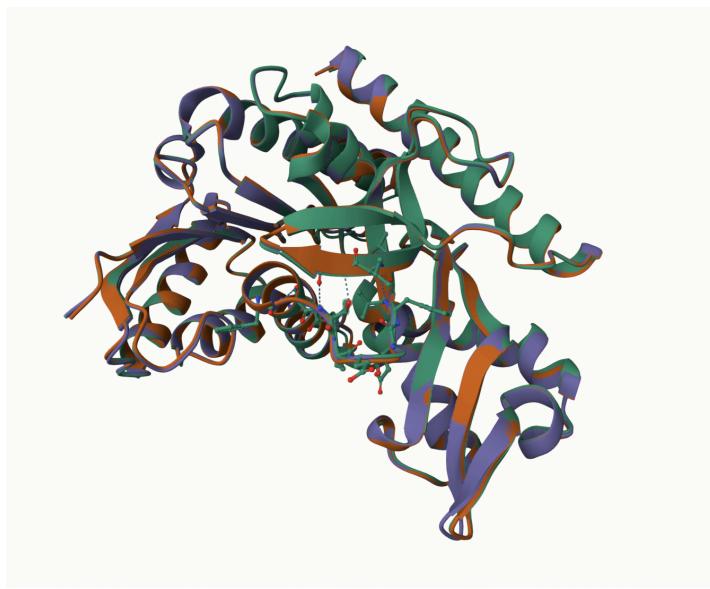
Variation: Phosphorylation of T261

Description

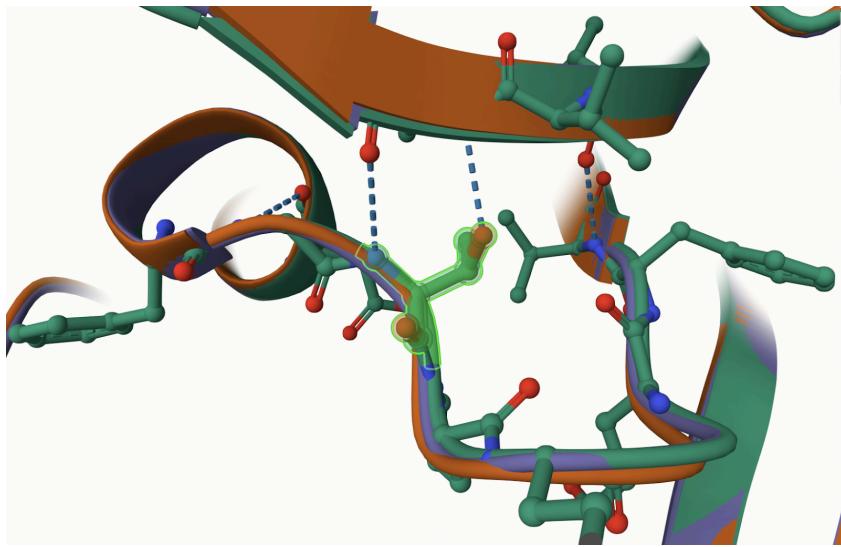
Threonine 261 was identified in Humans, *Homo sapiens* as a post-translationally modified site (Malone University). The study recognized the possibility that the PTM amino acid could have a possible effect on the stability of the MDH1 molecule. At this time there are no other functional studies of this site of the amino acid.

Comparison of MDH1 models and phospho modified MDH1

1. Alignment of MDH1 (green), MDH1 with PhosphoT 261 (orange) and T261D (violet)



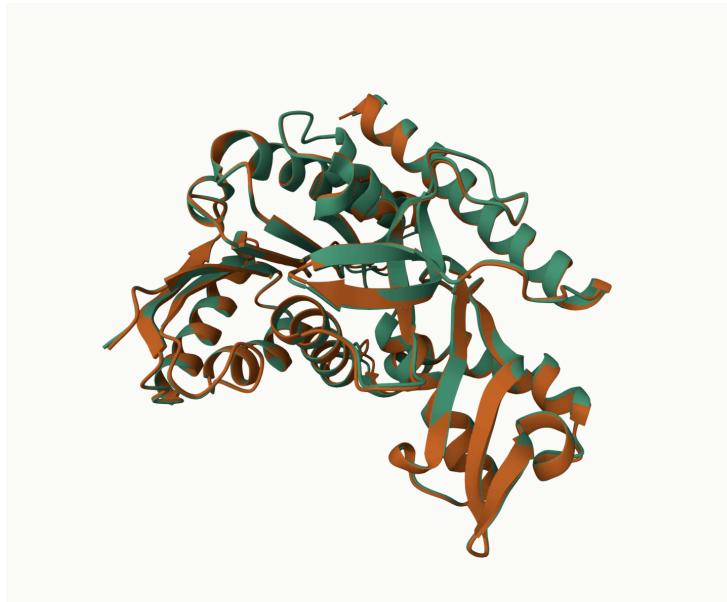
Modification site alignment in MDH1



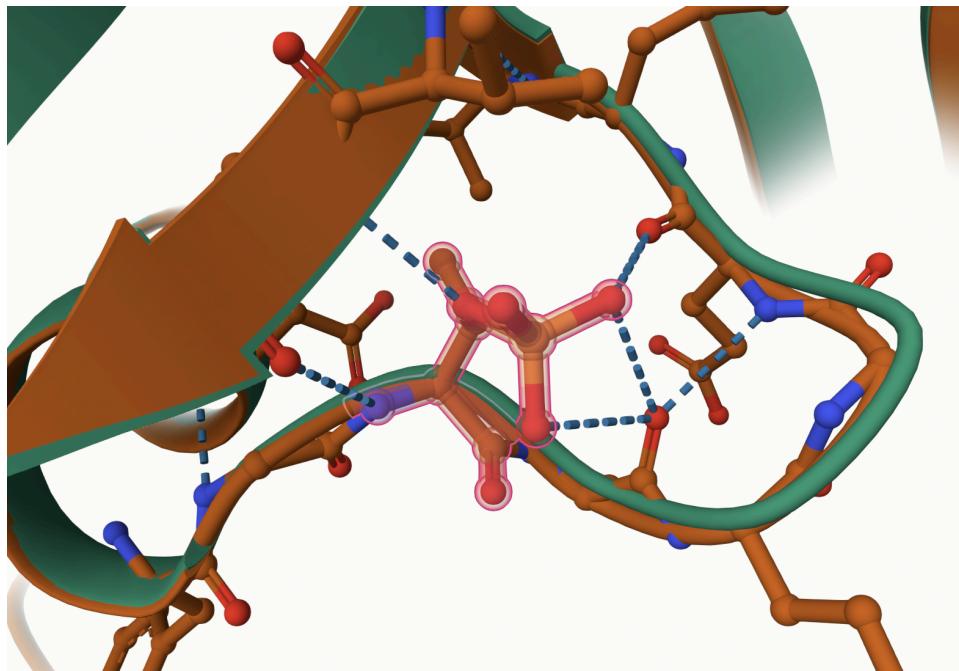
The modification site is near and most active with I292 which when altered could affect hydrogen bonds and make it less stable.

Effect of the sequence variant and PTM on MDH dynamics

The RMSD value of MDH1 (green) and MDHT261D (orange) is .45 Å



The simulations show that the two proteins are very similar the lower the Å the more closely the two molecules are to one another.

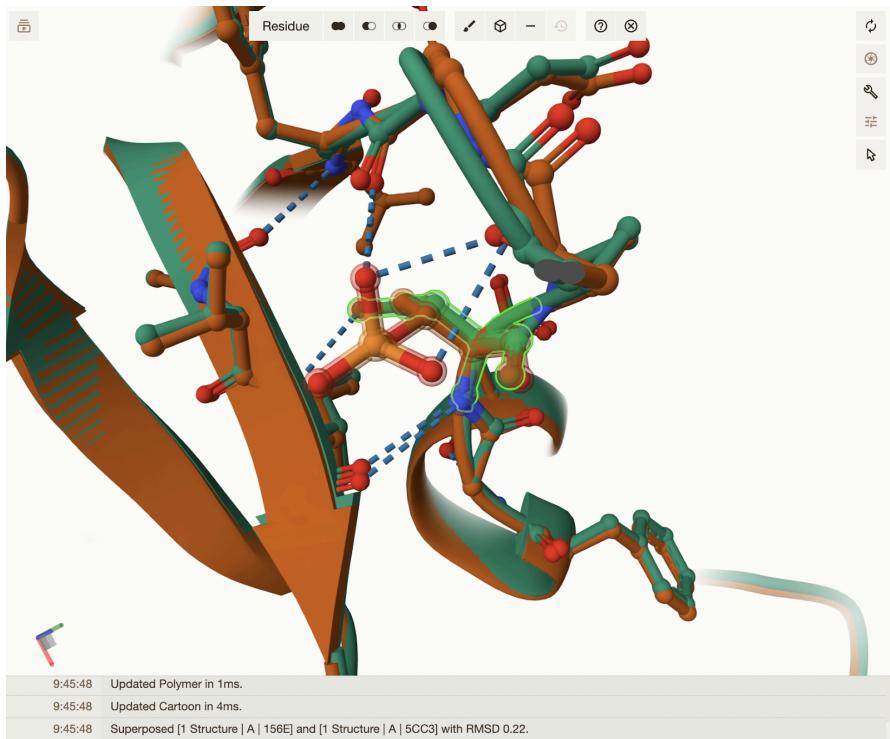


Comparison of the enzyme dynamics

Effects of the modification on the pKa values

Comparison of the mimic and the authentic PTM

The authentic PTM and mimic superimposed on one another. The RMSD value was .22 Å. This means that there was no major difference in structure or position of the proteins.



Authors

Thomas A. Stillwell