Site-specific docking: Frequently Asked Questions & answers for starters

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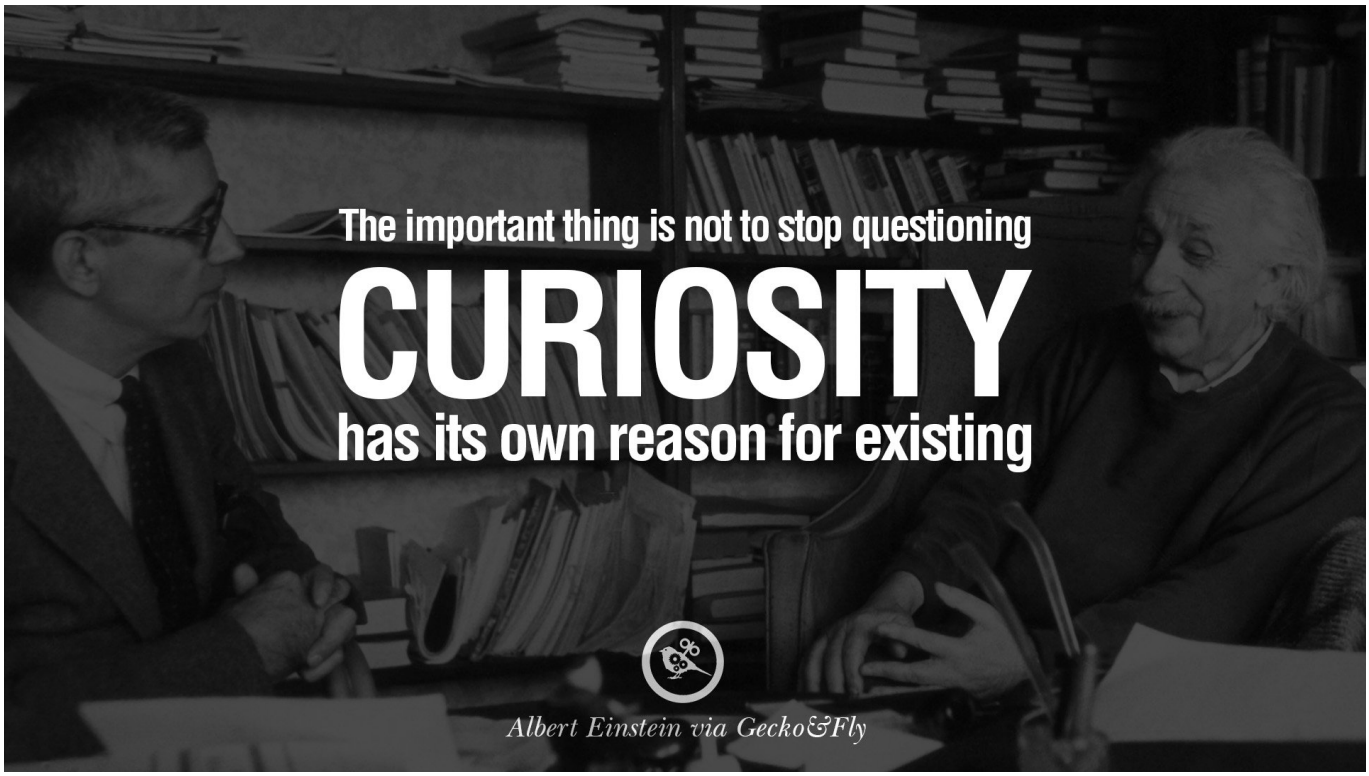

I have been getting several E-mails from researchers and students alike regarding *in-silico* docking. Most questions are similar in nature, so I thought of answering them once and for all. In this article, I have collected some frequently asked questions and provided the link to their answers present in our question answer section of Bioinformatics Review.

It is good to have questions in mind and they can be solved in a way as quoted by Sir Einstein:

> "We cannot solve our problems with the same thinking we used when we created them"

In this article, I have collected some of the most Frequently Asked Questions while performing site-specific and/ or blind docking. You have to consider a lot of factors before performing an actual docking on a protein with a specific ligand.

Question: How do you predict protein's binding sites?

Question: ***What is the difference between the blind docking and binding site based docking?***

Question: Since the protein is homo-dimer, should I get the same binding affinity values of ligand in two monomers?

Question: Since I know the binding sites in both monomers, so while doing docking do I necessarily need to mimic (preserve) the attachment of the ligand to these binding sites, so as to get the binding energy?

Question: ***While doing docking, if, in addition to the known binding site attachments, the ligand is showing few more attachments with some residues. Do they contribute to the binding energy ?? if Yes, do I need to dock the ligand in such a way so that, it shows attachments with the ligand as it is showing in PDB file when viewed in Pymol?***

Question: ***What about the conformation of the docked ligand ?? Should the docked ligand exactly fall on the ligand which we already have?***

Question: ***I have to find the 4 Armstrong neighborhood of a ligand. When I take the receptor molecule without adding hydrogen bonds and find 4A nbd of ligand, it gives one result. But when I first add hydrogens to the receptor molecule and then after finding the 4A nbd of ligand, it obviously gives different results. I want to know which one is better ??***

Second thing, if I have to find the distance between a ligand and any residue in receptor molecule. Do I have to take the central atom distances or minimum distance between any two atoms of the ligand and receptor molecule can be considered ??

Question: ***Why are the hetatoms removed from the protein PDB file before docking?***

Question: ***Why do we choose only one chain of protein for docking?***

If these are not the questions you are looking for, then feel free to ask in our ‘Bioinformatics Discussion‘ section or write to muniba@bioinformaticsreview.com.

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