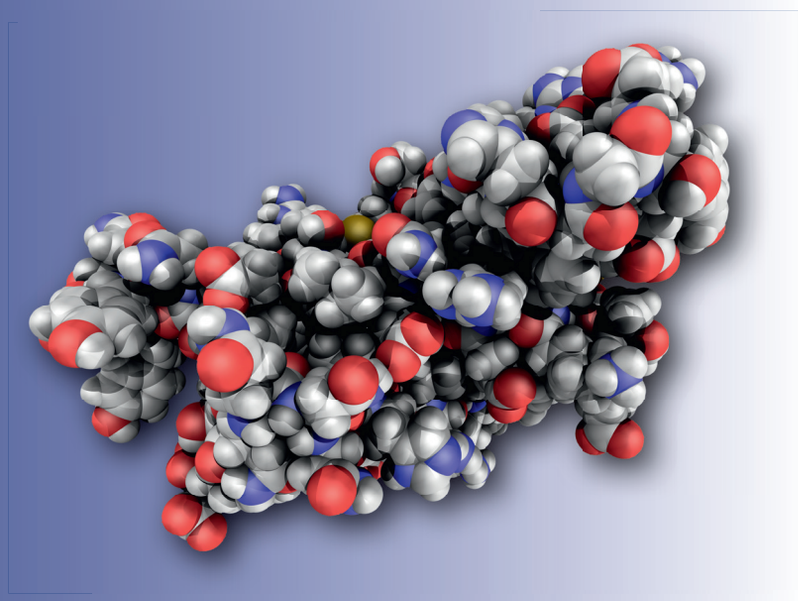
LEUKOCARE

formulation expertise meets data science

De-risk biologics development with Molecular Modeling



PROFILE YOUR DRUG SUBSTANCE AND POTENTIAL LIABILITY SITES

Choose the best lead candidate

Drug discovery involves screening hundreds to thousands of candidates. The identification of a high-quality lead is critical to the success of any drug discovery program. To ensure you pick the most suitable candidate for developmental success, Leukocare offers Molecular Modeling services to empower your selection process through characterization of your lead hits and their liability sites, so you can make an informed choice on which candidate to develop into a drug product.

Formulations tailored to your drug substance

Utilizing molecular modeling in the formulation development process gives you an insight into the potential liability sites of your molecule, de-risking your drug product development. Knowing the features and liability sites of the drug substance in combination with Leukocare's data science based formulation approach and regulatory approved excipient database, we can find the optimal combination and concentration for the drug product formulation by combining *in-silico* with *in-vitro* experiments to speed up your development times.

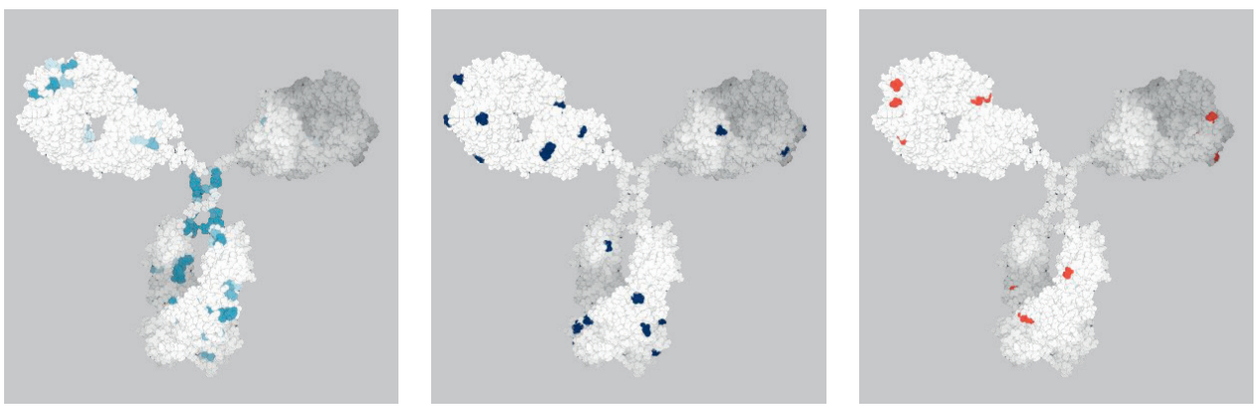
Molecular Modeling analysis can:

- Identify liability sites on the molecule
- Compare candidates' aggregation propensities
- Visualize charge and electrostatic properties across candidates
- Compare CDR properties to hundreds of therapeutic antibodies
- Enable molecular dynamic simulations for peptides

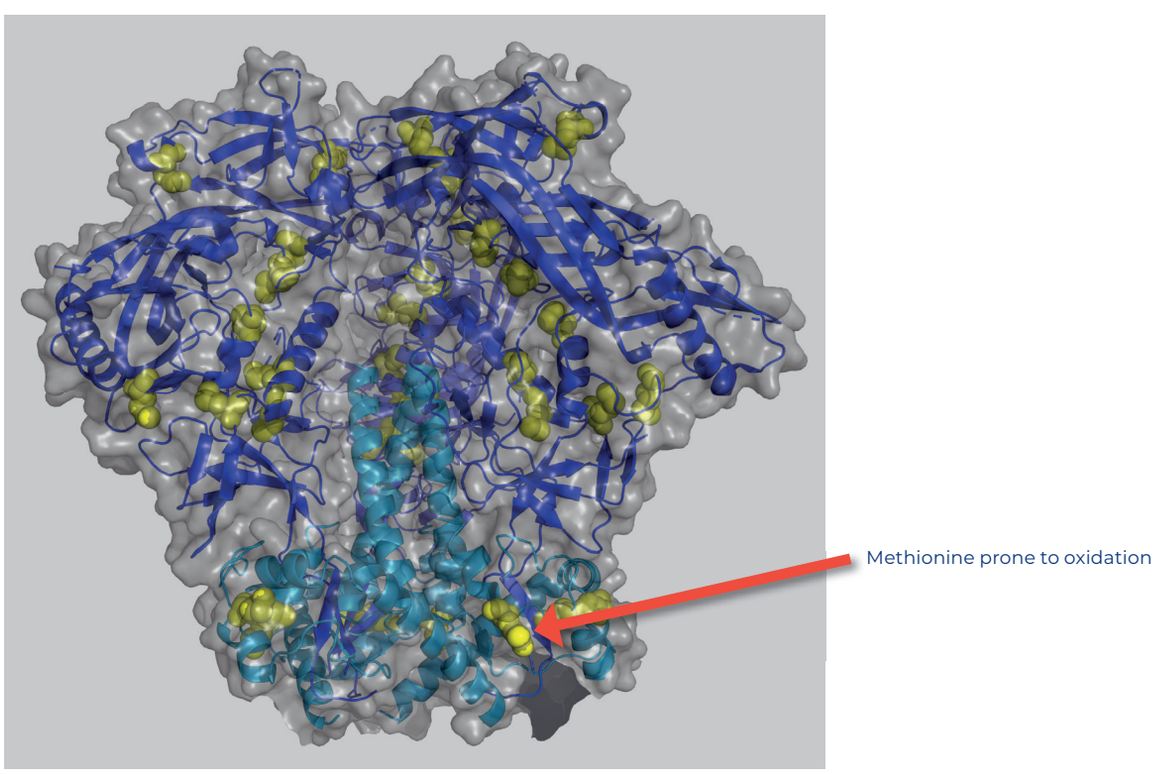
Identify degradation pathways of the drug substance

In candidate selection, as well as later selection of stabilizing excipients, the identification of liability sites is key. Molecular modeling of a target drug substance is an important ***in-silico*** tool to predict the biological effects and behaviors of molecules and results in an improved picture of the molecules':

- Degradation propensity
- Aggregation prone regions
- Hydrophobic patch areas
- Charge distribution



Molecular modeling of the 3D protein structure, aggregation-prone residues (light blue, left), de-amidation sites (dark blue, middle) and isomerization sites (red, right) on the monoclonal antibody.



3D structure of the envelope glycoprotein gp160 of human immunodeficiency virus type 1 (HIV-1). The model shows methionine residues which are not on the surface (dark yellow) and methionine residues which are on the surface (light yellow) and therefore accessible and prone to oxidation.

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