



école _____
normale _____
supérieure _____
paris-saclay _____



Erika Balog



Bálint Dudás

Activation mechanism of an autoinhibited small GTPase: RalF



Jacqueline Cherfils

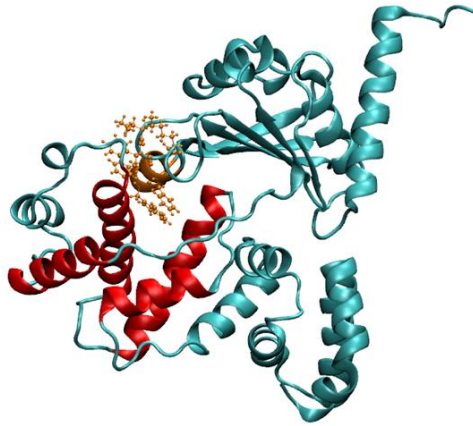


David Perahia

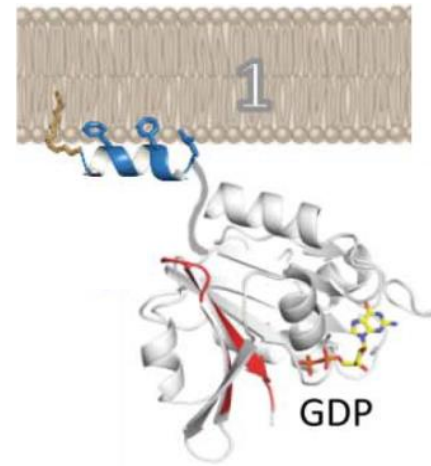


François Peurois

autoinhibited RalF



Arf-GDP



How does it open?

close conformation \longrightarrow open conformation

- how does it open?
- what is the open conformation that binds Arf?

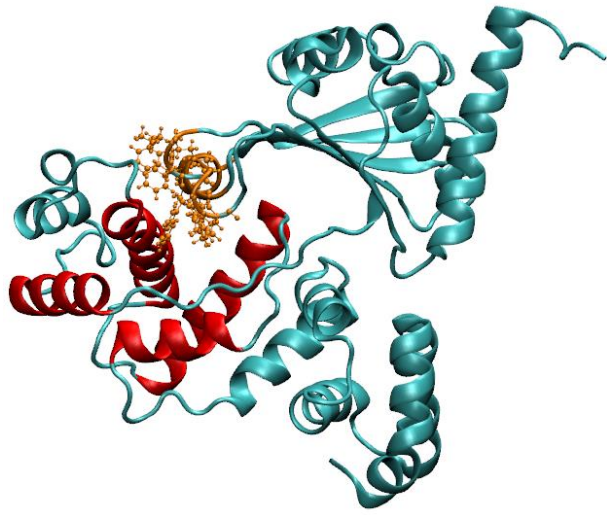
➤ no experimental method

➤ computer simulation:

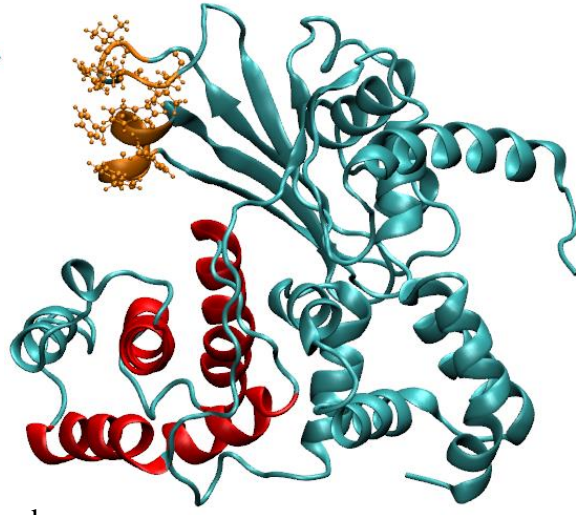
- Molecular Dynamics (MD) does not reach this scale

challenging...

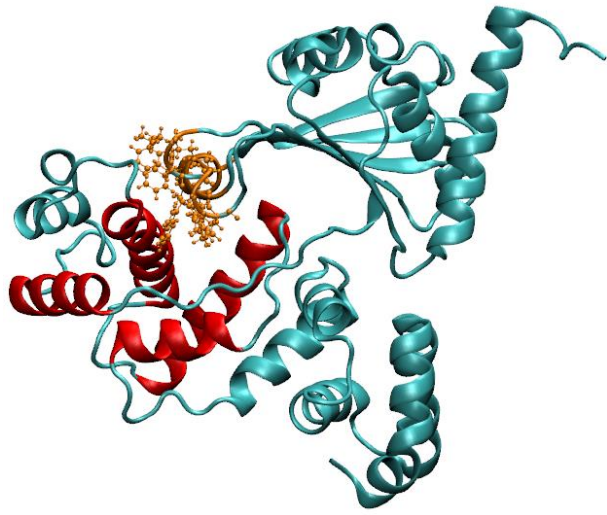
- Molecular Dynamics with excited Normal Modes (MDeNM) – David Perahia



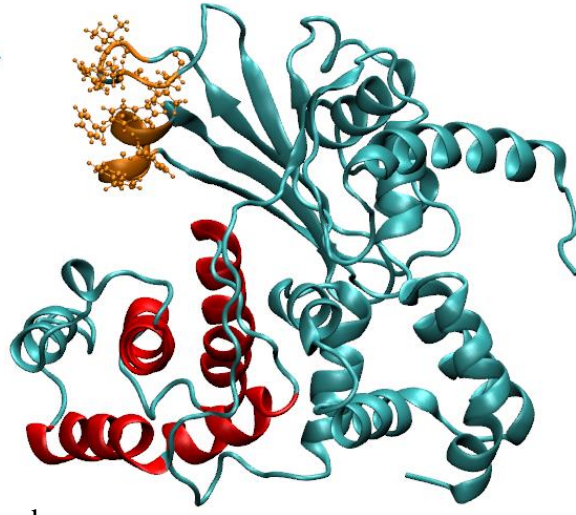
a



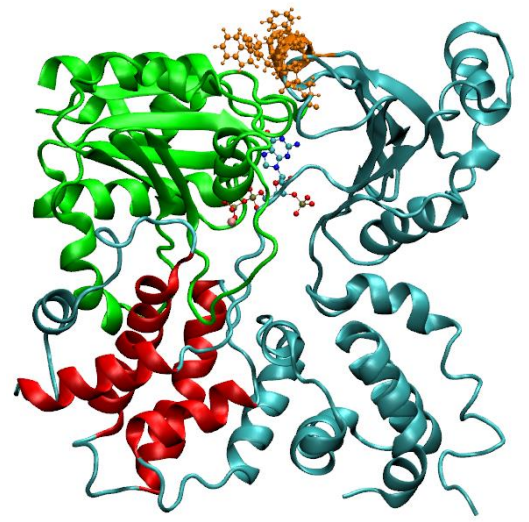
b



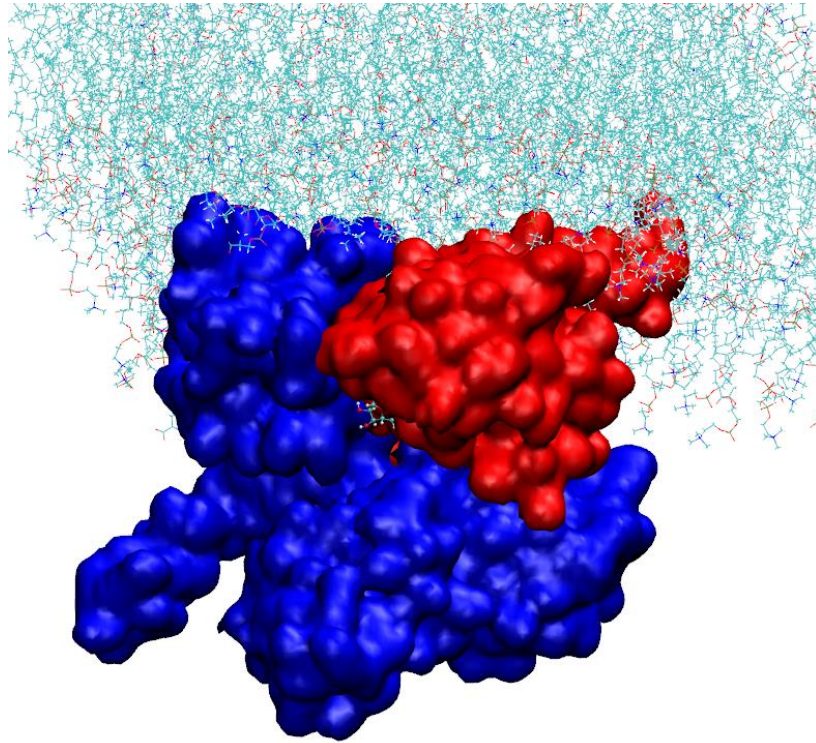
a



b



c



- ❖ Long term collaboration with David Perahia (over 15 years)
- ❖ Future: elucidate the activation mechanism of other biologically relevant macromolecules