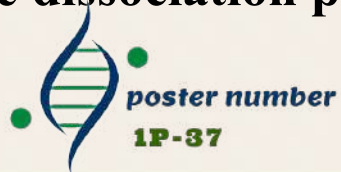




Investigating the dissociation process and binding free energy of the p53-DBD/DNA complex

Tokyo Tech



poster number
1P-37

by PaCS-MD and MSM

Mohamed Marzouk^{1,2} and Akio Kitao¹

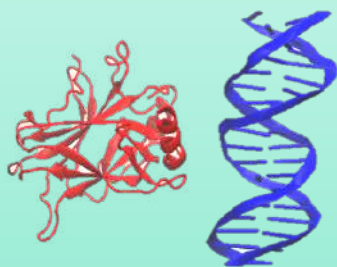
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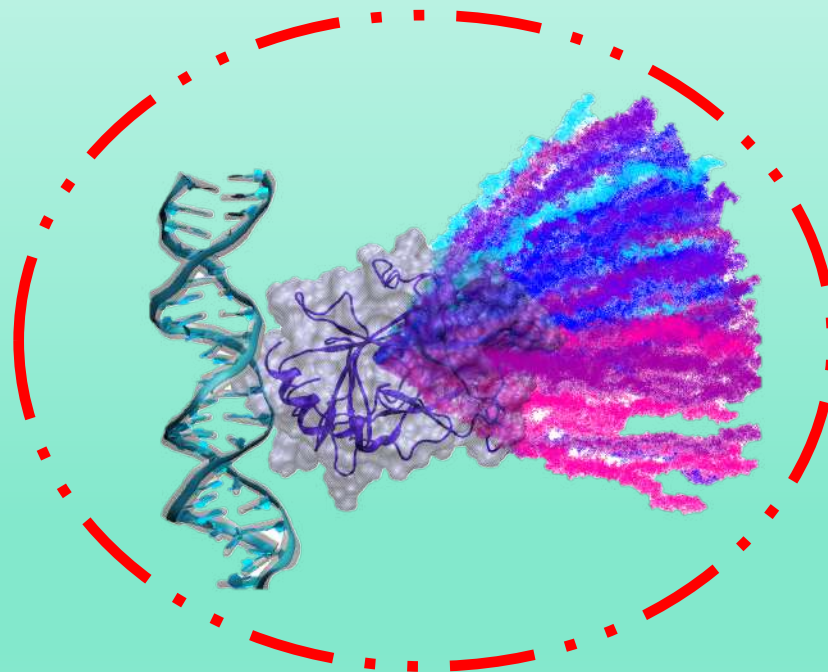
Dissociation simulation



PaCS-MD

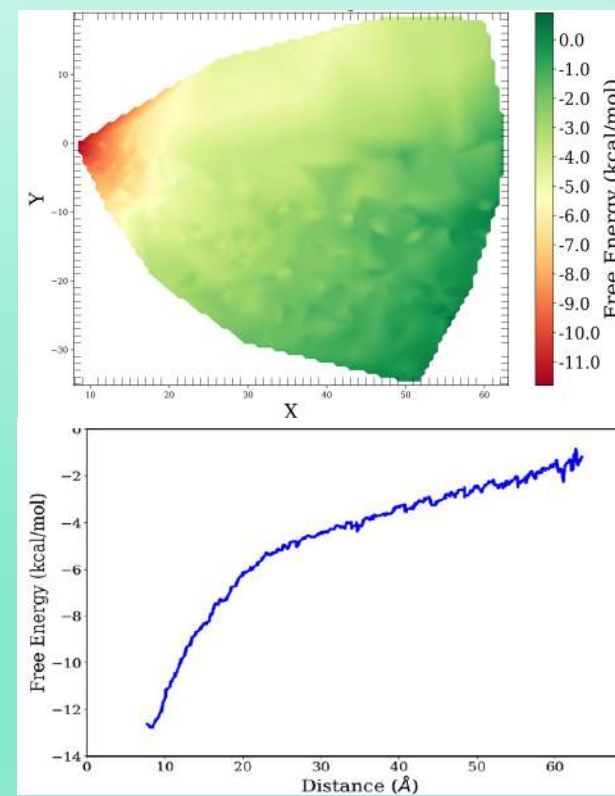
Parallel cascade selection molecular dynamics

Dissociation pathways



75 different dissociation pathways obtained by ran PaCS-MD for five different starting conformations

Free energy analysis by MSM



Binding free energy

● Predicted value : 11.8 kcal/mol

● Experimental value : 11.1 kcal/mol