

Surface Properties and Structural Developability

Hydrophobic Patches, Charge Densities, and Electrostatic Dipole Profiling

Predict and resolve formulation hurdles directly from 3D structural coordinates. AbLead computes Surface Hydrophobicity (SPH), Positive Charge Patches (SPP), Negative Charge Patches (SPN), and Charge Dipole (SPCD) using solvent-accessible surface area (SASA) and spatial neighbor decay to prevent stickiness, fast clearance, and viscosity liabilities.

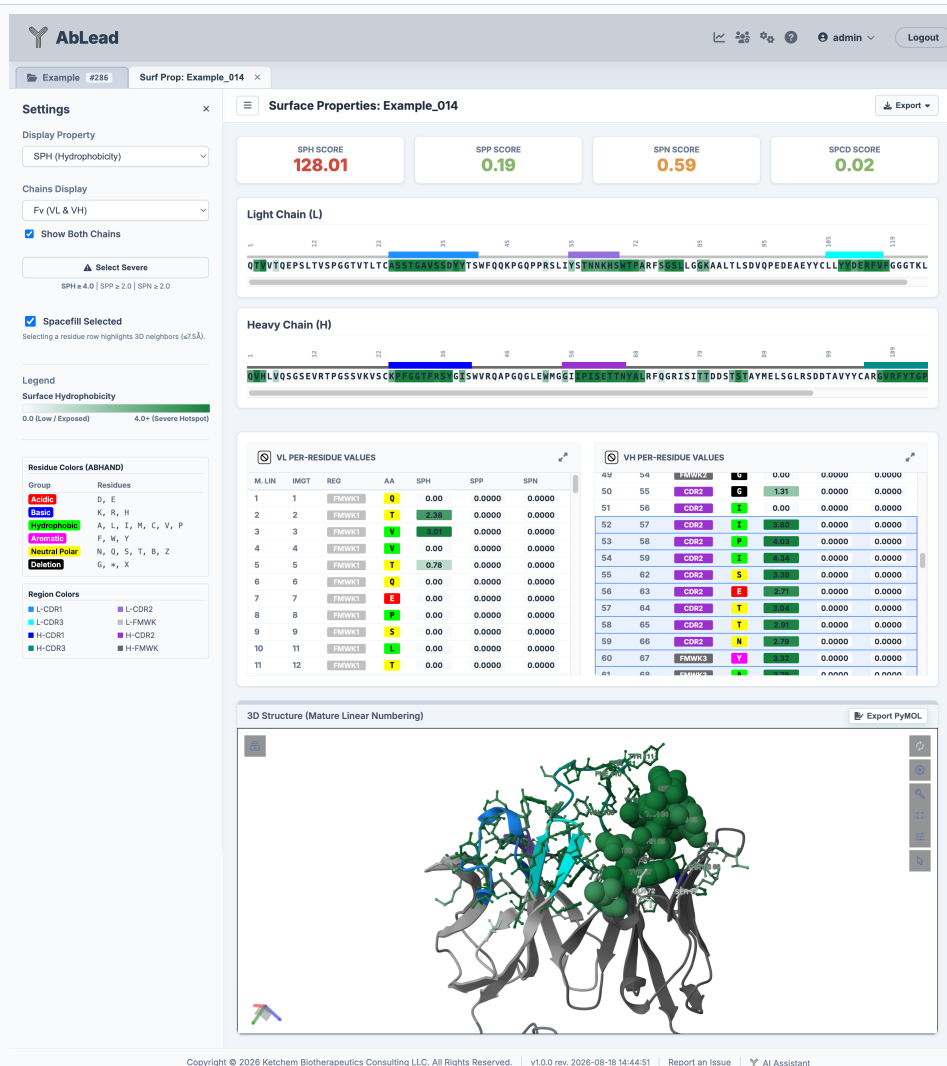


Figure: Surface Properties Workspace detailing spatial hydrophobicity (SPH), charge patches (SPP/SPN), dipole asymmetry (SPCD), and 3D structure.

CORE CAPABILITIES

- **3D Spatial SASA Calculations:** Implements the Shrake-Rupley algorithm with 7.5 Å spatial cutoff decay and pairwise salt-bridge neutralization.
- **Surface Hydrophobicity (SPH):** Measures exposed hydrophobic patches that drive self-association, aggregation, and rapid clearance.
- **Charge Patch Densities (SPP/SPN):** Pinpoints dense basic (Lys/Arg/His) or acidic (Asp/Glu) surface clusters that cause non-specific binding and high viscosity.
- **Electrostatic Dipole (SPCD):** Evaluates inter-chain charge asymmetry and polarization across the VH-VL interface.

DEVELOPABILITY ADVANTAGE and IMPACT

- **Prevent High-Concentration Viscosity:** Identifies dense electrostatic and hydrophobic clusters early, safeguarding high-concentration subcutaneous delivery.
- **Reduce Clearance and Off-Target Binding:** Neutralizes patches responsible for non-specific binding and fast in vivo clearance.
- **Isolated Domain Formulation QC:** Evaluates exposed interface liabilities in non-mAb formats (scFvs, VHH nanobodies) to prevent severe aggregation.
- **Targeted Solubilizing Designs:** Directly launches mutation designs on identified surface hotspots to improve biophysical developability profiles.

The AbLead Advantage: High-concentration viscosity and rapid clearance are frequently rooted in surface charge and hydrophobic patches. AbLead pinpoints these structural liabilities so you can optimize formulation profiles before entering the clinic.

Accelerate Your Antibody Lead Optimization and De-Risk Development

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