Integrating AI Based Tools Significantly Enhances the Usability of the Reference Chemistry Database for Research and Education

**Abstract:**

The rapid evolution of AI based tools is transforming both chemistry research and education. Traditional keyword-based database searches often fail to capture the contextual meaning of user queries, limiting their effectiveness and requiring significant user intervention. Recent advances in large language models (LLMs) and vector-based semantic search enable more intuitive querying and allowing retrieval based on conceptual similarity rather than exact text matching.

Concurrently, AI based predictive retrosynthesis tools are reshaping how organic synthesis is carried and taught. While traditional instruction emphasizes named reactions and mechanistic understanding, modern tools allow researchers and students to systematically design synthetic routes using comprehensive reaction databases and algorithmic predictions. These technologies not only accelerate route design but also encourage exploration of alternative, potentially more sustainable reaction pathways.

We explore the synergy between semantic search, navigating reaction conditions and predictive retrosynthesis in both research and educational settings. By integrating LLM-driven search capabilities with retrosynthetic planning tools, chemists and students can more efficiently access relevant chemical knowledge and apply it to synthesis design. We propose workflows demonstrating how these approaches can streamline problem-solving, enhance learning outcomes, and better prepare students for modern chemical research environments.