DNA-dcm-Vsr Endonuclease DNA-TATA box binding protein DNA-p53 tumor suppressor protein DNA-Integration host factor DNA-MATα2 homeodomain DNA-TnpA Transposase 5IU — G -nick

Nikolova, Zhou, Gottardo, Alvey, Kimsey, Al-Hashimi *Biopolymers* 2013 v. 99 p. 955

Simulation philosophy

- Unbiased dynamics: Make as few assumptions as possible about what degrees of freedom are important
- Full atomistic (explicit water): high resolution; include effect of water on hydrogen bonding
- Calculate rates, observe mechanisms:
 Compare with experiment and provide new insight