

Homology Modeling

'tis a tale told by an idiot; full of sound and fury; signifying nothing.

-William Shakespeare, Macbeth

Homology, or comparative modeling has come a long way. It used to be the stuff of mockery. Now you can frequently obtain reliable results. Further, the actual analysis you need to do is free and almost embarrassingly painless.

You may want to make a model if structural data is not available. However, the modeling requires that a similar sequence has a known structure. You may want to make a model from a known structure to hypothesize or predict structural changes when making mutations to a protein of interest.

Websites - homology modeling servers

- EsyPred3D

Personally, I've only tried it once and did not find it very quick.

- Swissmodel

The Swiss have made a nice server that gives reliable results or, in the case of inappropriate models, no results at all. The answer comes back quickly; frequently within a few minutes. The Swiss model works well in a standalone format. However, Swissmodel works nearly seamlessly with DeepView.

- WhatIf

Gert Vriens' old webserver.

It is still the standard. As always, read the fine print. If WhatIf cannot rigorously assign a minimized structure, it will do something ridiculous and human-obvious so that casual observance would identify the un-minimizable residues. Presumably, the humans can then do something appropriate to adjust the malfeasant side chain.

Websites - homology modeling tutorials

If you are seriously trying to create a model, you owe it to yourself to run through some of the tutorials.

- DeepView based This is the site I used.

- San Diego State The San Diego site summarizes several approaches to the subject.