

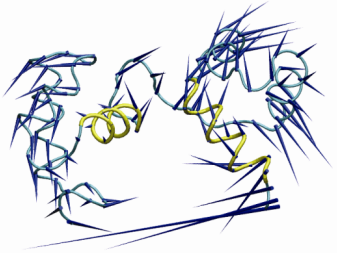
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Molecular dynamics simulation reveals DNA-specific recognition mechanism via c-Myb in pseudo-palindromic consensus of *mim-1* promoter

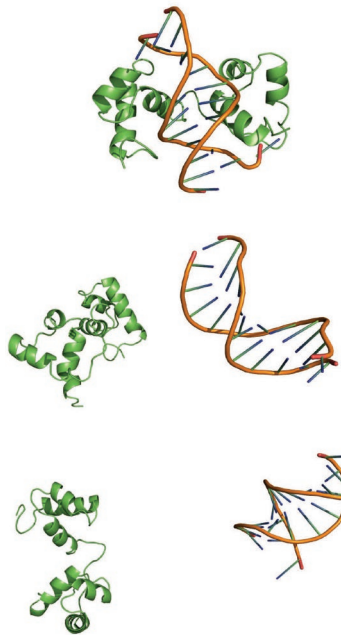
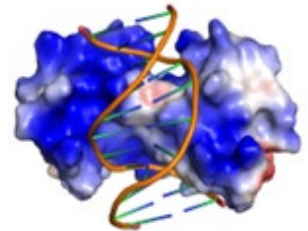
Key words: c-Myb; DNA-specific recognition mechanism;
molecular dynamics simulation; major groove
width; electrostatic potential

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:

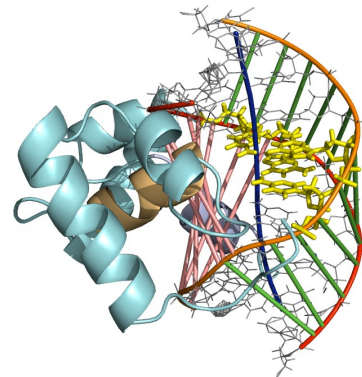


- A pseudo-palindromic sequence of c-Myb binding site in *mim-1* was chosen as a target to study the binding specificity



- 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.

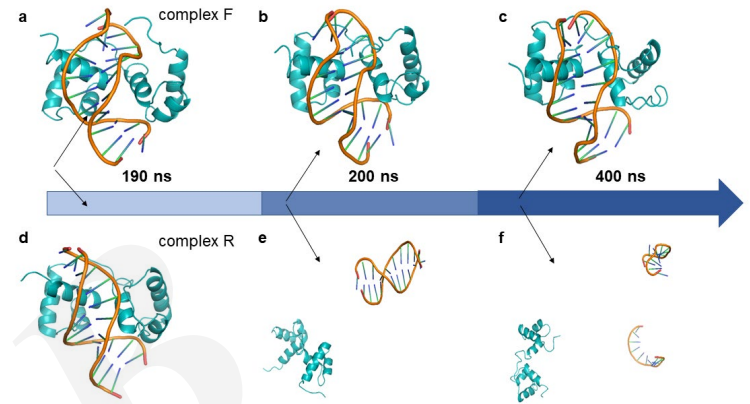


Figure 2

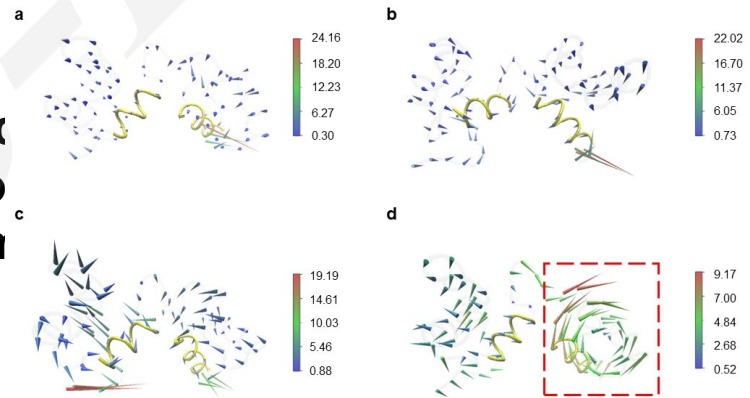


Figure 5

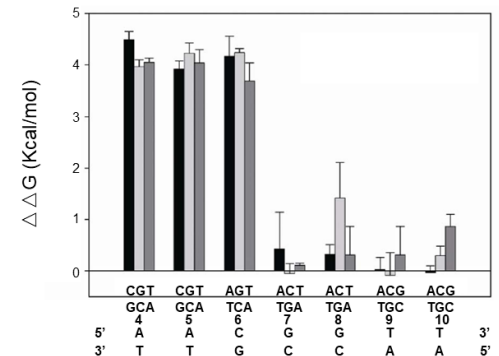


Figure 10