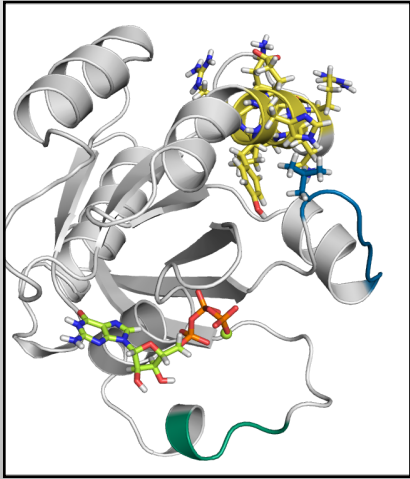




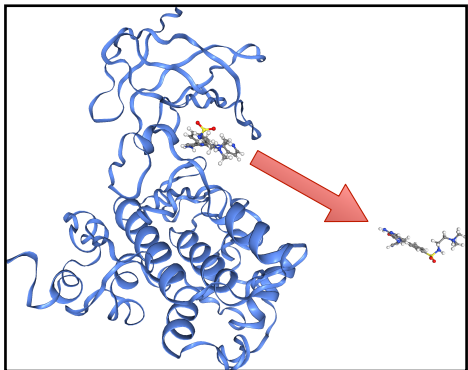
Answers

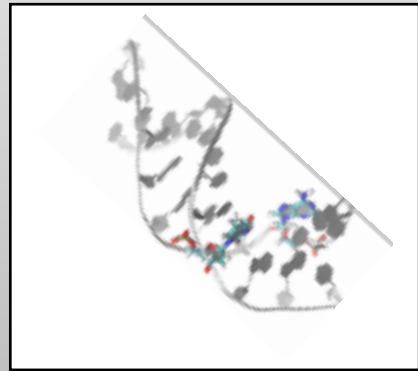


Path sampling simulations identify the differences in dynamics that lead to the K-Ras Q61L mutant causing cancer.



New on-the-fly state definitions in path sampling will help us characterize the role of intermediates in drug unbinding.





Path sampling simulations show that the outside channel is preferred in the WC-HG transition in DNA.

**Roet, Hooft, Bolhuis, DWHS, Vreede. In prep.**



**DWHS, de Groot, Bolhuis. In progress.**

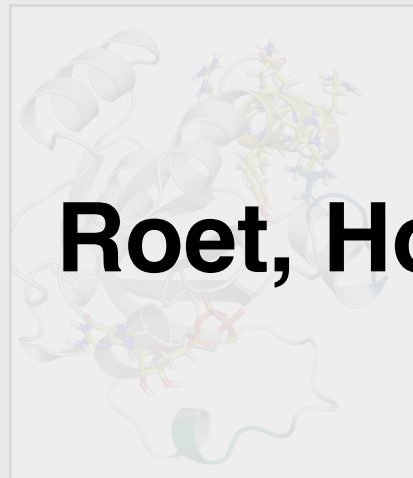
**Vreede, Bolhuis, DWHS. Submitted.**

# Answers



**Vreede, Bolhuis, DWHS. Submitted.**

Path sampling simulations show that the cut-off of the transition state in the WC-HG transition in DNA.



**Roet, Hooft, Bolhuis, DWHS, Vreede. In prep.**

Path sampling simulations identify the different states in the K-Ras Q61L mutant causing cancer.

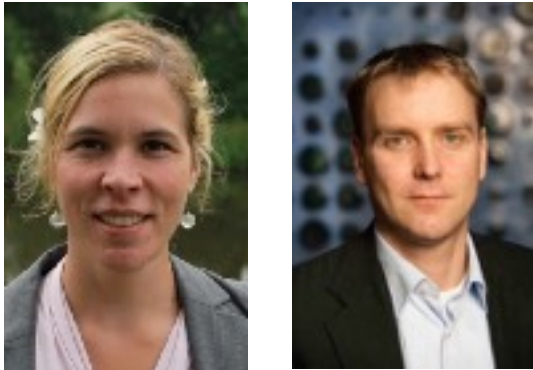


**DWHS, de Groot, Bolhuis. In progress.**

New on-the-fly state definitions in path sampling with the role of intermediates in drug unbinding.

# Acknowledgments

## DNA



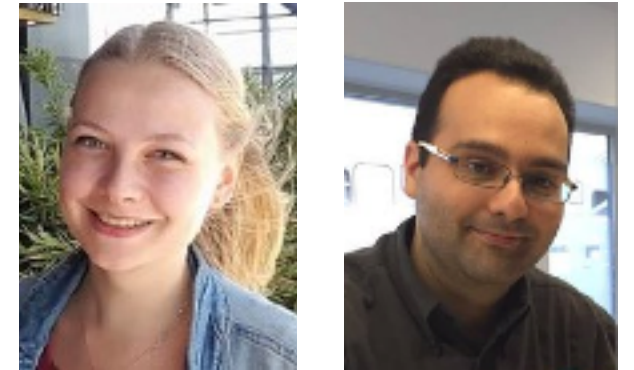
Jocelyne Vreede (UvA)  
Peter Bolhuis (UvA)

## K-Ras



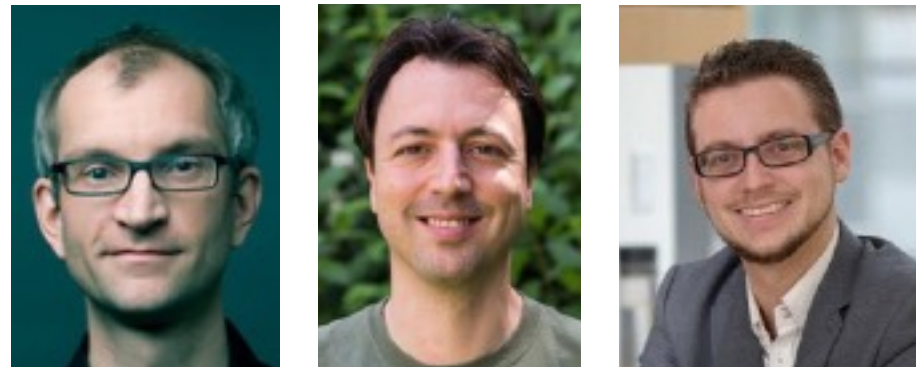
Sander Roet (UvA)  
Ferry Hooft (UvA)  
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## GSK3B



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## OpenPathSampling



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