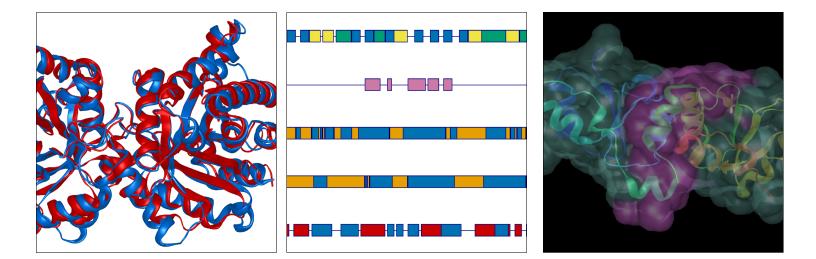


# LASERGENE PROTEIN AND NOVA APPLICATIONS

# Software for protein modeling and 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 using the award-winning AlphaFold 2 or I-TASSER algorithms
- 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 and NovaFold AI

- NovaFold utilizes the award-winning I-TASSER protein structure prediction algorithm, which combines threading and *ab initio* folding technologies.
- NovaFold AI uses the AlphaFold 2 algorithm from DeepMind to predict distance and create dihedral maps using deep multiple sequence alignments as input.
- Predict protein structure, function, ligand binding, and enzyme activity

#### **Protein-Protein Docking with NovaDock**

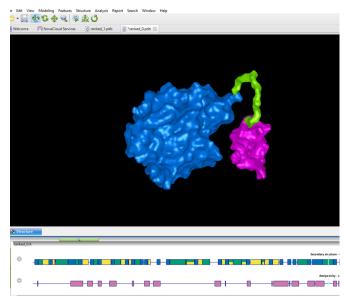
- Based on SwarmDock, a high-resolution docking algorithm
- · Model protein docking and binding interactions
- Explore protein flexibility during docking

# **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

# **Advanced Protein Design**

- Create, model, and analyze variants on structure
- Calculate energy changes caused by mutations
- Perform serine and alanine variant scans
- Improve protein fold stability with an automated workflow



A completed NovaFold AI prediction of two CASP 14 targets modeled with a linker.

		Model 🔺	Energy	Cluster size	Ligand cont
0		1	-26.73	б	232
		2	-22.29	3	224
C L L L L L		3	-21.98	5	308
		4	-19.84	5	208
		5	-18.66	3	233
	$\checkmark$	6	-16.50	1	223
	$\checkmark$	7	-16.45	1	221
	$\checkmark$	8	-15.56	1	229
	$\checkmark$	9	-15.01	4	277
		10	-14.62	1	163
en checked in new document ort as image Iodel 1					
as image					Re:
	Mol	ecule:	м	lodel 1	✓ 1:C
	Ene	rgy:	-1	lodel 1 26.73	<ul><li>✓ 1:C</li><li>✓ 1:V</li></ul>
	Ene Clus	rgy: :ter Size:	-2	26.73	<ul> <li>✓ 1:C</li> <li>✓ 1:V</li> <li>✓ 1:IU</li> </ul>
image	Ene Clus Clus	rgy: :ter Size: :ter Energ	-1 6 Iy: -2	26.73 21.68 +/- 3.28	<ul> <li>✓ 1:C</li> <li>✓ 1:V</li> <li>✓ 1:I</li> <li>✓ 1:A</li> </ul>
	Ene Clus Clus	rgy: :ter Size:	-1 6 Iy: -2	26.73 21.68 +/- 3.28	✓       1:C         ✓       1:V         ✓       1:II         ✓       1:A         ✓       1:A         ✓       1:A
	Ene Clus Clus Liga	rgy: :ter Size: :ter Energ	-1 6 Iy: -2	26.73 21.68 +/- 3.28	✓     1:C       ✓     1:V       ✓     1:II       ✓     1:A       ✓     1:A
as image	Ene Clus Clus Liga Cha	rgy: ster Size: ster Energ and atom o	-2 6 ly: -2 contacts	26.73 21.68 +/- 3.28 : 232	✓       1:C         ✓       1:V         ✓       1:II         ✓       1:A         ✓       1:A         ✓       1:T
	Ene Clus Clus Liga Cha	rgy: ster Size: ster Energ and atom ins: <u>1</u> <u>A</u>	-2 6 1y: -2 contacts	26.73 21.68 +/- 3.28 : 232	✓         1.0           ✓         1.1           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4
	Ene Clus Clus Liga Cha	rgy: eter Size: eter Energ and atom ins: <u>1</u> <u>A</u> en model i	-2 6 1y: -2 contacts	26.73 21.68 +/- 3.28 : 232	3         1:C           4         1:A           7         1:A           7         1:A           9         1:P
	Ene Clus Clus Liga Cha	rgy: eter Size: eter Energ and atom ins: <u>1</u> <u>A</u> en model i	-2 6 1y: -2 contacts	26.73 21.68 +/- 3.28 : 232	✓         1.0           ✓         1.1           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4           ✓         1.4

The NovaDock report showing the top ligand-receptor docking models for a completed prediction.

3801 Regent Street Madison, WI 53705

www.dnastar.com info@dnastar.com