BIOLOGICS BY DESIGN

Cutting-edge software for modeling different types of biologics, including monoclonal antibodies, vaccine antigens, enzymes, and peptides

ACCELERATE RESEARCH AND DEVELOPMENT PROJECTS

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IMPROVE WORKFLOW EFFICIENCY AND STREAMLINE EFFORTS

- Easily follow logically-organized tasks and flexible workflows bringing the power of computational chemistry and biology to advanced and occasional users
- Work efficiently through Schrödinger's unique unified modeling and simulation interface for biologics design

SCHRÖDINGER®

ANTIBODY MODELING

- Reliable structure prediction from sequence
- Automated intuitive workflows
- Advanced *ab initio* CDR loop prediction using PRIME
- Antibody humanization by CDR grafting
- Regularly updated and curated antibody database

LIABILITY PREDICTION

- Rapid protein surface analysis
- Protein aggregation prediction with AggScore
- Chemical liability prediction
- QSAR analysis for biologics

ADVANCED PROTEIN ENGINEERING

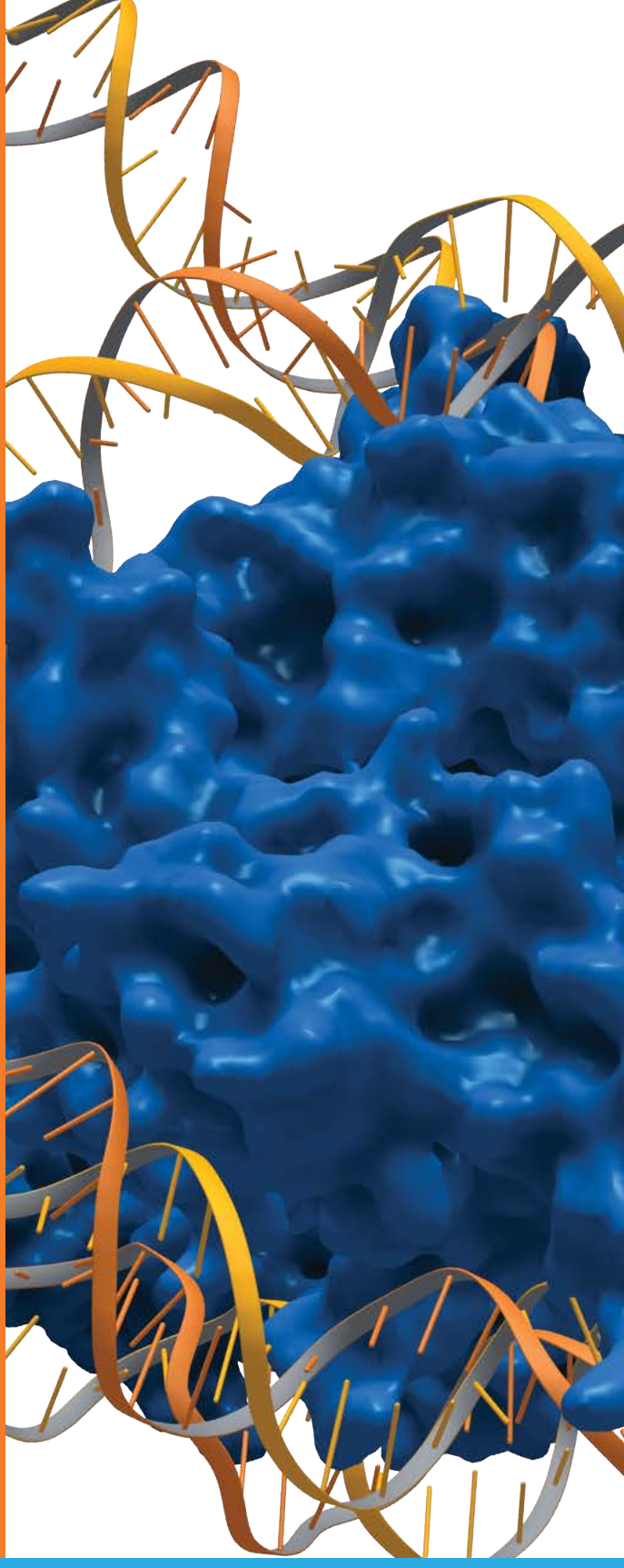
- *In silico* mutagenesis and scoring
- Cysteine scanning and design of disulfide bridges
- Protein FEP+ for prediction of relative free energy changes
- Fusion protein linker design

PROTEIN DOCKING

- Well-validated docking code, PIPER
- Proven track record in community-wide blind prediction competitions
- Antibody and Standard (Protein or Nucleic Acid) modes
- Protein-Peptide docking

COMPREHENSIVE PROTEIN MODELING

- Advanced tools for sequence alignment, with extensive annotation options
- Complete set of homology modeling tools, including both rapid and high-accuracy methods
- Easy to interpret protein structure quality analysis
- Residue-based analysis of energies, solvent-accessible surface areas, and hydropathy
- Molecular Dynamics simulation using Desmond



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