Molecular Modelling: An easy way of life?

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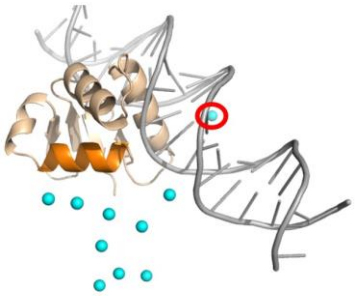
Nowadays, molecular modelling is coming back in front of the scene to help understand biological processes but at which cost?

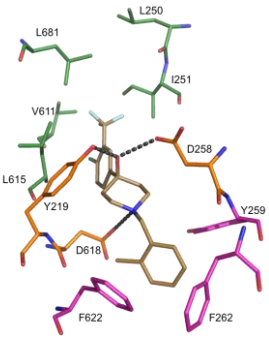
One of the examples

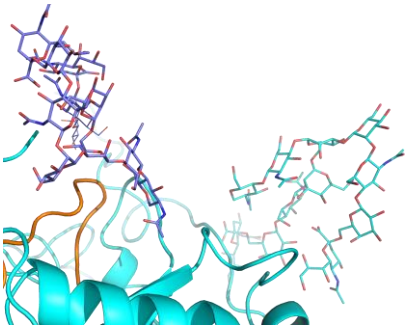
Ets-1 oncoprotein is a transcription factor that promotes target gene expression in specific biological processes. Typically, Ets-1 activity is low in healthy cells, but elevated levels of expression have been found in cancerous cells, specifically related to tumor progression. Like the vast majority of the cellular effectors, Ets-1 does not act alone but in association with partners. Given the important role that is attributed to Ets-1 in major human diseases, it is crucial to identify its partners and characterize their interactions. In this context, two DNA repair enzymes, PARP-1 and DNA-PK, have been identified recently as interaction partners of Ets-1.

We here identify their binding mode by means of protein docking. The results identify the interacting surface between Ets-1 and the two DNA repair enzymes centered on the α-helix H1 of the ETS domain, leaving α-helix H3 available to bind DNA. We rationalize the binding mode using a series of computational analyses, including alanine scanning, molecular dynamics simulation and residue centrality analysis. Our study constitutes a first but important step in the characterization, at the molecular level, of the interaction between an oncoprotein and DNA repair enzyme.

Others examples will be described and an open table is desired.







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