

Isoelectric Point (pI) Engineering

Structure-Based Charge Modification, Formulation Optimization, and Humanness Safeguards

Modulate antibody isoelectric point (pI) to optimize formulation and serum stability. AbLead couples sequence-based Bjellqvist titration with empirical 3D structure-based PROPKA 3 electrostatics, monitoring real-time humanness (Sapiens) and stability (AbLang) during combinatorial charge engineering.

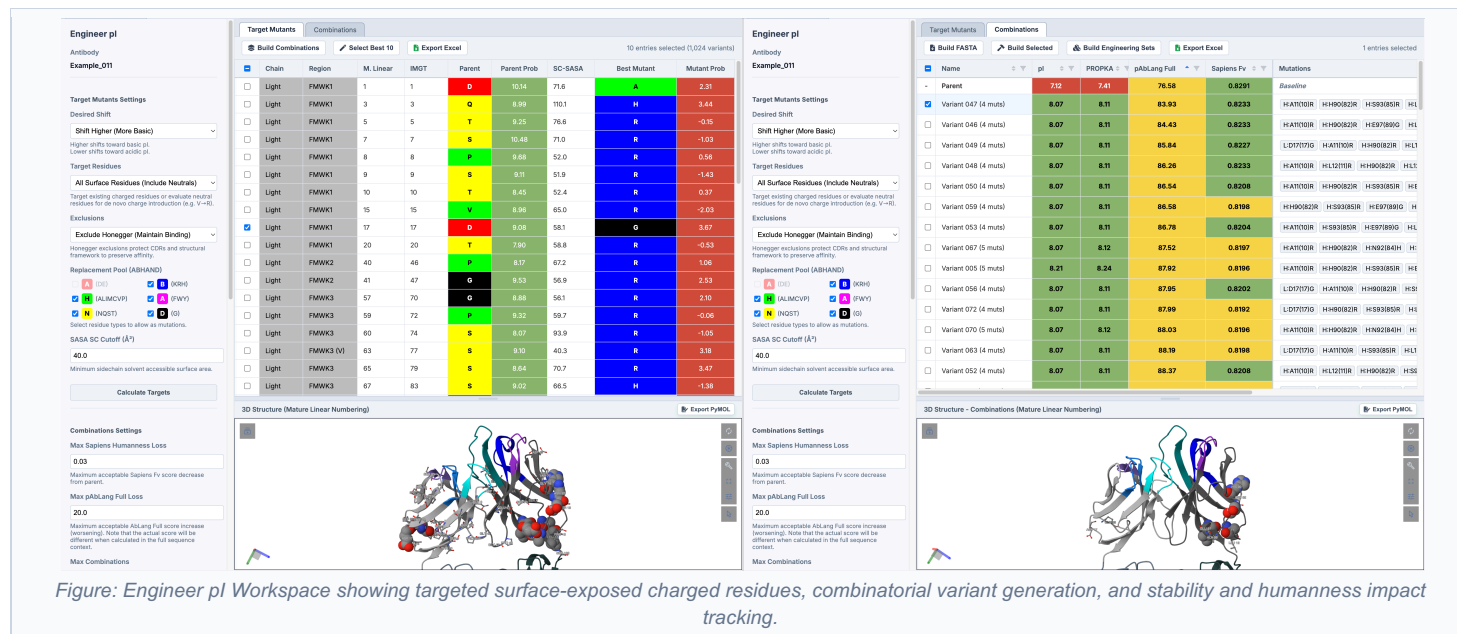


Figure: Engineer pI Workspace showing targeted surface-exposed charged residues, combinatorial variant generation, and stability and humanness impact tracking.

CORE CAPABILITIES

- **Dual Calculation Methodologies:** Combines theoretical sequence Bjellqvist titration with empirical 3D structure-based PROPKA 3 electrostatics.
- **Hybrid Full-Length Modeling:** Evaluates Fv electrostatics in 3D atomic coordinates and couples them with constant domain titration curves.
- **Rapid Delta Titration:** Calculates folded pI predictions for thousands of combinatorial variants instantly on exposed residues.
- **Real-Time Humanness Monitoring:** Monitors every charge-shifting substitution against Sapiens deep learning scores.

DEVELOPABILITY ADVANTAGE and IMPACT

- **Formulation Stability Optimization:** Shifts pI in the desired direction for optimal formulation stability.
- **Reduce Potential Serum Particulation:** Shifts molecular pI away from serum pH to prevent in vivo particulation.
- **Bispecific Heterodimer Purification:** Engineers pI asymmetry between homodimers and heterodimers to enable clean ion-exchange chromatography separation.
- **Direct Engineering Handoff:** Seamlessly exports prioritized charge-engineered combinations into project results or FASTA synthesis lists.

The AbLead Advantage: Shifting antibody isoelectric point has profound impacts on serum particulation, solubility, viscosity, and manufacturing purification. AbLead automates structure-guided charge engineering while safeguarding therapeutic stability and humanness.

Accelerate Your Antibody Lead Optimization and De-Risk Development

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