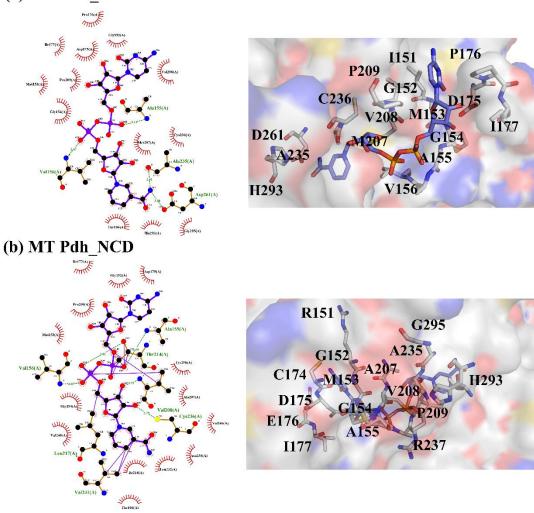
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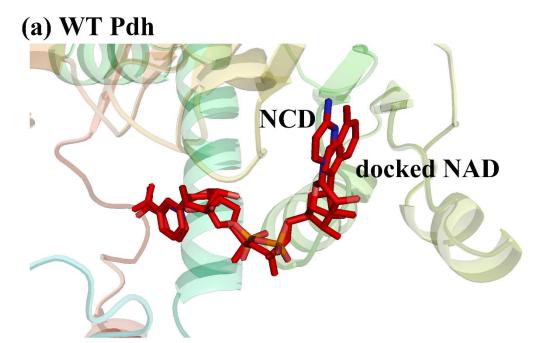
## Figure S1

## (a) WT Pdh\_NCD



**Figure S1 The surrounding residues of Pdh\_NCD.** (a) the surrounding residues of WT Pdh\_NCD, (b) the surrounding residues of MT Pdh\_NCD.

## Figure S2



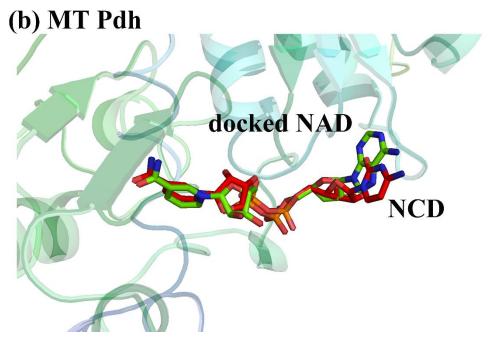


Figure S2 Comparison of NAD's docking results with the original position. (a) the position of docked NAD and NCD in WT Pdh, (b) the position of docked NAD and NCD in MT Pdh.