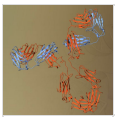

Jul 24, 2019

A Whole-heart Provider for Compartmental Modeling Antibody Services

Echo Han[1]

[1]na

1 Works for me dx.doi.org/10.17504/protocols.io.5r6g59e

Echo Han

1 About Creative Biolabs

Firstly started up at the beginning of 21 century in New York, USA, Creative Biolabs was set up by a group of biological scientists who are devoted to the development of antibodies. Aiming at facilitating drug or scientific research, high-tech antibody maturation platforms like PreciAb™, comprehensive antibody design services (*i.e.* Antibody Structure Modeling) and advanced technologies are provided. For more than 10 years of exploration and expansion, it is now regarded as the leading provider with services for people or companies in need in areas of scientific research and medical R & D. throughout the world.

2 On the basis of advanced *in silico* technologies, Creative Biolabs offers customized compartmental modeling antibody services by taking advantage of computational modeling approaches to help customers predict the antibody three-dimensional structure, and hence to contribute greatly to clients' antibody development projects with a variety of antibody structure modeling services:

Homology antibody modeling
Loop structure refinement
Modeling of the framework regions
Side chain modeling
Antibody modeling assessment

3 1. Homology modeling, one of the most commonly used antibody modeling methods of which the services provided adopts the 3-D antibody protein structures with alike sequences as a sample, and based on which produce a structure combined with the AA differences between the sample and the modeled one. Homology modeling works very well when it is predicting the structure of the Fv region framework, because of the extensively conserved fold of antibodies. A unique computational 3D structure prediction platform to generate an antibody homology model has been established by Creative Biolabs to fulfill projects in the following procedures.

1) Discover a template highly similar to our unknown protein, which has a known structure.
2) A sequence alignment is offered, and prior to aligning the two sequences, the template structure is cleaned.
3) Construct a series of homology models automatically and select the top notch.

Several methods for homology model analysis are also provided with a crucial step in building an antibody homology model that can not be overlooked: identification and refinement of CDR Loops.

4 1. High-quality loop structure refinement service is offered by Creative Biolabs to assist the customer to generate an expected antibody structure. There are 3 main steps to make a prediction of the structure of the loop: decoy generation, filtering, and ranking.

1) Decoy generation means to form several candidate conformations, or decoys, which relate to the residues on each side of protein structure gap.
2) Filtering is required to remove the invalid decoys, and it may be integrated with the other parts of the loop modeling process.
3) Ranking is an essential step. In spite that decoys close to the native structure have been produced, a useless ranking system implies that the structure selected as the final prediction will be inaccurate.
To improve the accuracy of antibodies structure prediction by a large margin, Creative Biolabs offers a two-phase strategy

5 3. Modeling of antibody framework regions is conducted by Creative Biolabs in the following steps.

1) Construct a model based on a single Fv framework template.
2) Construct a model by using a chimeric template.
3) Construct a model depended on five overall Fv framework templates.

6 4. Best in class side chain modeling service can be found to contribute customers' success, which includes side chain conformation prediction of antibody utilizing CIS-RR method and Rapid Side-chain Predictor (RASP) method.

7 4. Creative Biolabs offers professional antibody modeling assessment services for antibody modeling with the help of experienced scientists to guarantee to deliver fully comprehensive and professional assessment to satisfy the project development of clients globally, with which two major criteria are adopted to assess the quality and accuracy of the models.

1) MolProbity server is using a group of metrics offered to assess the quality of experimental proteins and nucleic acid structures.
2) RMSD values, combined with molprobilty, together help to assess the backbone structure of different regions of the Fv.

8 With the comprehensive antibody structure modeling services, designing and engineering novel antibodies like compartmental modeling antibodies are possible. Creative Biolabs customize the service according to the specific requirements from the customers. More information can be reached at https://www.creative-biolabs.com/preciab/.