

Developability Liabilities and 3D Structural Mapping

Comprehensive PTM Motif Detection, AI Stability Gating, and Real-Time 3D Visualization

Detect, categorize, and resolve chemical and structural degradation liabilities before advancing leads to production. AbLead combines the comprehensive Satlawat et al. (2024) motif library with cutting-edge antibody language models (AbLang, AbLang2, IgBert) and covariance analysis, synchronized with an interactive 3D molecular viewer.

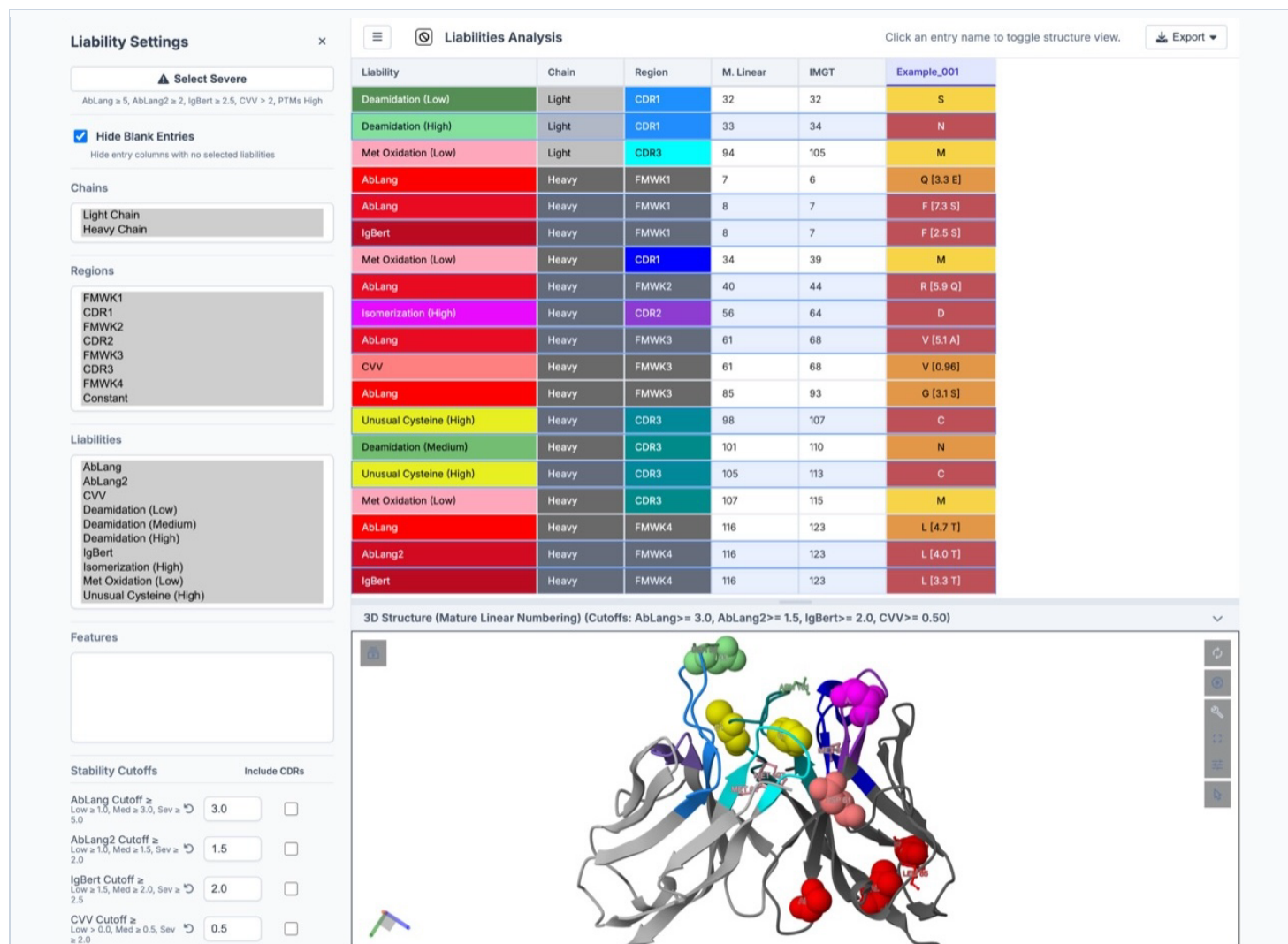


Figure: Interactive Liabilities Dashboard combining residue-level motif tables, AI stability penalty scores, and synchronized 3D structural viewer.

CORE CAPABILITIES

- Comprehensive Motif Detection:** Flags deamidation, isomerization, fragmentation, hydrolysis, unpaired cysteines, as well as user-based motifs.
- Multi-LLM Stability Gating:** Computes residue likelihood differences ($\Delta \ln P$) using AbLang, AbLang2, and IgBert to detect conformational destabilization.
- Covariance Violation Analysis:** Identifies co-varying constraint violations (CVV) that disrupt canonical antibody framework packing.
- Synchronized 3D Molecular Viewer:** Clicking any liability in the grid instantly highlights and spacefills the affected residue on the 3D atomic structure.

DEVELOPABILITY ADVANTAGE and IMPACT

- Improve Product Developability:** Drives optimization designs with direct visualization, allowing for combinatorial design decisions to maintain efficacy.
- Multi-Antibody Comparative Matrix:** Compares liability profiles across discovery cohorts side-by-side to de-select high-risk molecules early.
- 1-Click PyMOL Script Export:** Generates ready-to-run PyMOL visualization scripts with color-coded selections and custom zoom presets.
- Direct Engineering Workflow:** Select any identified liability to launch targeted mutation designs or execute 1-click First Pass Optimization.

The AbLead Advantage: Addressing stability and chemical liabilities computationally can save substantial time and money during cell line and process development, often improving yields and stability.

Accelerate Your Antibody Lead Optimization and De-Risk Development

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