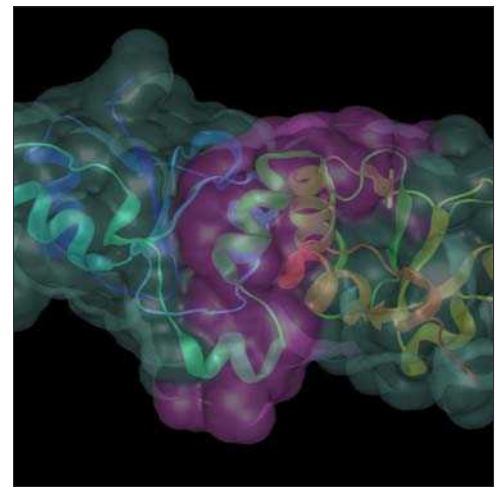
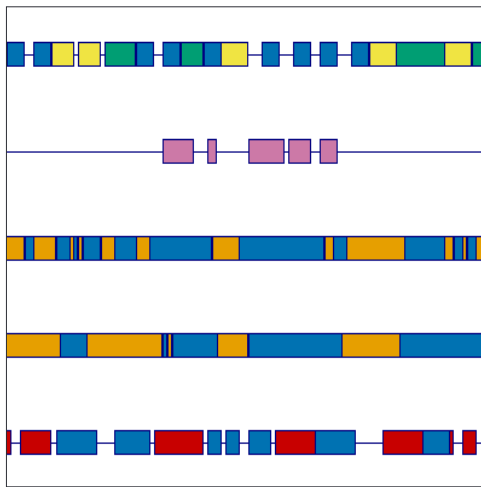
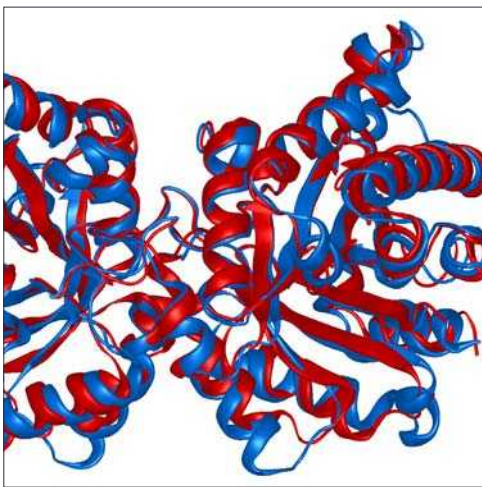


# LASERGENE PROTEIN

## Software for protein structure and sequence analysis



### PROTEIN SEQUENCE ANALYSIS

- Utilize integrated views and analysis methods for sequence, secondary structure, and tertiary structure
- Predict secondary structure characteristics

### PROTEIN STRUCTURE ANALYSIS

- Predict B-cell epitopes
- Create molecular and solvent accessible surfaces to visualize predicted epitopes
- Align entire structures or selected regions
- Create publication quality graphics
- Visualize conformational changes of nearly 400 animated macromolecular structures

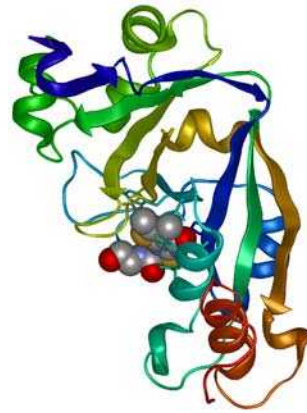
### PROTEIN MODELING

- Predict 3D structure for any protein sequence
- Model antibody structures and identify antibody/antigen binding sites
- Predict protein function, ligand binding sites, and enzyme activity
- Model docking for any receptor and ligand pair
- Predict binding interactions and energy
- Create and model variants on protein structures
- Perform hot-spot scans and improve fold stability with protein design tools

# Comprehensive tools for protein modeling

## Protein Structure Prediction with NovaFold

- Based on the top-rated algorithm: I-TASSER
- Large molecule support, up to 2000 residues
- Predict protein structure, function, ligand binding, and enzyme activity
- Advanced user restraint controls & custom templates



Diphtheria toxin fragment A

Residues: 153  
Sequence: GADGVYDSKPFVMEVNSYHSTKPGYVDSQKQKPSGTQAHYDDWNGPST  
PHTVDAAGVYDDENPISAGAGVHYTPYSGTYVALKPNATIKELSLSTPAHQGTTE  
PKRFGDASRVLSLPPAFSGSSVEYVNAVQMALESVELEHFTKRGKQDAMVEYMAQACAG  
NHYER

Templates

Rank	Template	Z-score	Threader	% Coverage	% ID	Map
1	1J8RAS	3.91	MUSTER	97	100	
2	1J8RAS	5.68	dPPAS	97	100	
3	1J8RAS	6.43	-uPPAS	97	100	
4	1J8RAS	4.83	-uMUSTER	96	100	
5	1J8RAS	6.05	-uPPAS	97	100	
6	1J8RAS	7.05	dPPAS2	97	100	
7	1J8RAS	5.57	PPAS	97	100	
8	1J8RAS	7.13	Em-PPAS	97	100	
9	1J8RAS	1.09	MUSTER	100	96	
10	1J8RAS	1.92	dPPAS	100	97	

Open checked template fragments aligned to: [1J8RAS](#)

Model Overview

Model 1

TM-score: 0.99±0.04  
RMSD: 1.61±1.42

C-score: 1.93  
Cluster size: 2000 of 2000  
Density score: 1.120

[Open model in new document](#)  
[Spin the model](#)

NovaFold results

## Protein-Protein Docking with NovaDock

- Based on SwarmDock, a high-resolution docking algorithm
- Model protein docking and binding interactions
- Explore protein flexibility during docking

NovaFold model with  
predicted ligand binding  
TM-Score: 0.99±0.04;  
RMSD: 1.61±1.42

## Antibody Modeling with NovaFold Antibody

- Model Fv, Fab, VH, sdAb in minutes
- Search a library of antibody frameworks, or provide custom templates
- Ab initio loop modeling for H3 - up to 15 residues
- Automated annotation of CDR loops

## Protein Design with NovaDesign - NEW!

- Create, model, and analyze variants on structure
- Calculate energy changes of mutations
- Perform serine and alanine variant scans
- Improve protein fold stability with an automated workflow - **COMING SOON!**

Model Overview

[Open checked in new document](#)  
[Export as image...](#)

Model 1

Molecule: Model 1

Energy: -26.73  
Cluster Size: 6  
Cluster Energy: -21.68 +/- 3.28  
Ligand atom contacts: 232

Chains: 1 A

[Open model in new document](#)  
[Spin the model](#)

Model	Energy	Cluster size	Ligand conta
1	-26.73	6	232
2	-22.29	3	224
3	-21.98	5	308
4	-19.84	5	208
5	-18.66	3	233
6	-16.50	1	223
7	-16.45	1	221
8	-15.56	1	229
9	-15.01	4	277
10	-14.62	1	163

Residue list:

- 1:CV
- 1:VA
- 1:IL
- 1:AS
- 1:GL
- 1:AS
- 1:TR
- 1:LY
- 1:PH
- 1:AL
- 1:CY

NovaDock report

## Contact Us

608.258.7420 tel  
866.511.5090 toll free

0.808.234.1643 U.K.  
0.800.182.4747 Germany

3801 Regent Street  
Madison, WI 53705

www.dnastar.com  
info@dnastar.com

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