ChemReact: Integrated Retrosynthesis Planning & Visualization System

1. Project Overview

ChemReact is a sophisticated chemoinformatics and retrosynthesis automation framework designed to bridge the gap between high-level chemical reasoning and executable laboratory procedures. By leveraging the advanced molecular manipulation capabilities of **RDKit** and a **Multi-Persona LLM Architecture**, ChemReact provides a closed-loop system for molecular design, auditing, and high-fidelity visualization.

2. Core Architecture: Competitive Multi-Persona Reasoning

Unlike monolithic planning systems, ChemReact utilizes a "checks and balances" approach through specialized agent personas, ensuring that every synthetic route is both strategically sound and tactically executable.

Persona	Responsibility	Focus
Top-Level Designer	Strategic Planning	Skeletal disconnection, convergent vs. linear strategy, core ring system construction.
Reaction Designer	Tactical Execution	Detailed reagent selection, solvent/catalyst optimization, selectivity control (Regio/Stereo).
Auditor	Quality Assurance	Mass balance verification, protecting group (PG) loop detection, safety/toxicity screening.
Visualization Specialist	Visual Communication	Creative direction for molecular rendering, identifying key intermediates and reaction centers for highlighting.

3. Visual Results and Demonstrations

The system's strength lies in its ability to translate abstract JSON data into intuitive visual artifacts. Below are representative outputs from a standard run (`run_001`) performing the retrosynthesis of **Losartan**.

3.1 Target Molecule Analysis

The system identifies the core biphenyl-tetrazole-imidazole scaffold, providing a clean 2D representation for strategic mapping.

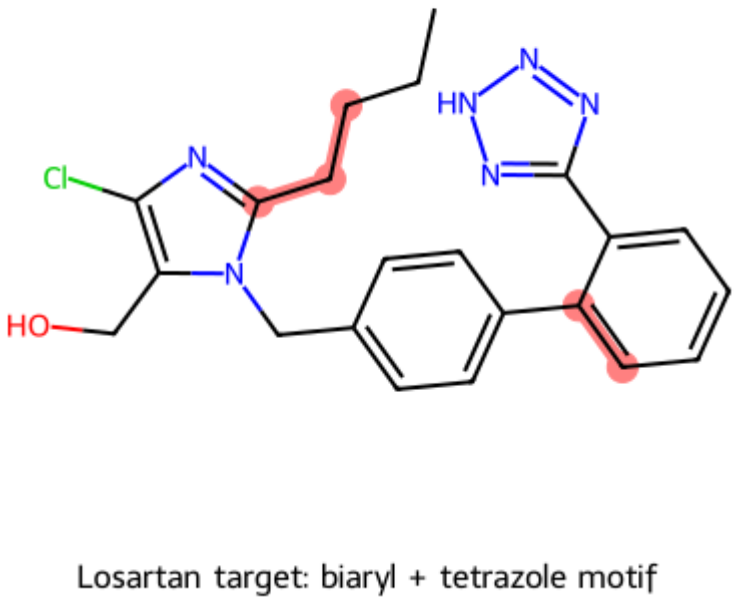

Fig 1. Target Molecule (Losartan) 2D Rendering.

3.2 Retrosynthesis Tree (The "Tree View")

A cornerstone of the ChemReact system is the orthogonal tree visualization, which clearly maps the target to its primary precursors, illustrating the convergent nature of the synthesis.

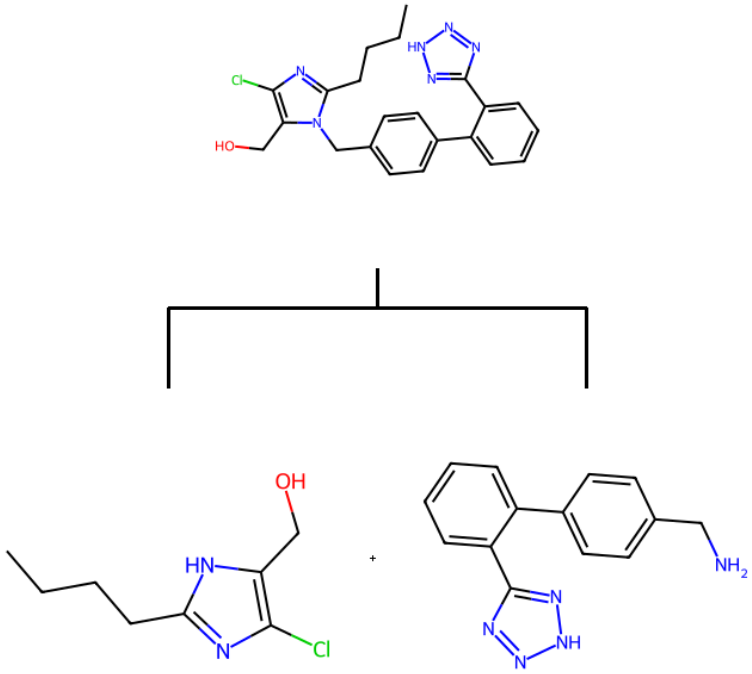

Fig 2. Route 1: Strategic Disconnection Tree.

3.3 Reaction Step Detailing

For each step, the system generates high-fidelity reaction mappings, highlighting the transformation of functional groups and atomic changes.

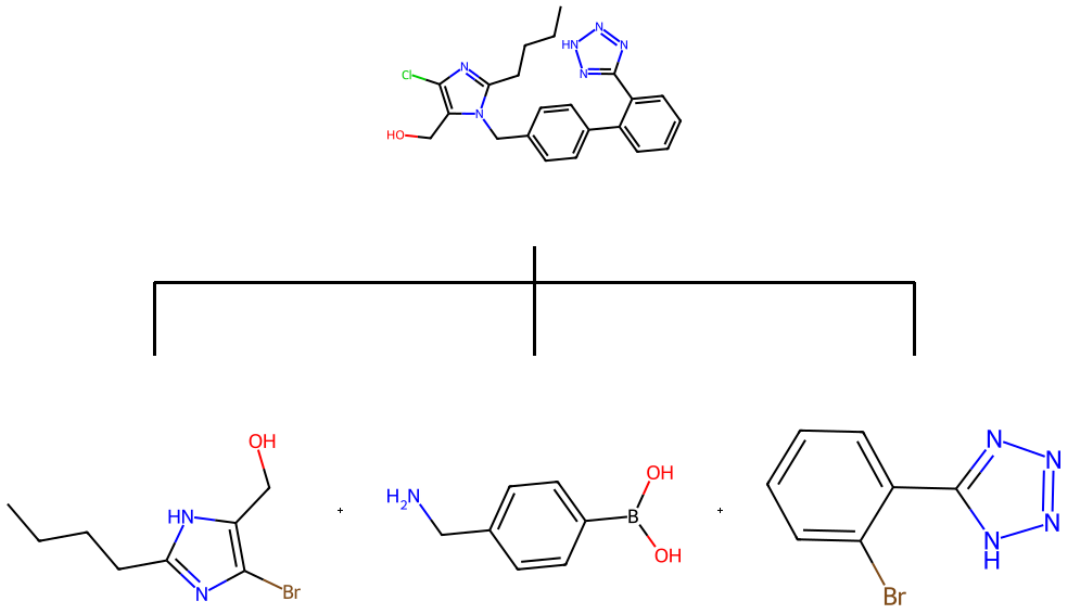

Fig 3. Detailed Reaction Mapping: Step 1 (Coupling).

4. Key Technical Innovations

- **Closed-Loop Verification**: Integration with `verify_skill.py` ensures that all RDKit-derived properties (LogP, MW, Fingerprints) are consistent throughout the planning process.
- **Persona-Driven Prompting**: Specialized prompts in `prompts_personas.py` reduce hallucination by forcing agents to focus on their specific domain (e.g., the Auditor cannot ignore PG loops).
- **Automated Reporting**: The `report_generator.py` compiles JSON audit trails and PNG assets into a single, cohesive Markdown document for peer review.

5. Conclusion

ChemReact transforms retrosynthesis from a solo "guessing" game into an audited, visual, and documented engineering process. By combining the precision of RDKit with the flexibility of multi-persona LLMs, it offers a scalable solution for early-stage drug discovery and process chemistry.

Released Version: v0.1.0