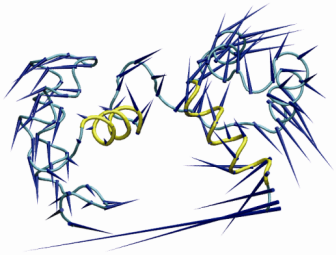
Cite this as: Jinru WENG, Shuo YANG, Jinkang SHEN, Hongsen LIU, Yuzi XU, Dongyun HAO, Shan WANG. Molecular dynamics simulation reveals DNA-specific recognition mechanism via c-Myb in pseudo-palindromic consensus of *mim-1* promoter[J]. Journal of Zhejiang University Science B, 2023, 24(10): 883-895. http://doi.org/10.1631/jzus.B2200634

Molecular dynamics simulation reveals DNA-specific recognition mechanism via c-Myb in pseudo-palindromic consensus of *mim-1* promoter

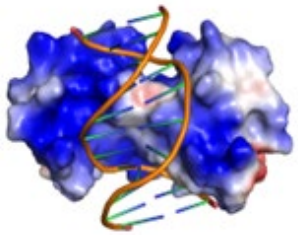
Key words: c-Myb; DNA-specific recognition mechanism; molecular dynamics simulation; major groove width; electrostatic potential

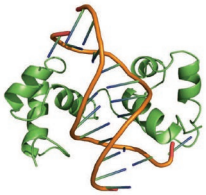
Research Summary

This article aims to answer a question of what might be the DNA-specific binding mechanism of c-Myb transcription factor during the regulation of cell early differentiation and proliferation:

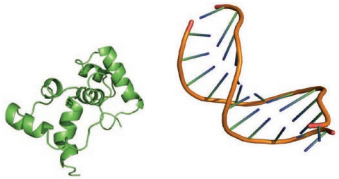


- **A pseudo-palindromic sequence of c-Myb binding site in *mim-1* was chosen as a target to study the binding specificity**



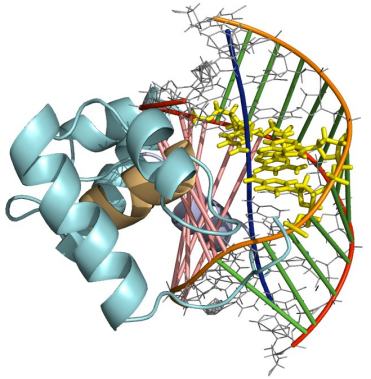


- **MD simulation studies identified the DNA-specific recognition mechanism by c-Myb in the 3D-structure level**





- **The trials in vitro confirmed the simulation results**



Innovation points

- **MD simulation studies revealed that c-Myb binding with *mim-1* in the forward strand is more stable than that in the reverse strand.**

- **PCA dynamics trajectory analyses suggested an opening motion of the recognition helices of R2R3, resulting in the dissociation of DNA from c-Myb in complex R at 330 K**

- **The major groove width of DNA are vital for the specific recognition of c-Myb.**

- **The trials in vitro confirmed the simulation results, that is, c-Myb specifically bound to mim-1 in the forward strand.**

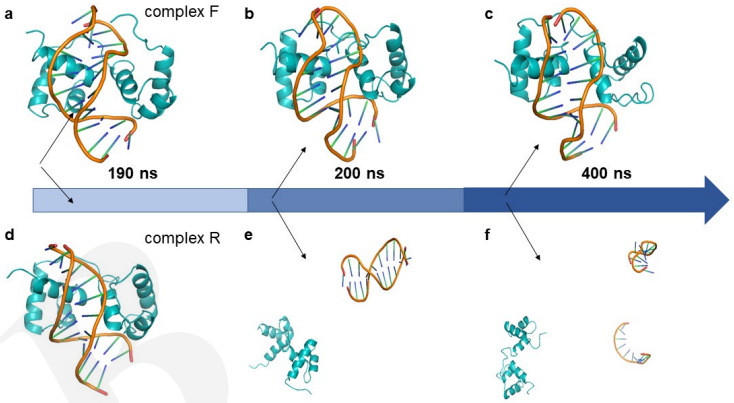


Figure 2

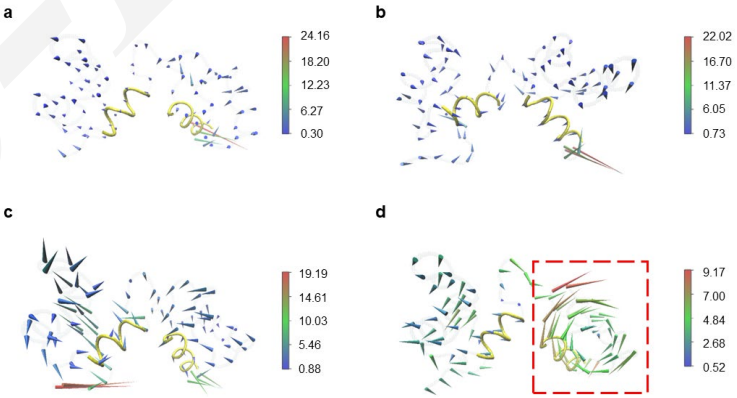


Figure 5

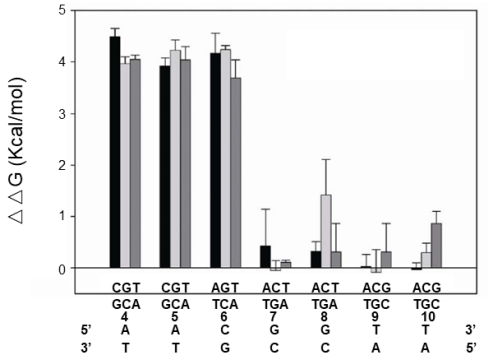


Figure 10