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Automated electrosynthesis reaction mining with multimodal large language models (MLLMs)[†]

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Leveraging the chemical data available in legacy formats such as publications and patents is a significant challenge for the community. Automated reaction mining offers a promising solution to unleash this knowledge into a learnable digital form and therefore help expedite materials and reaction discovery. However, existing reaction mining toolkits are limited to single input modalities (text or images) and cannot effectively integrate heterogeneous data that is scattered across text, tables, and figures. In this work, we go beyond single input modalities and explore multimodal large language models (MLLMs) for the analysis of diverse data inputs for automated electrosynthesis reaction mining. We compiled a test dataset of 65 articles (MERMES-T24 set) and employed it to benchmark five prominent MLLMs against two critical tasks: (i) reaction diagram parsing and (ii) resolving cross-modality data interdependencies. The frontrunner MLLM achieved $\geq 96\%$ accuracy in both tasks, with the strategic integration of single-shot visual prompts and image pre-processing techniques. We integrate this capability into a toolkit named MERMES (multimodal reaction mining pipeline for electrosynthesis). Our toolkit functions as an end-to-end MLLM-powered pipeline that integrates article retrieval, information extraction and multimodal analysis for streamlining and automating knowledge extraction. This work lays the groundwork for the increased utilization of MLLMs to accelerate the digitization of chemistry knowledge for data-driven research.

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Introduction

Despite today's increasingly data-driven scientific landscape, most of the past chemical knowledge remains locked in one way or another, using legacy data formats such as the hypertext markup language (HTML) and portable document format (PDF), or hidden behind paywalls. One way forward is the automated data mining from these "locked" scientific data

stemming from publications and patents. If fully automated, this task would be essential to help construct databases which can be leveraged as collective knowledge to significantly expedite materials and reaction discovery and uncover fundamental governing chemistries.^{1–13} Despite advancements in specialized text mining or diagram parsing tools,^{14–18} extracting accurate and comprehensive experimental data records remains challenging due to at least two main hurdles: (i) key chemical and/or materials information is usually scattered across various data modalities within both the main text and ESI,[†] including tables, figures/schemes, and textual descriptions and (ii) the user-desired data is typically overwhelmed by a substantial amount of extraneous content, *i.e.*, "data flooding". These two challenges underscore the need for robust yet flexible data mining workflows capable of multimodal analysis, while efficiently filtering and processing the specialized data at hand.

Recently, large language models (LLMs) such as Claude,^{19,20} Gemini,²¹ GPT²² and LLaMA²³ among others^{24,25} have demonstrated immense potential in text-based knowledge extraction from scientific publications, using a combination of prompt engineering, model fine-tuning and in-context learning techniques.^{3,22,26–40} Compared to traditional natural language processing (NLP) methods that rely heavily on rule-based syntax or dictionary-matching, LLM-powered literature mining exhibits higher adaptability and generalizability due to the

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natural language processing, conversational capabilities, and general-purpose versatility of LLMs. Nonetheless, the integration of visual information poses an additional layer of complexity. The emergent development of multimodal large language models (MLLMs), with the ability to receive and process multiple data types including images, text, language, audio, and other heterogeneity, offers a more well-rounded task-solver.^{41–44} These MLLMs have reported promising accuracies in various vision-language multimodal tasks such as image captioning and visual question-answering in generic everyday context, across different evaluation benchmarks. The next logical question for us arises: can state-of-the-art MLLMs effectively process and integrate textual and visual inputs from scientific literature for specialized, domain-specific tasks such as reaction mining?

In this study, we demonstrate that MLLMs exhibit multimodal cognition capabilities that are suitable for chemical applications. We focus on two essential subtasks in automated reaction mining. The first subtask involves parsing reaction conditions into categorical data (10 different categories), which is a requirement due to the conventional use of graphical representations to summarize novel reactions (Fig. 1A). The second subtask involves resolving cross-modality interdependencies, where reference labels within figure images are defined elsewhere in the text (Fig. 1B). This capability is also required since substrate-specific variations in reaction conditions are typically conveyed through such index cross-references. Being able to identify and connect these distributed pieces of information together is thus crucial to maintain data coherency and integrity during the automated mining process. Using 65

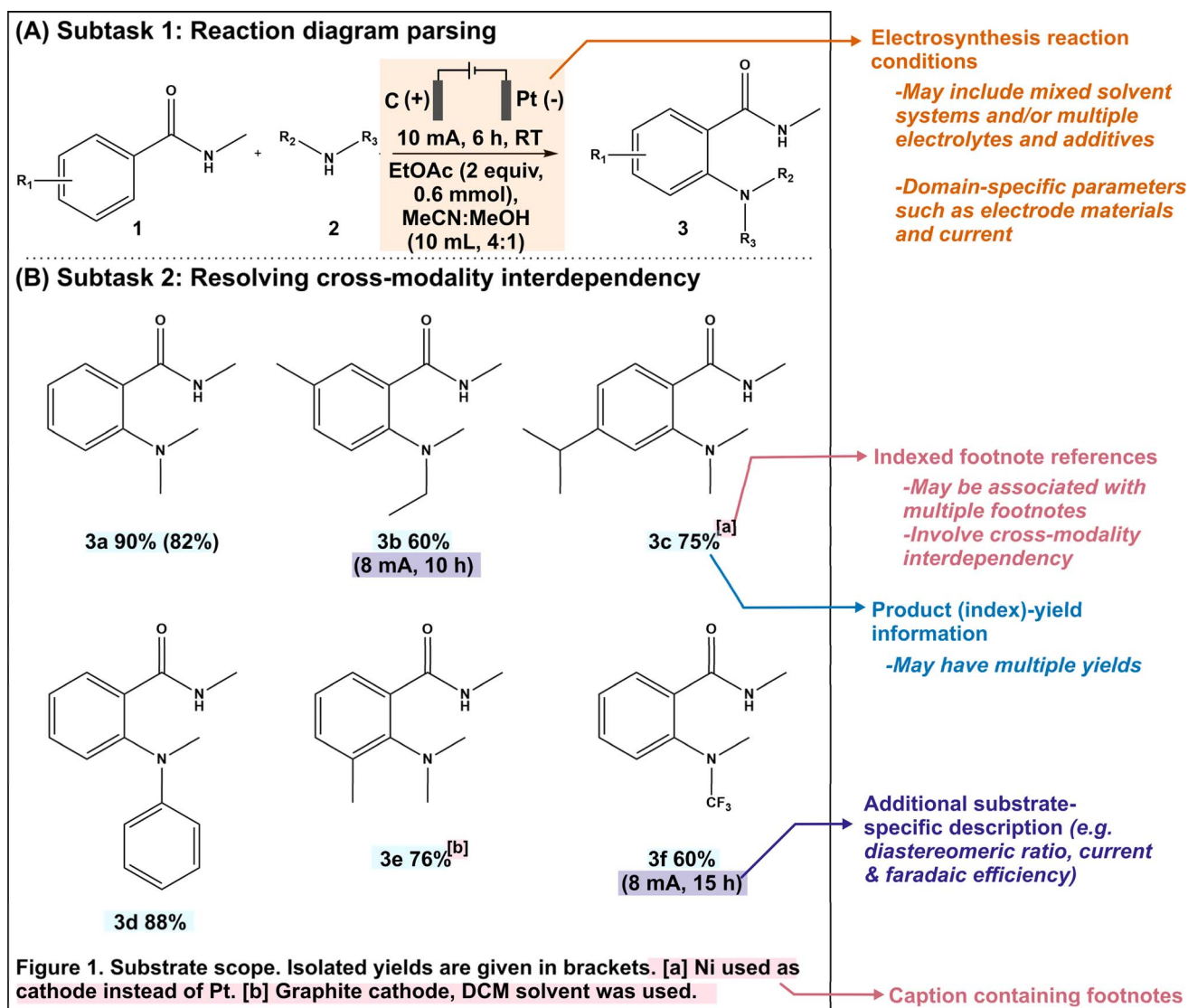


Fig. 1 [Task overview] An example of a typical figure depicting the overall reaction diagram and substrate scope, with the corresponding caption. The figure is a non-copyrighted image drawn by the authors for illustrative purposes. We highlight two key challenges of automated reaction mining: (A) reaction diagram parsing and (B) resolving cross-modality data interdependency in terms of footnote cross-references. In addition, substrate-specific information that are presented in non-standardized formats across figures may also be present.

Prompt for reaction diagram parsing

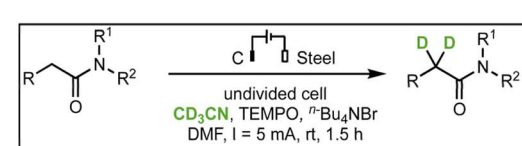


This is an electrolysis reaction. Output a JSON dictionary for the standard conditions with the following keys:

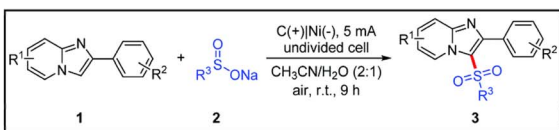
- 1) "anode material": a string that describes the anode material, which is the positive end. Abbreviations may be used in the image.
- 2) "cathode material": a string that describes the cathode material, which is the negative end. Abbreviations may be used in the image.
- 3) "electrolytes": a string that describes all the electrolytes and additives for the reaction. Provide all equivalents, amounts and concentrations in brackets.
- 4) "solvents": a string that describes all the solvents for the reaction. Provide all volumes and ratios in brackets.
- 5) "current": a string that describes the current used.
- 6) "duration": a string that describes the duration of the reaction.
- 7) "air/inert": a string that describes if the reaction is performed in air or under inert conditions.
- 8) "temperature": a string that describes the temperature of the reaction.
- 9) "others": a string that describes any other reaction conditions not included in the previous keys.

In all the strings, only use information that are given. Put N.R. otherwise. Each compound should only appear once.

Minimize hallucinations



```
{ "anode material": "C", "cathode material": "Steel", "electrolytes": "CD3CN (N.R.), TEMPO (N.R.), nBu4NBr (N.R.)", "solvents": "DMF (N.R.)", "current": "5 mA", "duration": "1.5 h", "air/inert": "N.R.", "temperature": "rt", "others": "undivided cell" }
```



```
{ "anode material": "C", "cathode material": "Ni", "electrolytes": "N.R.", "solvents": "CH3CN/H2O (2:1)", "current": "5 mA", "duration": "9 h", "air/inert": "air", "temperature": "rt", "others": "undivided cell" }
```

Single-shot visual prompts of different presentation styles (example figure-response)

Fig. 2 [Single-shot visual prompting for electrosynthesis reaction diagram parsing] The full prompt used in this subtask for electrosynthesis reaction diagram parsing is provided. The example images are adapted with permission from ref. 59 and ref. 60, with permission from the Royal Society of Chemistry.

We analysed the results of reaction diagram parsing using two evaluation metrics with different tolerance levels: (i) hard match evaluation requires the correct matching of reaction parameters with their intended role, while (ii) soft match evaluation requires only correct identification of the parameter, regardless of its role. For instance, an anode material annotated as the cathode, or solvents classified as electrolytes/additives are considered incorrect under hard match evaluation but correct under soft match evaluation. Accurate hard matches for the anode and cathode material are especially critical for automated electrosynthesis reaction mining because swapping the electrode polarity would influence the actual yield and selectivity. In addition, it is important to note that we do not accommodate partial answers for reactions involving mixed solvent systems and/or multiple electrolytes/additives across both evaluation metrics. In other words, the identified parameter is only considered "correct" when all reported solvents/electrolytes/additives are present.

The outcomes of our preliminary evaluation of the zero-shot performances of the five MLLMs, summarized in Fig. 3A, reveal that GPT-4V surpasses the others in both hard and soft match evaluations (detailed discussion in ESI Note 1; supplementary

evaluation metrics provided in Tables S2–S5†). Given its strong performance, we chose GPT-4V for further refinement. The model's hard match accuracy was lowest for the identification of solvents and electrode materials (both cathode and anode), with scores of 83% and 85% respectively (Fig. 3A). In the case of solvents, misclassification primarily arises from mis-labelling solvents as electrolytes, in which the model achieved excellent 100% soft-match accuracy (Fig. 3A). For electrode classification, we deconvoluted the model's performance based on the presentation style of the electrode systems, categorized into four categories based on whether the anode and cathode materials are explicitly indicated by their respective polarities or inferred schematically from circuit symbols (Fig. 3B-i). While the model achieved 100% accuracy for the first two styles, its performance dropped to 75–78% and 70% for styles 3 and 4, respectively (Fig. 3B-iii). We hypothesize that these two styles are poorly predicted due to their ambiguous representations, which necessitate prior understanding of the commonly employed chemical nomenclature. In this regard, we demonstrate the effectiveness of single-shot visual prompting in boosting the "chemical-awareness" of the MLLM for improved adaptability to specialized image mining tasks. By providing single-shot

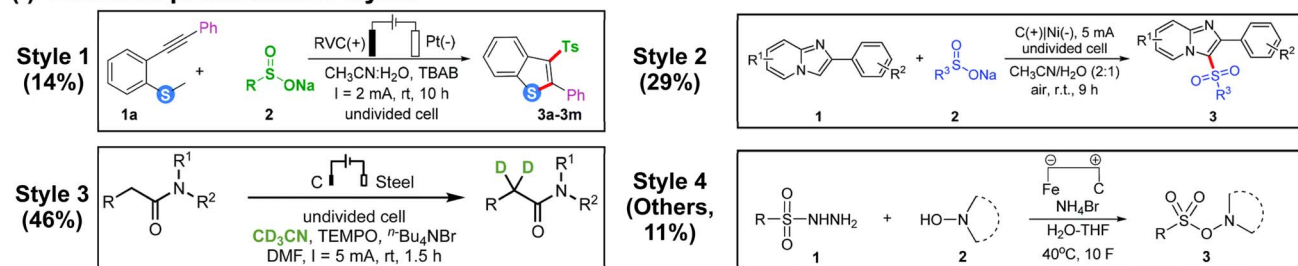


(A) Zero-shot performances of different MLLMs and previous pipelined approaches

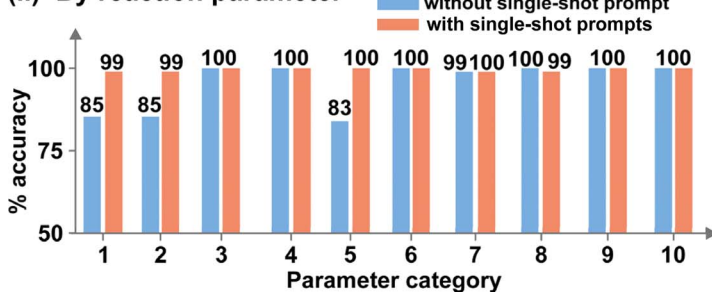
	% identification accuracy									
	Anode (+)	Cathode (-)	Electrolytes/additives	Amount of electrolytes/additives	Solvents	Solvent amounts	Current	Duration	Air/Inert	Temperature
GPT-4V	85% (93%)	85% (93%)	100% (100%)	100% (100%)	83% (100%)	100% (100%)	99% (99%)	100% (100%)	100% (100%)	100% (100%)
Gemini	61% (66%)	51% (66%)	89% (89%)	89% (89%)	59% (93%)	93% (93%)	98% (98%)	97% (97%)	99% (99%)	100% (100%)
Claude 3	56% (72%)	54% (69%)	95% (96%)	86% (86%)	68% (92%)	88% (91%)	99% (99%)	96% (96%)	100% (100%)	100% (100%)
LLaVA	16% (28%)	19% (38%)	53% (57%)	59% (63%)	31% (47%)	91% (64%)	25% (33%)	77% (81%)	74% (76%)	43% (55%)
InternVL	46% (60%)	43% (57%)	51% (52%)	47% (48%)	26% (51%)	50% (50%)	55% (57%)	55% (55%)	54% (54%)	34% (37%)
ReactionData Extractor2.0	— (23%)	— (23%)	— (31%)	— (33%)	— (31%)	— (31%)	— (32%)	— (36%)	— (33%)	— (33%)
RxnScribe	— (50%)	— (50%)	— (79%)	— (87%)	— (83%)	— (94%)	— (95%)	— (98%)	— (99%)	— (83%)

(B) Performance refinement for GPT-4V model (hard match)

(i) Different presentation styles



(ii) By reaction parameter



(iii) By presentation style

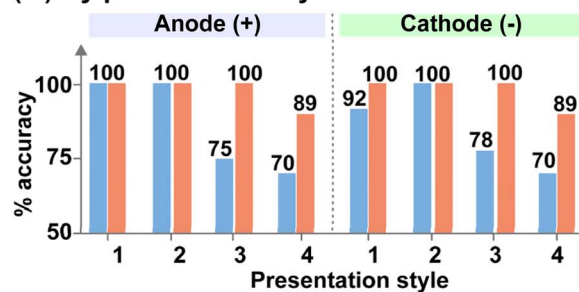


Fig. 3 [Performance evaluation of electrosynthesis reaction diagram parsing] (A) % hard match (soft match) identification accuracy for each parameter using different MLLMs and two specialized reaction diagram parsing toolkits previously reported, as benchmarks. For the benchmark models, only the soft match scores are tabulated because the different categories are not specified. The highest scores for each category are in green. (B) Evaluation of the effectiveness of single-shot visual prompts. (i) Examples of different reaction diagram presentation styles. The % distribution of each style within our dataset is included in brackets. The example images are adapted with permission from ref. 61 (style 1), ref. 59 (style 2), ref. 60 (style 3), and ref. 62 (style 4), with permission from the Royal Society of Chemistry. (ii) % of correctly identified for each reaction parameter category with and without the integration of single-shot visual prompts. Categories 1–10 refer to anode, cathode, electrolytes/additives, amounts of electrolytes/additives, solvents, amounts of solvents, current, duration, air/inert atmosphere, and temperature, respectively. (iii) % of correctly identified anode and cathode material for each presentation style under hard match evaluation.

examples of a representative reaction diagram from each presentation style before analysing the actual dataset, we observed notable improvements to 100% and 89% for the latter two styles, boosting the overall hard match electrode accuracy to 99% (Fig. 3B-ii and iii; Tables S6 and S7†). In addition, hard match accuracies for all other parameter categories also reached

near-unity (Fig. 3B-ii). Importantly, the model is robust against more intricate scenarios, such as those involving mixed solvent systems and/or multiple electrolytes and additives (present in 57% of investigated reaction diagrams), or in instances where multiple units such as ratio, % mol, mmol and molarity are utilized (present in all investigated reaction diagrams).



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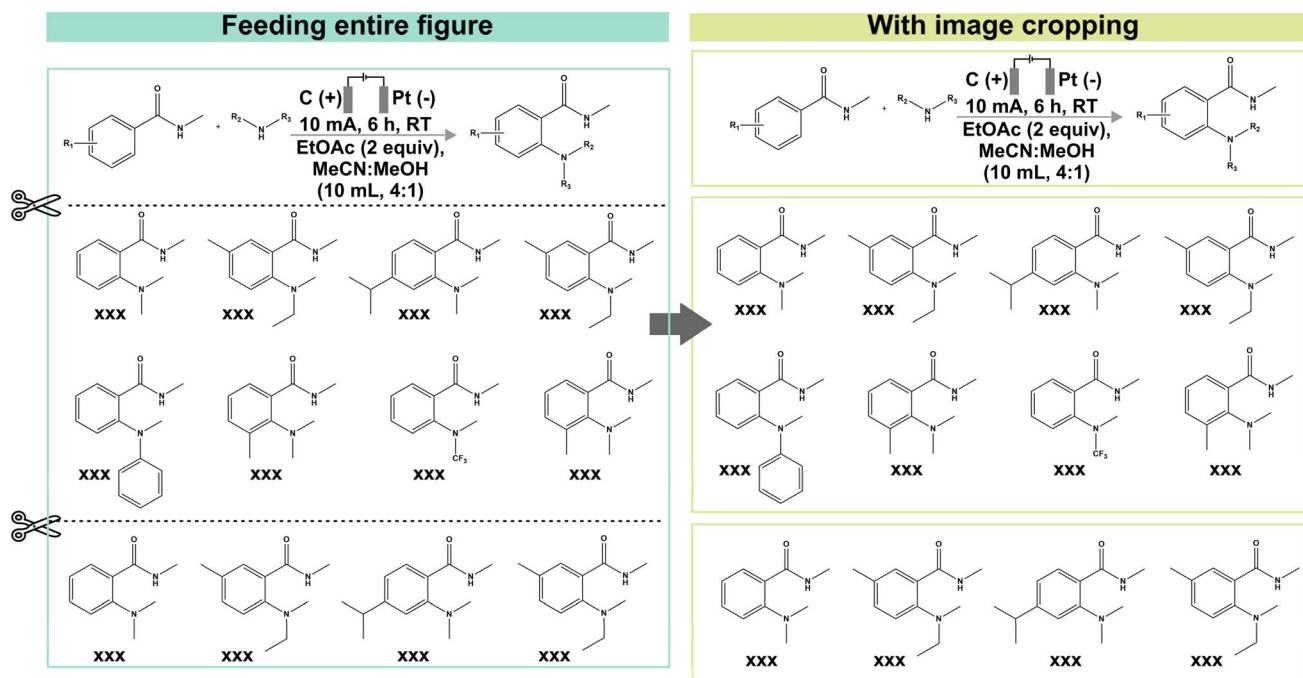
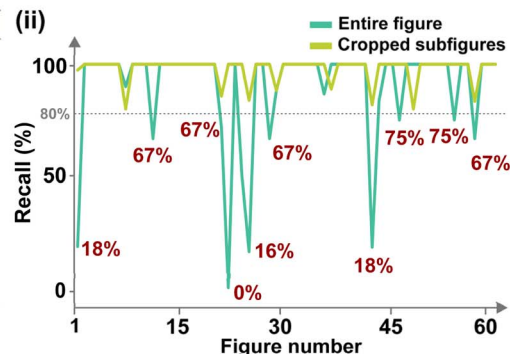


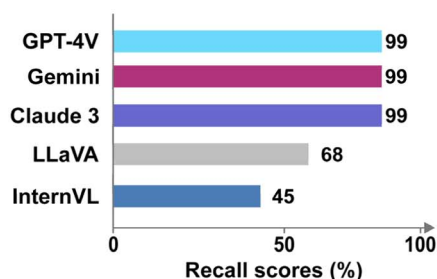
Fig. 4 [Image cropping prior to multimodal analysis] Schematic overview of image cropping prior to multimodal analysis. The figure is a non-copyrighted image drawn by the authors for illustrative purposes.

(A) Resolving footnote cross-referencing

(i)	MLLM	Precision	Recall	F1	Specificity	Accuracy
	GPT-4V	95%	73%	83%	99%	91%
	(without image cropping)					
	GPT-4V	96%	96%	96%	99%	98%
	(with image cropping)					
	Gemini	88%	59%	70%	96%	85%
	(with image cropping)					
	Claude 3	90%	86%	88%	96%	93%
	(with image cropping)					
	LLaVA	9%	7%	8%	70%	51%
	(with image cropping)					
	InternVL	5%	6%	6%	50%	37%
	(with image cropping)					



(B)(i) Index-yield pairs



(ii) Additional substrate-specific information

	MLLM	Precision	Recall	F1	Specificity	Accuracy
	GPT-4V	100%	92%	96%	100%	98%
	(without image cropping)					
	GPT-4V	99%	99%	99%	100%	99%
	(with image cropping)					
	Gemini	100%	94%	97%	100%	98%
	(with image cropping)					
	Claude 3	99%	100%	99%	99%	99%
	(with image cropping)					
	LLaVA	62%	50%	55%	85%	73%
	(with image cropping)					
	InternVL	24%	22%	23%	59%	45%
	(with image cropping)					

Fig. 5 [Performance evaluation for parsing of substrate scope information] (A) (i) Performance evaluation of different MLLMs at resolving cross-modality data interdependencies. The highest scores for each evaluation metric are in green. (ii) Comparison of individual recall scores for resolving footnote cross-referencing in each figure with and without image cropping, using GPT-4V model as the test model. Figures with low recall scores <80% are indicated. (B) Performance evaluation of different MLLMs at identifying (i) index-yield pairs and (ii) additional substrate-specific information. The highest scores for each evaluation metric are in green.

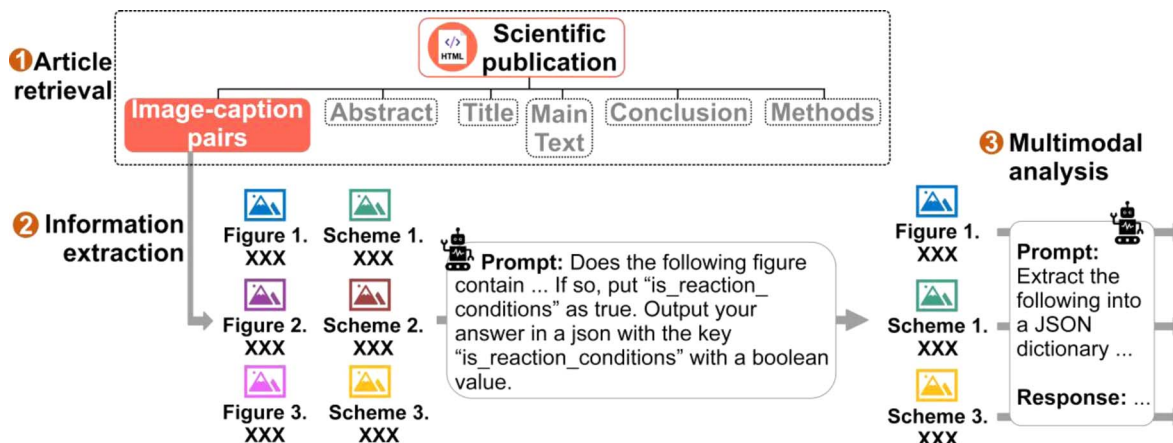


Fig. 6 Schematic illustration of multimodal pipeline for automated reaction mining featuring three sequential steps: article retrieval, information extraction, and multimodal analysis of filtered information.

multimodal analysis. Our automated workflow is designed to process articles in HTML format, which offers standardized, machine-readable document structure to facilitate automated data extraction. In brief, the article retrieval module initiates the job by downloading content and high-resolution images from the URLs of the articles (Step 1 in Fig. 6). Next, the information extraction module extracts the image–caption pairs and identifies those of relevance to our defined task *via* MLLM, guided by user-provided natural language prompts (Step 2 in Fig. 6). The filtered image–caption pairs are directed to the final multimodal analysis module, where the pertinent chemical information is extracted by natural language prompts (Step 3 in Fig. 6). When analysing the figures, we adopt the similar strategy to crop the figure into smaller subfigures parts to ensure the performance of the MLLM. We note that our framework can be easily extended to process other data contents in the article. Our future work will include extending the pipeline to efficiently mine other document formats, such as PDF, which remains challenging for machines to parse and sort the data. The full code is available in GitHub: <https://www.github.com/aspuru-guzik-group/MERMES>.

Conclusions

We demonstrate that multimodal large language models are capable of chemistry-relevant multimodal cognition skills to interpret and assimilate electrosynthesis information from scientific publications. Our findings reveal that the strategic integration of text-based preconditioning prompts and single-shot visual prompts for in-context learning enables MLLMs to grasp domain-specific concepts for accurate parameter identification and role assignment, achieving $\geq 99\%$ accuracy across 10 different parameter categories for the frontrunner MLLM. At the same time, they can resolve cross-modality data interdependency with excellent F1 scores of $\geq 96\%$, while offering enough flexibility to handle disparate amounts of information to extract additional, non-standardized details not consistently reported across all figures. This level of accuracy significantly

surpasses the 80% benchmark for manual data extraction by humans.⁶³ We developed a toolkit (MERMES) for carrying out these tasks, serving as a multimodal pipeline for automated reaction mining from scientific publications. Moving forward, we will equip MERMES with additional capabilities such as image-to-SMILES translation and utilize MERMES to create a comprehensive electrosynthesis reaction database as an invaluable data resource for numerous potential downstream applications from computer-aided reaction discovery and optimization, reaction prediction and other predictive tasks. From a broader perspective, by exemplifying the potential of harnessing multimodal large language models in (electro)chemical information processing, we envisage that MLLM-based reaction mining workflows such as MERMES will open new opportunities for data-driven research across numerous domains.

Data availability

The source code of our automated workflow extraction code, MERMES, together with additional data mining scripts, can be found in our Github repository (<https://www.github.com/aspuru-guzik-group/MERMES>). To improve the reproducibility of this work, a frozen version of the repository has been uploaded to Zenodo (<https://doi.org/10.5281/zenodo.12713560>).⁶⁴ The prompts used in this work, together with the raw responses from the tested MLLM models are compiled and uploaded to Zenodo (<https://doi.org/10.5281/zenodo.12701834>) for data transparency and reproducibility.⁶⁵

Author contributions

S. X. L., conceptualization, data curation, formal analysis, investigation, methodology, validation, visualization & writing – original draft preparation, review & editing. S. P.-G., conceptualization, formal analysis, methodology, supervision & writing – review & editing. Z. Z. conceptualization, methodology, software & writing – review & editing. A. A.-G., conceptualization, funding



acquisition, resources, project administration, supervision & writing – review & editing.

Conflicts of interest

A. A.-G is a founder of Kebotix, Inc., Axiomatic, Inc., and Intrepid Labs, Inc.

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