MOE
Biologics Design

Biologics Design and Protein Engineering

- Structure-Based Biologics Design
- Analyze and Edit Protein Sequences
- Protein Properties and Developability
- ADC and Fusion Protein Modeling
- Protein, Antibody and Peptide Modeling
- Protein Engineering
- Simulations

Chemical Computing Group

The Molecular Operating Environment (MOE) has a comprehensive suite of applications for computer-aided biologics design packaged in a workflow oriented interface for streamlined visualization and analysis. These applications aid in identifying and prioritizing potential mutagenesis experiments for affinity maturation, property modulation and liability screening.

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Biologics Design and Protein Engineering

Structure-Based Biologics Design
○ Easy-to-Use Interface for Biologics Modeling
○ Protein-protein Interface Visualization
○ Identify Protein-Protein Contacts
○ Surfaces and Property Maps for Analyzing Structures
○ Solvent Analysis for Protein Surfaces

Analyze and Edit Protein Sequences
○ Visualize, Manage and Edit Protein Sequences
○ Automatic Annotation of Protein Family Motifs
○ Align Multiple Sequences and Structures
○ Calculate Residue Identity and Similarity
○ Graft Sequences, Loops and Secondary Structures

Protein Properties and Developability
○ Patch Analysis to Identify Aggregation Prone Regions
○ Calculate Protein Property Descriptors
○ Identify Surface Accessible Residues
○ Liability Detection of Post-Translational Modifications
○ Use Protein Descriptors for QSAR and QSPR Modeling

ADC and Fusion Protein Modeling
○ Linker Modeler to Connect and Fuse Protein Domains
○ Domain Motif Searching to Identify Linkers
○ Optimize Protein Mutations with Protein Builder
○ Non-Natural Amino Acids for ADC Linkers
○ Identify ADC Conjugation Sites and Reactive Motifs

Protein, Antibody and Peptide Modeling
○ Specialized Protein Families and Antibody Databases
○ Generate Diverse Antibody Models from Fv to Ig
○ Protein Multimer Homology Modeling
○ In Situ Modeling of Loops and Sidechains
○ Peptide Library Design and Screening

Protein Engineering
○ Ala, Cys, SNP, Residue Scanning
○ Sequence Optimization and Mutagenesis
○ Evaluate Thermostability and Affinity
○ Generate Focused Mutant Libraries
○ Assess Solubility, Viscosity, Aggregation and Liabilities

Simulations
○ Protein-Protein Docking
○ Generate, Refine and Score Ensembles
○ Explicit and Implicit Solvent Models
○ Run MD to Model Surfactants and Solvents
○ Simulate Excipient Effects - Formulation

MOE
Biologics Design

Rank	1:Leu3	1:Ile5	1:Thr14	1:Thr16	1:Phe28	1:Tyr31
1	Leu	Val	Leu	Arg	Phe	Trp
2	Val	Leu	Arg	Val	Leu	Leu
3	Cys	Phe	Phe	Leu	Tyr	Phe
4	Phe	Ala	Trp	Trp	Trp	Met
5	Gly	Ser	Ser	Thr	Ile	Tyr
6	Thr	Ile	Val	Ser	Val	Val
7	Met	Trp	Thr	Phe	Ser	Ile
	Ser	Tyr	Lys	Ala	Val	Lys
	Ala	Thr	Ile	Tyr	Cys	Ile
	Trp	Cys	Gly	Lys	Thr	Gly
		His	Ala	Gly	Pro	Ser