Multimodal Search in Chemical Documents and Reactions

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Abstract

We present a multimodal search tool for retrieval of chemical reactions, molecular structures, and associated text from scientific literature. Queries may combine molecular diagrams, textual descriptions, and reaction data, allowing users to connect different chemical information representations. Indexing includes chemical diagram extraction and parsing, extraction of reaction data from text in tabular form, and cross-modal linking of diagrams with their mentions in text. We describe the system's architecture and retrieval features, along with expert assessments of the system. Our demo highlights the workflow and search components. Online demo: https://www.cs.rit.edu/~dprl/reactionminer-demo-landing

CCS Concepts

• **Information systems → Chemical and biochemical retrieval**.

Keywords

multi-modal search, reactions, chemical diagrams

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1 Introduction

The scientific literature contains vast chemical knowledge represented in prose and diagrams. Roughly speaking, molecular and reaction diagrams represent the structure and relation of compounds participating in reactions, while the main text and text labels on reaction diagram entities describe how and why reactions occur (e.g., at what temperature, the yield of a product molecule, pertinent molecular properties, etc.). As a result, the full story of a reaction is often told using a combination of text and diagrams.

Traditional Chemical Information Retrieval (CIR) systems and commercial platforms such as SciFinder® [1] and Reaxys® [2] provide text-based and structure-based search. However, these systems do not link molecular figures with their textual descriptions, making it difficult to retrieve reactions found in diagrams with their associated context provided in the text of a paper. These systems also return individual compounds or full documents as results, rather than returning text passages where reaction descriptions are found. These limitations present challenges for chemists, patent examiners, and researchers seeking to retrieve relevant compounds, reactions, or synthesis protocols along with their contexts efficiently.

To address these challenges, our system[3] supports direct retrieval of relevant passages along with their associated molecular structures. This includes structures extracted from molecular diagrams and referenced in the text by common name (e.g., 'chromene'), IUPAC name [19], or figure identifier (e.g., molecule '4b'). Automatically extracted reaction records are also generated from passages using *ReactionMiner* [23], and provided alongside passages and their associated compounds. The reaction records enable researchers to explore linked reaction steps.

Passages may be searched using text queries, molecular structure queries in SMILES (Simplified Molecular Input Line Entry System) strings [22], or their combination. SMILES is frequently used in chemoinformatics, and can be readily generated by a number of

[1] SciFinder®: https://scifinder.cas.org/
[2] Reaxys®: https://www.reaxys.com/
[3] https://www.cs.rit.edu/~dprl/reactionminer-demo-landing/

commonly used drawing tools (e.g., ChemDraw or Marvin). This multimodal search model facilitates direct navigation between reaction text, associated molecule diagrams, and extracted chemical entities. The system supports text-based search using BM25, and SMILES-based molecular search using structural similarity and substructure matching provided by RDKit.[4]

Related work. Early CIR systems such as ChemXSeer [12] focused on extracting and indexing chemical names from tables in PDFs to support search by molecule name or formula. Later efforts, such as TREC-CHEM [9], introduced the concept of document-level retrieval for chemistry-specific tasks in patents, and provided relevance assessment data. Recent advances in deep learning have focused on cross-modal learning to align structured molecular representations with textual descriptions. Both Text2Mol [3] and MoleculeSTM [7] adopt joint learning approaches that embed chemical structures and text into a shared embedding space, facilitating retrieval across modalities. Text2Mol employs graph neural networks (GNNs) [15] to predict the most appropriate SMILES representation given a textual query, aiming to support molecule retrieval from natural language descriptions. Similarly, MoleculeSTM is designed for structure-text retrieval, retrieving chemical structure from textual descriptions and vice versa by leveraging a multimodal transformer within a contrastive learning framework.

However, these systems focus on document-level rather than passage-level search. Our system enables structured retrieval by directly linking extracted molecular diagrams, textual mentions, and reaction descriptions. OpenChemIE [4] extracts reaction data from text, tables, and figures using modality-specific models, similar to our approach of combining text-based reaction extraction and molecular diagram parsing. Unlike OpenChemIE our system integrates extraction with passage-level retrieval.

2 Indexing Extracted Compounds and Reactions

In our system, textual and graphical content are processed through two parallel pipelines, whose outputs are later used to build a unified index of chemical entities, paragraph texts, and reactions.

Text mining for extracting reaction information. *ReactionMiner [23]* processes PDF document text to convert reaction descriptions to structured reaction records in JSON. First, the text is segmented into reaction-related sentences through product-indicative keywords and topic modeling [2]. A large language model, LLaMA3.1-8b [5], fine-tuned with LoRA [6], is used to identify relevant chemical entities including reactants, products, and catalysts, along with key conditions (e.g., temperature, reagents, or solvents). Each extracted reaction is associated with a PDF text bounding box (see Figure 1), enabling direct navigation to the underlying paragraph.

Extracting SMILES from document text. We also extract individual compounds from document text. These additional SMILES annotations ensure that compounds mentioned both inside and outside of reaction descriptions can be retrieved through the search interface. For indexing compounds in text, we first use PyTesseract to convert document page images to text, which is then passed to *ChemDataExtractor2.0's* [11] Chemical Named Entity Recognition (CNER) system to identify molecule names. Each recognized name is converted into a SMILES string via *OPSIN* [8], and any passage containing at least one valid SMILES is retained for indexing.

Molecular diagram extraction and parsing. We use YOLOv8, an improved version of scaled YOLOv4 [21], for detecting molecular regions in documents. We then employ *ChemScraper* [16] to parse molecular diagrams from detected PDF regions (see Figure 1) through two complementary pipelines: a *born-digital* approach for vector images representing characters and geometric objects, and a *visual parsing* [18] approach for pixel-based raster images. In the born-digital parser, *SymbolScraper* [17] accesses low-level PDF drawing commands to extract lines, polygons, and characters directly from the PDF. The visual parser works on raster images, applying the *Line Segment Detector (LSD)* [20] and watershed algorithm to detect line primitives and text regions. Together, these methods yield a set of graphical elements (e.g., atoms, bond lines, named functional groups) and their local connections.

ChemScraper then constructs a *visual structure graph* using a Minimum Spanning Tree (MST) and rewrite rules for born-digital diagrams and a segmentation-aware, multi-task neural network for raster images. The visual graph is then converted to a molecular graph, where bonds become edges and implicit carbon atoms are inferred from line intersections. The final molecular graph is stored in *CDXML format* to retain both chemical and visual structure. This format is converted into SMILES for indexing.

Compound-passage linking and multimodal indexing. Once we have extracted reaction information from text, and molecular structures from text and diagrams, they are stored in a unified representation to support flexible querying. There are two passage types in our system: (1) those extracted by *ReactionMiner* (boxed text in Figure 1), and (2) those extracted from general text regions using PyTesseract (unboxed). For passages extracted by *ReactionMiner*, relevant text fields include reactants, products, catalysts, and yields. We link reactants and products in reaction records with corresponding molecular diagrams using two approaches:

(1) *Token-based text matching*. Text mentions of diagram labels for reactants and products are identified using regular expressions, and then matched with the nearest diagram text label by a normalized Levenshtein similarity ratio[5], ensuring minor variations in naming do not prevent linkage. An example is shown in red in Figure 1, where 'compound 5' is matched with the diagram labeled '5.'
(2) *SMILES-based fingerprint matching*. The text tokens are first processed through *ChemDataExtractor2.0* [11] and *OPSIN* [8], following the same approach described earlier for non-reaction text, while SMILES from diagrams are extracted by *ChemScraper* [16]. Each SMILES representation undergoes molecular fingerprinting, producing a binary vector encoding the molecular graph's connectivity patterns. To determine similarity, we compute the *Tanimoto Similarity* [1] measuring the overlap between fingerprint vectors, giving a similarity score between 0 and 1. The diagram with the highest *Tanimoto Similarity* score with a passage SMILES are linked. An example is shown in blue in Figure 1, where 'N-formyl amide' is matched with the diagram labeled '2.'

[4] https://www.rdkit.org

[5] https://rapidfuzz.github.io/Levenshtein/levenshtein.html#ratio

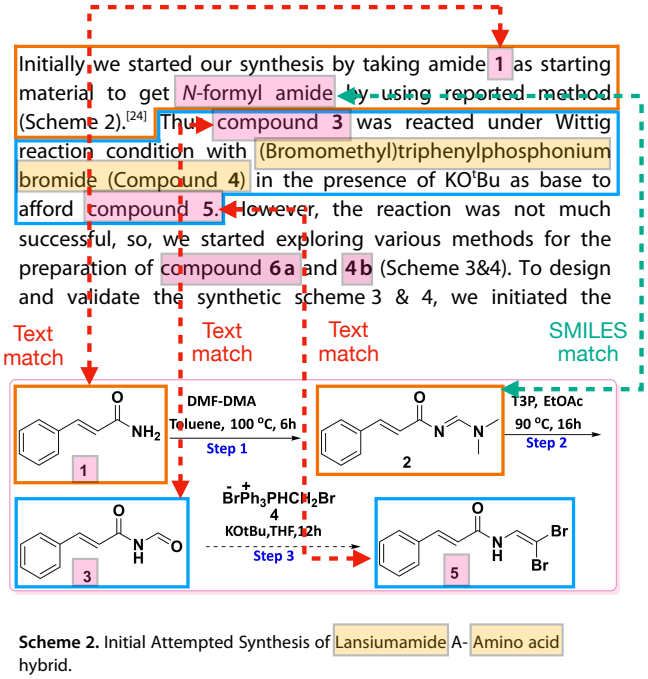

Figure 1: Text/diagram compound extraction and compound–passage linking. Two passage types are shown: (1) reaction passages from *ReactionMiner* (2 boxes) and (2) a single text passage containing both extracted compounds. Highlighted text denotes extracted chemical entities: pink for mentions in molecular diagrams, yellow for unmatched mentions. Matches come from (1) *Text matching* via Levenshtein distance and (2) *SMILES matching* via *Tanimoto Similarity*. Highlight colors (e.g., orange and blue) indicate molecules & reaction text linked to the same reaction passage.

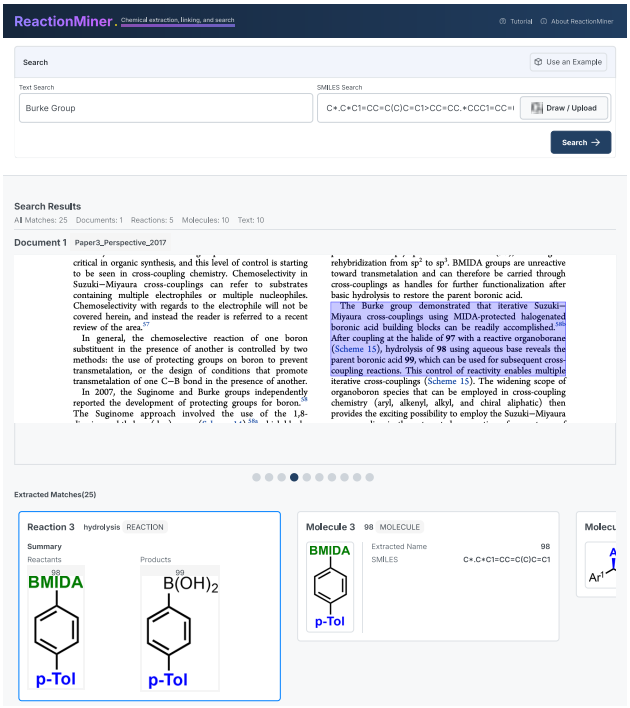

Figure 2: Multi-modal search results for a text and reaction SMARTS query. Results are organized by document, with matched passages highlighted and linked to extracted reactions, molecular structures, and text mentions (shown in 'cards' at bottom). Key reaction details, including reactant ('98') and product ('99') in both text and diagrams, along with their extracted SMILES representations are displayed. Users can navigate directly to passages associated with the cards at bottom by clicking on them.

If a compound can be linked by both strategies, the strategy with the higher score between the normalized *Levenshtein similarity ratio* and the *Tanimoto Similarity* is chosen. In the final index, text passages are annotated with their linked SMILES and reaction records. This enables retrieval of specific compounds and reaction information in text passages and extracted reaction records.

During indexing, IUPAC names in text are tokenized into constituent groups [13] to support partial matching. For example, IUPAC name 'N-((E)-2-bromo-2-phenylvinyl)-cinnamamide' is tokenized as 'N E 2 bromo 2 phenyl vinyl cinnamamide'.

3 Multimodal Search: Suzuki Coupling Papers

Our system supports three primary search models based on different query types: text search, molecular structure/substructure search (from SMILES), and multimodal search combining text and molecular queries. Text search is handled using BM25 [14] as implemented in PyTerrier [10], allowing users to search for compounds, reaction conditions, or chemical properties in text. Molecular structure search is provided by RDKit, enabling both exact molecule matching and substructure searching. Multimodal search integrates results from both models, by re-ranking results to prioritize passages that contain both textual and molecular matches.

For this demonstration, we indexed 7 main and 6 supplementary papers describing Suzuki coupling reactions, provided by chemists at the University of Illinois. The dataset includes 1282 extracted passages, of which 538 are indexed (passages without links to reactions or compounds are removed). Associated with these passages are 383 unique SMILES strings, and 219 extracted reactions. The passages are linked to diagrams and SMILES as described in the previous section. This structured linking allows users to retrieve molecular and reaction information, whether entities appear in text descriptions or are represented as molecular diagrams.

Molecular SMILES and SMARTS search. Query SMILES and candidate SMILES in the index are converted into fingerprint vector representations using Morgan Fingerprinting (2048 bits), and are ranked using *Tanimoto Similarity*, described earlier. The system also accommodates structured queries specifying entire chemical reactions using *Reaction SMARTS* (SMILES Arbitrary Targets Specification) notation. This format extends SMILES strings to include '>' separating reactants, reagents, and products, while '.' separates individual SMILES compounds within each category, as seen in Figure 2.

To process these queries, SMILES compounds are extracted from the SMARTS string, and each is matched against indexed molecular structures and reaction passages.

This allows retrieval of reactions in passages using SMARTS queries, while also providing access to details provided in *ReactionMiner* records linked to passages. Information such as reactants, products, catalysts, reaction conditions, and temperature are presented for retrieved passages, when associated reaction records are present in the index. This enables users to search for entire reactions rather than just isolated compounds.

Multimodal search. For multimodal queries containing text and SMILES (or Reaction SMARTS) as shown in Figure 2, the initial SMILES candidates are obtained using *sub-structure search*. We find that including all possible sub-structures as valid candidates for re-ranking text candidates leads to better performance: *Tanimoto Similarity* can be unpredictable for very specific information needs when combined with text. If multiple SMILES are provided, the retrieved passages for each individual SMILES query are aggregated. For hybrid queries, results from text-based and SMILES-based retrieval are fused to improve ranking. Text hits, retrieved using BM25, serve as the anchor. SMILES-based sub-structure search identifies compound hits, which are mapped back to their original passages. Overlaps between the two retrieval modes are detected, and passages linked to more SMILES hits are ranked higher. The final ranking is a two-level sort, ordering passages by their number of sub-structure matches, followed by BM25 text match scores.

Reaction navigation. The system also provides a dedicated reaction navigation feature for each retrieved document. When a user selects a passage, they can inspect all extracted reactions from the associated document in a structured list, with each reaction entry pointing to the relevant PDF page and bounding-box highlights, as shown in Figure 2. This approach lets users explore multiple reaction mentions in context, making it easier to follow complex procedures, compare alternative synthetic routes, or identify recurring reagents and intermediates within a single publication.

4 Expert Evaluation by Chemists

We conducted an expert assessment with two chemical researchers at the University of Illinois. The system effectively retrieved relevant chemical information, linking molecular diagrams and text-based reaction details to chemical names or SMILES queries. For example, as shown in Figure 2, a multi-modal search with the text query 'Burke group' and a Reaction SMARTS string successfully retrieved passages with relevant reactions which were associated with the 'Burke group', as shown in the highlighted text and corresponding reaction diagrams displayed below the document image. Chemists found the ability to click on molecule 'cards' and navigate directly to the corresponding section in the document particularly useful. The structured reaction output captured key experimental details such as yield, catalysts, solvents, and temperature, enhancing the accessibility of reaction data. The reaction and molecule cards serve as a structured extractive summary of the paper, while also providing navigation links to their original context. Note that the 'Reaction 3' in Figure 2 does not show these additional details as they were not available in the text.

Notably, the system retrieved derivatives of a queried molecule, such as 'benzo[b]thiophen-2-ylboronic acid,' which was relevant to the SMILES query 'C1=CC=C2C(=C1)C3=CC=CC=C3S2' (dibenzothiophene) but not explicitly searched for. Overall, the chemists were able to find the information they were hoping for, and the retrieved results were useful for their research.

While reaction details were generally well extracted, experts recommended incorporating additional metadata such as 'equivalents' and mol% of catalysts, which are essential for exporting data to electronic lab notebooks. When using a combination of text and SMILES queries, the chemists found it challenging to determine whether retrieved results were more influenced by text-based or structure-based matching, suggesting a need for greater transparency in the effect of text vs. SMILES on ranked results. Additionally, filtering options to view reactions, molecules, and text separately would improve usability, allowing chemists to focus on the most relevant data. Another key area for improvement is enhanced diagram-text linking, as some extracted text mentions were not associated with their corresponding molecular diagrams. Addressing these issues would further enhance the system's utility for chemical research.

5 Conclusion and Future Work

We have presented a multimodal search system that integrates text and molecular structure retrieval, enabling passage-level search with structured linking between chemical entities in text, molecular diagrams, and reaction descriptions. By combining BM25 for text, RDKit-based molecular similarity search, and a fusion mechanism for multimodal queries, our system improves access to chemical knowledge in scientific literature. The expert evaluation with chemists demonstrates the system's usability, with researchers successfully retrieving relevant chemical information, including useful molecular derivatives and structured reaction details.

Future work will focus on enhancing retrieval effectiveness with dense embeddings and cross-modal search, leveraging transformer-based models to improve ranking and semantic matching across text and molecular representations. While the system currently matches chemical names to diagrams via SMILES translation, inspired by Text2Mol [3], we aim to explore query expansion within an aligned multimodal embedding space. This approach would expand text queries to incorporate corresponding molecular diagrams or SMILES representations and extend SMILES queries to include relevant text-based descriptors, improving retrieval flexibility.

Additional directions include scaling the system to index larger collections, integrating external chemical databases, and adding filtering mechanisms to improve user experience. A more mature version of our system may find use in chemical research, industry, and patent analysis, reducing time spent on literature review and supporting efficient retrieval of structured chemical information.

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