



AI-Driven Molecular Screening Prompt Frameworks

STRUCTURAL ARCHITECTURE FOR GENERATIVE LIGAND & POLYMER DISCOVERY

Accelerate R&D Discovery: Generative models can act as powerful ideation partners during early-stage molecular screening when guided by highly structured prompt constraints. This toolkit provides advanced engineering frameworks to blueprint ligand target mechanics and initial polymer estimations without losing chemical logic.

1. Structural In Silico Screening Frameworks

Target-Specific Receptor Docking Framework

LIGAND INTERACTIONS

Optimized for designing mock structural libraries targeting a specific enzyme binding pocket or receptor domain based on geometric parameter groups.

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Act as an expert computational medicinal chemist. I need to design a small structural library of small-molecule ligands targeting the active site of [TARGET PROTEIN/RECEPTOR, e.g., main protease of SARS-CoV-2].
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Provide 5 structural core scaffolds that optimize for:
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1. High binding affinity based on matching hydrogen bond donor/acceptor positions within [SPECIFIC ACTIVE RESIDUES, e.g., His41 and Cys145].
2. Strict compliance with Lipinski's Rule of 5 parameters.
3. Easy synthetic accessibility (low synthetic score complexity).

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Output each candidate structure with its IUPAC name, a clear description of its functional mechanism, and its expected binding mode properties.
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Polymeric Material Property Estimation Engine

POLYMER METRICS

Engineered to map structure-property relationships for macro-molecular backbones, optimizing for mechanical, thermal, and green degradation profiles.

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Act as a materials scientist specializing in high-performance polymers. I am designing a new polymer matrix for [APPLICATION, e.g., sustainable food packaging barriers] that requires high thermal stability and biodegradability.
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Analyze a hypothetical polymer backbone constructed from [MONOMER BUILDING BLOCKS, e.g., polylactic acid co-glycolic acid units functionalized with furan rings].
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Estimate and break down the following initial properties based on chemical structural logic:
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1. Expected Glass Transition Temperature (Tg) and Melting Point (Tm) behavior.
2. Tensile modulus capabilities and structural crystallinity variations.
3. Environmental degradation timeline and expected non-toxic breakdown moieties.

2. Computational Verification Controls

Critical Prompt Rule: Enforce Structural Notation Validity

Large Language Models do not possess intrinsic spatial awareness of molecular coordinates. To prevent molecular hallucinations, always force the AI tool to output structures using explicit SMILES (Simplified Molecular Input Line Entry System) string notations or InChI keys alongside IUPAC definitions. Always cross-verify these strings using open-source parsers like RDKit or PubChem before adding them to physical screening loops.

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