Fine-tuning ChatGPT Achieves State-of-the-Art Performance for Chemical Text Mining

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Abstract

Extracting knowledge from complex and diverse chemical texts is a pivotal task for both experimental and computational chemists. The task is still considered to be extremely challenging due to the complexity of the chemical language and scientific literature. This study fine-tuned ChatGPT for five intricate chemical text mining tasks: compound entity recognition, reaction role labelling, metal-organic framework (MOF) synthesis information extraction, nuclear magnetic resonance spectroscopy (NMR) data extraction, and the conversion of reaction paragraph to action sequence. The fine-tuned ChatGPT demonstrated impressive performance, significantly reducing the need for repetitive and extensive prompt engineering experiments. It achieved exact accuracy levels ranging from 69% to 95% on these tasks with minimal annotated data. For comparison, we fine-tuned open-source pre-trained large language models (LLMs) such as Llama2, T5, and BART. The results showed that the fine-tuned ChatGPT excelled in all tasks. It even outperformed those task-adaptive pre-training and fine-tuning models that were based on a significantly larger amount of in-domain data. Given its versatility, robustness, and low-code capability, leveraging fine-tuned LLMs as toolkits for automated data acquisition could revolutionize chemical knowledge extraction.

Main

Chemical text mining is a crucial foundation in chemical research. It creates extensive databases that provide access to physicochemical properties and synthetic routes for experimental chemists. Additionally, it accumulates rich data and insights for computational chemists to use for modelling and predicting. More than just extracting information from chemical texts, the rule-based transformation of chemical text is particularly interesting. For instance, synthetic procedures

can be converted into action sequences[1] or programming languages[2-4]. This allows them to be understood and executed by robotic systems for automated syntheses.

Converting structured data from intricate scientific literature is a challenging task, especially due to the complexity and heterogeneity of chemical language. As a result, a number of text-mining tools have been developed. For instance, ChemDataExtractor[5,6] was created to extract chemical entities and their associated properties, measurements and relationships. ChemRxnExtractor[7] was designed to extract the product and label associated reaction roles such as reactant, catalyst, solvent, and temperature. Historically, the focus has been on designing models and algorithms specific to certain tasks, often using regular expressions with rule-based syntax or dictionary-matching. These tools require extensive domain knowledge and sophisticated data processing, which limits their versatility.

Recently, large language models (LLMs), represented by ChatGPT released in November 2022, have shown the potential of Artificial General Intelligence (AGI). LLMs, such as GPT-3.5 and GPT-4, can generate logical insights or content that meets requirements based on human instructions. We are entering a new era where AGI and medicinal chemists might work together. There have been assessments of ChatGPT's chemistry capabilities, including tasks like synonym transformation, property prediction, retrosynthesis, and molecule design[8-10]. However, LLMs tend to "hallucinate", meaning they generate unintended text that misaligns with established facts and real-world knowledge[11,12]. Moreover, objectively evaluating the results of open-ended questions remains a significant challenge.

At this juncture, LLMs may struggle to accurately answer factual and knowledge-based questions. However, using LLMs for knowledge extraction tasks should greatly alleviate hallucination and fully leverage their powerful text comprehension and processing capabilities,

making them promising universal tools for chemical text mining. For instance, Zheng et al.[13] used prompt engineering to guide ChatGPT in extracting information about metal-organic framework (MOF) synthesis. Yet, Chen et al.[14] reported that ChatGPT performed significantly worse on biomedical text mining compared to existing models. This finding contradicts the common belief in the LLMs' superior comprehension abilities. Either way, LLMs have limitations due to their model architecture and memory, including a maximum length of prompt tokens. Additionally, human expressions can be ambiguous, incomplete, vague, and difficult to refine. Outputs may not strictly adhere to formatting requirements, leading to misunderstanding and poor performance in mining complex text, such as patents or scientific literature. Therefore, zero-shot or few-shot prompts are often insufficient to address the diversity of scenarios.

In this study, we fine-tuned ChatGPT for five challenging tasks in chemical text mining: compound entity recognition, reaction role annotation, metal-organic framework (MOF) synthesis information extraction, nuclear magnetic resonance spectroscopy (NMR) data extraction, and conversion reaction paragraphs into action sequences. We found for the first time that fine-tuning ChatGPT significantly enhances performance in text mining tasks, compared to prompt-only version, while also reducing dependency on the repetitive and extensive prompt engineering experiments. Meanwhile, we also evaluated other newly emerged generative pre-trained language models, such as Llama2[15], T5[16], and BART[17]. Among these, the fine-tuned ChatGPT achieved state-of-the-art (SOTA) performance across all five tasks. Remarkably, it even outperformed models that have been trained specifically for each task and subsequently fine-tuned, based on a significantly larger amount of in-domain data. This study highlights the potential of fine-tuning LLMs, like ChatGPT, to revolutionize complex knowledge extraction with their versatility, robustness, and low code capability. Fine-tuned LLMs can be easily generalizable and can

optimize the labour-intensive and time-consuming data collection workflow, even when trained with few data. This will accelerate the discovery and creation of novel substances, making them powerful tools for universal use.

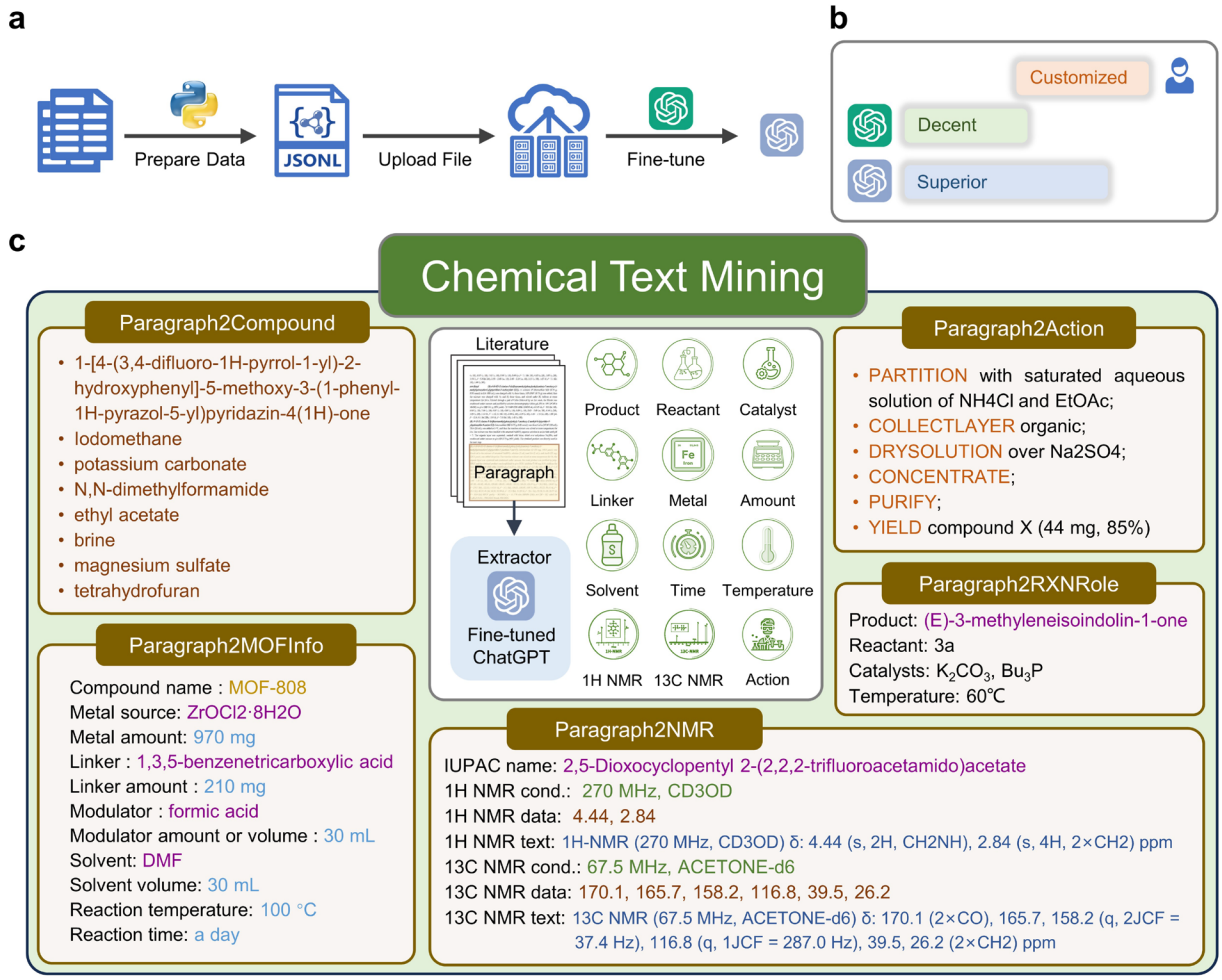


Fig. 1 | Schematics of fine-tuning ChatGPT for chemical text mining. a, The pipeline of fine-tuning ChatGPT on proprietary data. The green OpenAI logo symbolizes official gpt-3.5-turbo, while the blue one symbolizes fine-tuned gpt-3.5-turbo. **b,** Supervised fine-tuned ChatGPT outperforms prompt-only ChatGPT in some customized scenarios. **c,** Illustration of cheminformatics insights to be extracted from paragraph. And illustration of the five practical tasks in chemical text mining with respective example outputs, including Paragraph2Compound, Paragraph2RXNRole, Paragraph2MOFInfo, Paragraph2NMR, and Paragraph2Action.

Overview of Chemical Text Mining Tasks

Given the complex and diverse information embedded in chemical literature, we designed five extraction tasks to demonstrate the potential and practicality of LLMs in chemical text mining. Paragraph2Compound task is to extract all chemical compound entities from the given chemical paragraph. Paragraph2RXNRole task is to label the reaction roles including product, reactant, catalyst, temperature, solvent, time, and yield in the paragraph. Paragraph2MOFInfo task is to extract all MOF synthesis conditions including compound name, metal source, metal amount, linker, linker amount, modulator, modulator amount or volume, solvent, solvent volume, reaction temperature and reaction time. Paragraph2NMR task is to extract the IUPAC name, experimental condition including frequency and solvent as well as chemical shift data for both 1H NMR and 13C NMR spectra. Paragraph2Action task is to convert experimental procedures to structured synthetic steps (action sequences). All tasks are unified to sequence-to-sequence formats to facilitate the uses of LLMs.

Paragraph2Compound—Extract all chemical compound entities.

Fig. 2a illustrates the sampling process, which narrows down from 100,000 to 10, out of millions of pre-processed annotations, followed by the training process. Fig. 2b demonstrates the performance of prompt-only models and fine-tuned models, which are evaluated on a consistent evaluation set of 1,000 samples across varying training data sizes. These results are obtained from three independent trials. In the case of prompt-only models, randomness is intentionally introduced by altering the prompt and examples (Fig. 2c). Given the task's straightforward nature and clear instructions, even the prompt-only language models achieved decent F1 scores over 0.6. For fine-tuned models, the sampling and training process for the training set is repeated three times, as

depicted in Fig. 2a. As shown in Fig. 2b, all fine-tuned models demonstrate a performance improvement, especially in terms of the F1 score and Jaccard index, proportional to the increase in dataset size. These models outperform the prompt-only models designed for this task. When the training data size is substantial enough, the F1 scores of ChatGPT, Llama2, and T5 can reach close to 0.9, and the Jaccard index can approach 0.8. Notably, gpt-3.5-turbo, when fine-tuned, showed minimal fluctuations and superior performance. However, it is essential to emphasize that the cost of fine-tuning gpt-3.5-turbo increased tenfold with each tenfold increase in data volume. Our experimentation with gpt-3.5-turbo were capped at 10,000 training samples for 3 epochs due to OpenAI's limitations, resulting in a nearly 90-dollar expense—a significant investment in computational resources. In contrast, other fine-tuned language models have displayed notable cost advantages in this simple task.

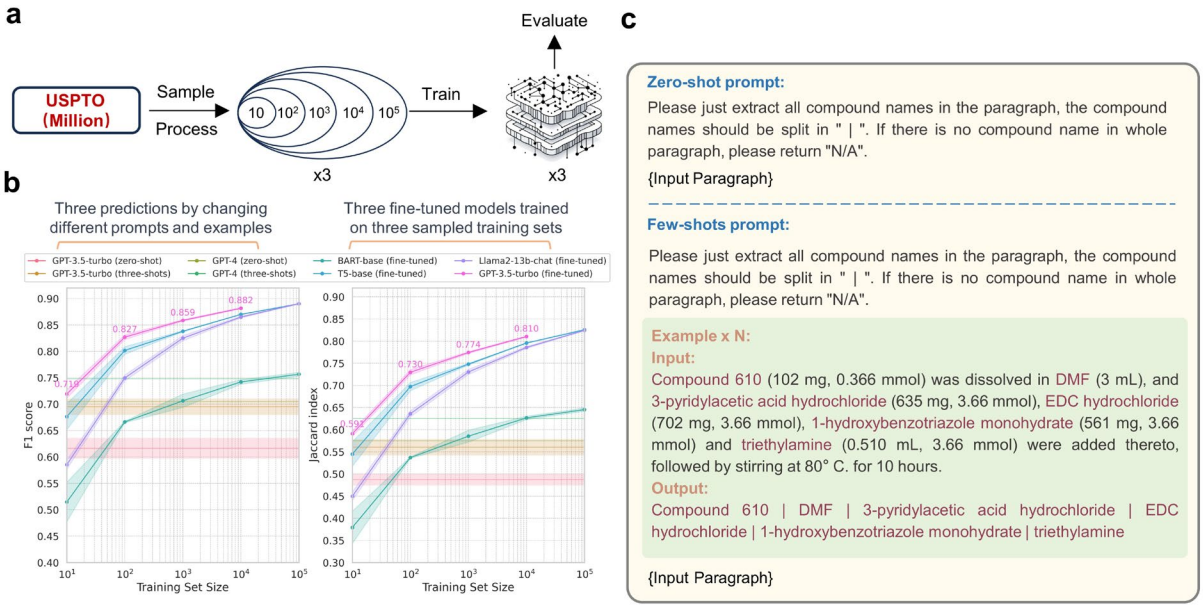


Fig. 2. | Design and Performance for Paragraph2Compound task. a, The workflow of sampling and training based on USPTO dataset for Paragraph2Compound task. **b**, The performance of different models across varying size of training set. The data point and the shaded areas represent respectively the mean values and standard deviations derived from three independent trials. **c**, Example of the zero-shot and three-shots prompts utilized for Paragraph2Compound task.

Paragraph2RXNRole—Product Extraction and Reaction Role Labelling.

According to Guo et al.[7], the Paragraph2RXNRole task comprises two subtasks. The first is to extract the central product, and the second is to label the associated reaction roles within specified paragraphs (Fig. 3a). For these tasks, Guo et al. developed two-stage BERT-like token-multi-classification models. To enable a fair comparison with generative language models, we converted the data into sequence-to-sequence formats by adding <Role*Compound*Role> annotations to the input paragraphs. We then converted the language models' outputs back into lists of BIO-tags, followed by post-processing to align with the original BIO-tags labels for assessment. For product extraction, our fine-tuned ChatGPT (best over one epoch) achieved a F1 score of 77.1%, slightly surpassing the previous SOTA approach, ChemBERT, which scored 76.2% (Fig. 3b). For reaction role labelling, our fine-tuned ChatGPT (best over five epochs) achieved a F1 score of 83.0%, significantly outperforming the previous SOTA approach, ChemRxnBERT, which scored 78.7% (Fig. 3c). It's notable that the fine-tuned ChatGPT models, which cost only $1 and $5 respectively, demonstrated extremely high cost-effectiveness with small training datasets. In contrast, ChemBERT was domain-adaptive pre-trained on 9,478,043 sentences from 200,000 journal articles, and ChemRxnBERT was further task-adaptive trained on 944,733 reaction-inclusive sentences. We should also mention that the outputs of fine-tuned ChatGPT and Llama2 align almost perfectly with the input text, with 100% and 99% post-processing-free ratios respectively. On the other hand, the outputs of fine-tuned T5 and BART require additional alignment due to their tokenization and vocabulary limitations, with a ratio of only 31% that does not require post-processing. Even after post-processing, the F1 scores of T5 and BART were significantly lower than those token-classification models or LLMs such as ChatGPT and Llama2.

By the way, when utilizing prompt engineering with 30-shot examples, ChatGPT just achieved an F1 score of less than 30% due to the disorganized dataset.

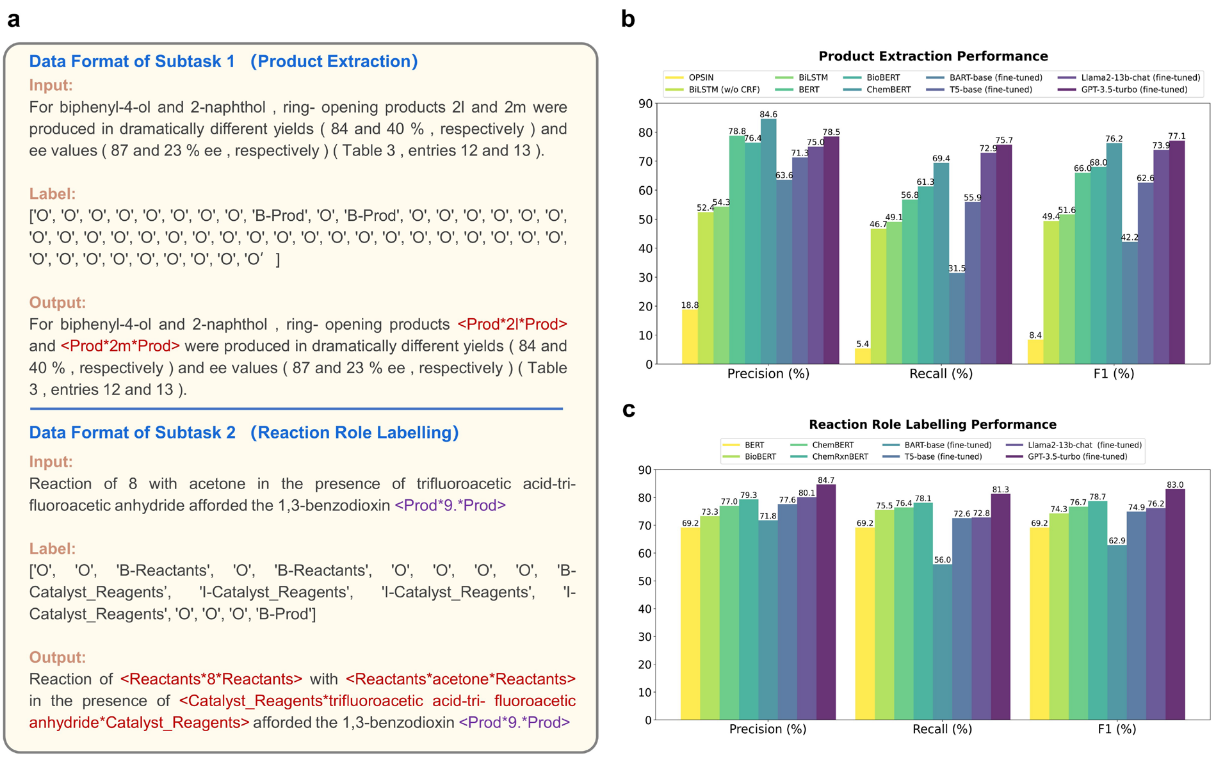
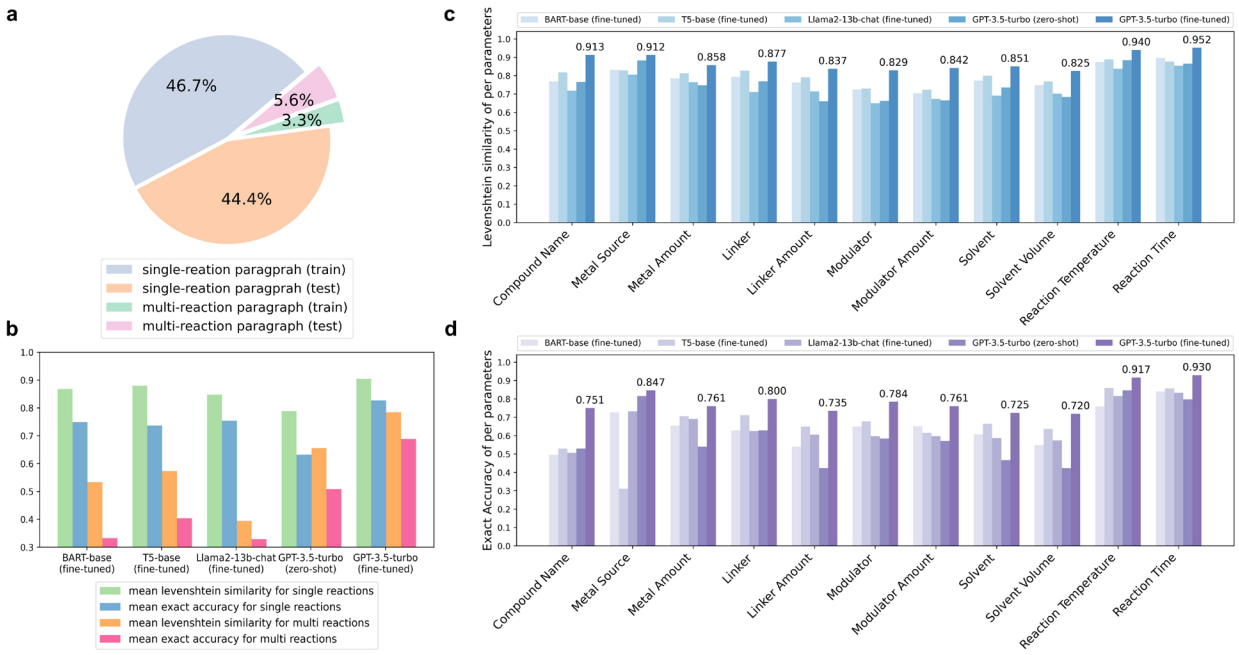


Fig. 3. | Design and Performance for Paragraph2RXNRole task. a, Data formats of two subtasks in paragraph2RXNRole task. **b**, Performance of product extraction. **c**, Performance of reaction role labelling.

Paragraph2MOFInfo—Extraction of MOF Synthesis Information.

Our re-annotated dataset for the Paragraph2MOFInfo task displayed in Fig. 4a, mostly contains single reaction paragraphs with a few featuring multiple reactions. We used Levenshtein similarity and exact accuracy as metrics to objectively assess the models' ability to extract formatted data that fully complies with customized requirements in the task. This approach contrasts with the manual analysis used by Zheng et al.[13] and requires less human intervention. The fine-tuned ChatGPT significantly outperforms the ChatGPT with prompt engineering, improving exact extractions by over 20% for both single and multiple reactions (Fig. 4b). It also surpasses other fine-tuned models, especially when handling complex multi-reaction paragraphs.

Exact accuracy rates for single and multiple reactions are 82.7% and 68.8%, respectively (Fig. 4b). As depicted in Fig. 4c and Fig. 4d, while most models achieve high Levenshtein similarity across the 11 parameters, only a few maintain high exact accuracy, which is the golden metric that we mainly focus on. Considering that some MOF synthesis paragraphs may include multiple reactions, we provide an example of multi-reaction extraction by various models in Fig. 4e. The paragraph includes two reactions, the first with (R)-H3PIA and bipy as linkers, providing all reaction conditions explicitly, and the second with the substitution of (R)-H3PIA with (S)-H3PIA, keeping all other conditions unchanged. Most models successfully interpreted the semantics and extracted two reactions from the MOF synthesis paragraph. However, only the fine-tuned ChatGPT perfectly extracted information that matched our annotated ground truth. Other models showed varying degrees of incompleteness, particularly with items involving multiple components and their quantities.



e

Paragraph

Synthesis of [Cd1.5((R)-PIA)(bipy)1.5(H2O)]n (1-D): a mixture of (R)-H3PIA (0.031 g, 0.1 mmol), bipy (0.023 g, 0.15 mmol), Cd(NO3)2·4H2O (0.061 g, 0.20 mmol), distilled water (1 mL), methanol (2 mL) and DMF (2 mL) was stirred in a 23 mL teflon cup, and then heated at 100 °C for 48 hours. The colorless block-like crystals of 1-D were obtained in 50% yield based on (R)-H3PIA. Elemental analysis calcd (%) for 1-D: C 49.26, H 3.14, N 7.92; found C 48.14, H 3.32, N 7.66.Synthesis of [Cd1.5((S)-PIA)(bipy)1.5(H2O)]n (1-L): Complex 1-L was synthesized in a similar way to that described for 1-D except using (S)-H3PIA instead of (R)-H3PIA. The colorless block-like crystals of 1-D were obtained in 45% yield based on (S)-H3PIA. Elemental analysis calcd (%) for 1-L: C 49.26, H 3.14, N 7.92; found C 48.41, H 3.41, N 7.45.

Extractions

Model	Compound name	Metal source	Metal amount	Linker	Linker amount	Modulator	Modulator amount	Solvent	Solvent volume	Reaction temperature	Reaction time
BART-base (fine-tuned)	[Cd1.5((R)-PIA)(bipy) 1.5(H2O)]n (1-D)	Cd(NO3)2·4H2O	0.0601 g, 0.20 mmol	(R)-H3PIA | bipy	0.031 g, 0.1 mmol | 0.023 g, 3.15 mmol	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL| 2 mL	100 °C	48 hours
	[CD1.3((S)-H3PIA)1.05(H3O)]ni (1–L)	Cd[NO3]2·6H2S	0.061 g%, 0. 20 mmol	(S–H3PBIA | DMF	0.029 g, 1.15 mL | 0.)023 g. 0.15 °C	NaN	NaN	distilled water | meethanol	NaN	100 °C	48 hours
T5-base (fine-tuned)	[Cd1.5((R)-PIA)(bipy)1.5(H2O)]n (1-D)	Cd[NO3]2·6H2S	0.061 g, 0.20 mmol	(R)-H3PIA | bipy	0.031 g, 0.1 mmol | 0.023 g, 0.15 mmol	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	48 hours
	Cd1.5((R)-PIA)(bipy)1.5(H2O)]n (1-D)	Cd(NO3)24H2O	0.061 g, 0.20 mmol	(S)-H3PIA | (R)-H3PIA	0.031 g, 0.1 mmol | 0.023 g, 0.15 mmol	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	48 hours
Llama2 (fine-tuned)	1-D	Cd(NO3)2·4H2O	0.061 g, 0.20 mmol	bipy	0.023 g, 0.15 mmol	R-H3PIA	0.031 g, 0.1 mmol	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	48 hours
GPT-3.5-turbo (zero-shot)	[Cd1.5((R)-PIA)(bipy)1.5(H2O)]n	Cd(NO3)2·4H2O	0.061 g, 0.20 mmol	(R)-H3PIA	0.031 g, 0.1 mmol	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	48 hours
	[Cd1.5((S)-PIA)(bipy)1.5(H2O)]n	Cd(NO3)2·4H2O	0.061 g, 0.20 mmol	(S)-H3PIA	NaN	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	NaN
GPT-3.5-turbo (fine-tuned)	[Cd1.5((R)-PIA)(bipy)1.5(H2O)]n (1-D)	Cd(NO3)2·4H2O	0.061 g, 0.20 mmol	(R)-H3PIA | bipy	0.031 g, 0.1 mmol | 0.023 g, 0.15 mmol	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	48 hours
	[Cd1.5((S)-PIA)(bipy)1.5(H2O)]n (1-L)	Cd(NO3)2·4H2O	0.061 g, 0.20 mmol	(S)-H3PIA | bipy	0.031 g, 0.1 mmol | 0.023 g, 0.15 mmol	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	48 hours
Ground truth	[Cd1.5((R)-PIA)(bipy)1.5(H2O)]n (1-D)	Cd(NO3)2·4H2O	0.061 g, 0.20 mmol	(R)-H3PIA | bipy	0.031 g, 0.1 mmol | 0.023 g, 0.15 mmol	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	48 hours
	[Cd1.5((S)-PIA)(bipy)1.5(H2O)]n (1-L)	Cd(NO3)2·4H2O	0.061 g, 0.20 mmol	(S)-H3PIA | bipy	0.031 g, 0.1 mmol | 0.023 g, 0.15 mmol	NaN	NaN	distilled water | methanol | DMF	1 mL | 2 mL | 2 mL	100 °C	48 hours

Fig. 4. | Design and Performance for Paragraph2MOFInfo task. a, A statistic of the dataset. **b**, Mean performance of Levenshtein similarity and exact match accuracy by different models. **c**, Levenshtein similarity for 11 parameters in the Paragraph2MOFInfo task. **d**, Exact match accuracy for 11 parameters in the Paragraph2MOFInfo task. **e**, An example of extractions by different models from a multi-reaction MOF synthesis paragraph. The cells in yellow represented the ground truth. The cells in green represented the exact match predictions. The cells in blue represented the incorrect predictions.

Paragraph2NMR—Extraction of experimental conditions and NMR chemical shifts.

The impact of training set sizes and the use of prompt engineering on the performance of fine-tuning ChatGPT in extracting NMR information is illustrated in Fig. 5a. Regardless of the training data size for fine-tuning (ranging from 25 to 300), or the presence of prompt engineering, there are hardly any significant fluctuations in performance. This holds true for metrics such as Levenshtein similarity and exact match accuracy of the fine-tuned ChatGPT when the numbers of training samples exceed 50. This demonstrates the strong learning capability and robustness of LLMs. Fig. 5b illustrates the performance of different generative language models using the same 200 training data. In terms of Levenshtein similarity, a metric based on edit distance, almost all fine-tuned language models achieved impressing scores, outperforming ChatGPT that solely relies on prompt engineering (Fig. 5b). However, when considering the exact match accuracy metric, where each character must perfectly align with the ground truth count, LLMs such as ChatGPT and Llama2 take the lead. While fine-tuned T5 and BART manage to extract the majority of the text, they often miss or mistakenly copy several characters. This contributes to a significant decrease in their exact match accuracy metric, as shown in Fig. 5c. In this context, the extraction of long complex text by LLMs is more standardized and high-quality, aligning more closely with human expectations. It is worth noting that fine-tuning Llama2 provides an alternative approach for deploying text mining locally, given its exceptional exact match accuracy.

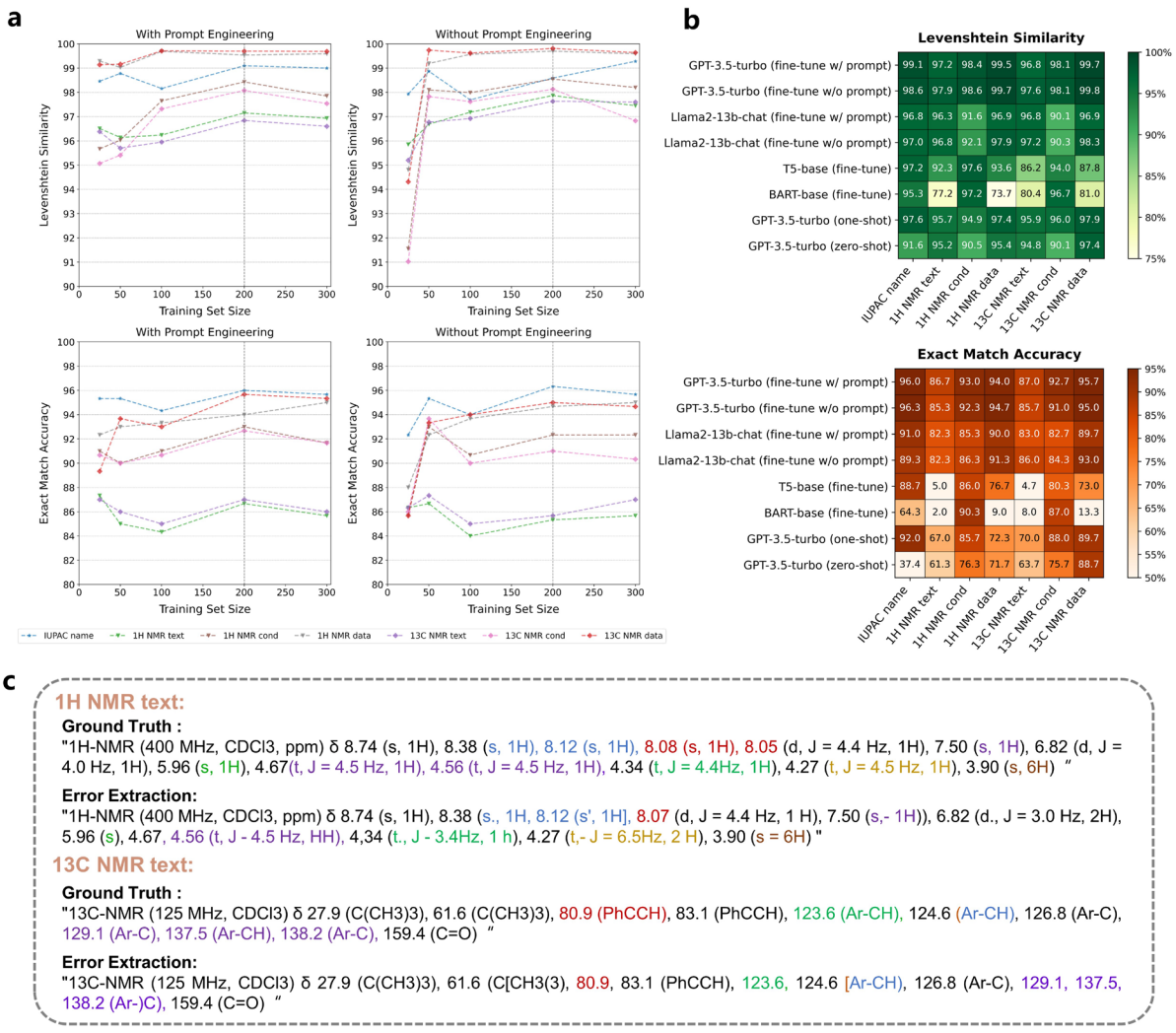


Fig. 5. | Performance for Pargraph2NMR task. a, The performance of fine-tuning ChatGPT with and without prompt engineering as it varies with training data size. **b**, Heat map illustrating Levenshtein similarity and exact match accuracy of various models in extracting each NMR information. **c**, Examples of error extractions by T5 and BART, compared with the ground truth.

Paragraph2Action: Action sequence extracted from an experimental procedure.

The above-mentioned extraction tasks simply require the model to replicate specific information from the paragraph. However, the Paragraph2Action task requires the model to understand and transform the paragraph. Clearly, ChatGPT with prompt engineering has difficulty with this task, especially when it involves multiple complex conversions and insufficient prompt descriptions. To gauge the maximum potential of ChatGPT using only prompts, we incrementally

increased the number of transformation examples from 6 to 30. Despite encompassing all types of actions at least once and nearly reaching the token limit of 4,096 with 30 examples, ChatGPT's performance in a few-shot scenario remains disappointingly poor. It only achieved 13.9% full sentence exact accuracy, a BLEU score of 49.5, and a Levenshtein similarity of 66.0. In contrast, fine-tuning pre-trained language models with a small amount of data can yield decent results, achieving over 50% full sentence exact accuracy and over 80% for both BLEU Score and Levenshtein similarity. Remarkably, after 3 epochs of fine-tuning ChatGPT on 1,060 hand-annotated training data, we achieved 62.5% full sentence exact accuracy, an 84.8 Modified BLEU score, and an 87.6 Levenshtein similarity. This process took only 1 hour and cost $3 for fine-tuning. These metrics surpass the SOTA results previously reported by Vaucher et al.[1], which used an ensemble of three modes, each task-adaptively pre-trained on 2 millions rule-based data and refined on 14,168 augmented data. Interestingly, further improvement was achieved by augmenting the training data size to 14,168. This resulted in 69.0% full sentence exact accuracy, an 86.4 Modified BLEU score, and an 89.9 Levenshtein similarity (Table 1). For tasks involving "fuzzy rules" or hard-to-define extraction, fine-tuning ChatGPT offers significant advantages in tailoring the transformation with a small amount of annotated data.

Tabel 1 | Performance on Paragraph2Action task.

Model	Training data strategy	100% accuracy	90% accuracy	75% accuracy	Modified BLEU score	Levenshtein similarity	Cost
GPT-3.5-turbo (6-shots)	No training	8.2	16.8	34.7	38.6	59.4	905 mean tokens
GPT-3.5-turbo (12-shots)	No training	8.8	19.3	42.3	43.1	62.3	1,374 mean tokens
GPT-3.5-turbo (18-shots)	No training	13.1	23.3	42.6	44.4	64.3	1,670 mean tokens
GPT-3.5-turbo (24-shots)	No training	14.8	25.9	45.5	47.0	65.8	2,598 mean tokens
GPT-3.5-turbo (30-shots)	No training	13.9	26.4	47.2	49.5	66.0	3,610 mean tokens
Transformer (single model) *	No task-adaptive pretraining, no augmentation (1,060)	13.1	15.1	21.9	22.5	45.9	-
BART-base (fine-tuned)	No task-adaptive pretraining, no augmentation (1,060)	51.1	65.9	77.6	73.2	83.9	-
T5-base (fine-tuned)	No task-adaptive pretraining, no augmentation (1,060)	57.7	71.6	83.2	81.8	86.8	-
Lama2-13b-chat (fine-tuned)	No task-adaptive pretraining, no augmentation (1,060)	56.8	66.8	80.7	80.3	86.0	40 min for training
GPT-3.5-turbo (fine-tuned)	No task-adaptive pretraining, no augmentation (1,060)	**62.5**	**72.7**	**82.9**	**84.8**	**87.6**	3 epochs, $ 3, 1h
Transformer (single model) *	No task-adaptive pretraining, augmented unique (14,168)	37.8	47.7	62.8	64.7	76.4	-
BART-base (fine-tuned)	No task-adaptive pretraining, augmented unique (14,168)	52.0	68.5	80.1	74.4	84.8	
T5-base (fine-tuned)	No task-adaptive pretraining, augmented unique (14,168)	59.7	74.1	82.4	84.1	87.1	-
Llama2-13b-chat (fine-tuned)	No task-adaptive pretraining, augmented unique (14,168)	60.2	70.4	83.5	81.6	87.9	9 hours for training
GPT-3.5-turbo (fine-tuned)	No task-adaptive pretraining, augmented unique (14,168)	**69.0**	**78.1**	**86.9**	**86.4**	**89.9**	5 epochs, $ 92, 1.5 h
Transformer (single model) *	Task-adaptive pretraining (2 million), no augmentation (1,060)	56.8	67.3	80.4	81.5	85.7	-
Transformer (single model) *	Task-adaptive pretraining (2 million), augmented unique (14,168)	59.4	70.5	81.8	84.3	86.7	-
Transformer (ensemble models) *	Task-adaptive pretraining (200w+), augmented unique (14,168)	**60.8**	**71.3**	**82.4**	**85.0**	**86.6**	-

The symbol "*" represented the result reported by Vaucher. The result in black bold is the best previous performance. The result in red bold is the best new performance.

Discussion

Chemical text mining expedites scientific discovery in chemistry. Previously, tasks involving complex chemical language and sophisticated processing required the development of specific domain-focused models. Now, the fine-tuning of universal LLMs offers a highly generalized and cost-effective solution. We have demonstrated the impressive efficacy and high exact accuracy of fine-tuning LLMs, especially ChatGPT, across five tasks in text mining. An examination of incorrect predictions revealed that only a small proportion were entirely incorrect, while most were acceptable alternatives to the ground truth or even pointed out the incorrect labels (Supporting Information). These errors can be attributed to inconsistent annotation standards and the inherent ambiguity of terms with multiple interpretations or functions. Therefore, improving the formatted

data extraction requires continuous efforts, including the refinement of specific rules and the enrichment of annotations prone to misinterpretation during training and inference. With detailed specifications and high-quality formatted data, the fine-tuning method based on LLMs is highly reliable. It can be easily extended to tasks related to extracting information from scientific literature and transforming data into customized format. This approach will significantly contribute to the development of extensive databases like SciFinder[18] and Reaxys[19], which gather comprehensive synthesis data through automated curation and expert verification.

In this work, we have scratched the surface of the vast potential of LLMs in chemistry and materials science by fine-tuning LLMs for chemical text mining. Technically, advancements like wider context windows, faster inference approaches, and improved model architectures in the era of LLMs are anticipated to further enhance text mining. However, it's essential to consider what else can be achieved with LLMs and how we can develop more effective LLMs for chemistry and materials science. For instance, LLMs have the potential to revolutionize predictive modelling by incorporating the extensive "fuzzy knowledge" encapsulated within scientific literature, especially in chemistry and drug discovery. By combining empirical results with documented knowledge, LLMs could assist chemists identify patterns in experiments that might otherwise be missed, predict properties of compounds and outcomes of reactions, and even generate new chemical hypotheses and theories. Furthermore, the integration of LLMs' comprehension with specialized tools could substantially lower the barrier of chemists to use these tools throughout the entire workflow, thanks to interactive interfaces in natural language. Future research could investigate how to merge formatted laboratory data with wealth of information in scientific literature and develop the multimodal capability to enrich specific domain knowledge for LLMs. This endeavour will require a sustained, long-term effort.

For the first time, we have demonstrated the effectiveness of fine-tuning ChatGPT and the potential of LLMs n chemical text mining. We conducted five complex tasks: compound entity recognition, reaction role labelling, MOF synthesis information extraction, NMR data extraction, and the transformation from reaction procedures to action sequences. Chemical text mining remains a challenging professional domain when leveraging language model mining, even with prompt engineering. However, LLMs that are fine-tuned with appropriate annotations can produce structured outputs that perfectly fulfil human requirements not easily expressed in natural language. This feature fully utilizes their natural language understanding and formatting capability. Using chemical text mining as an example, this study provides guidance on fine-tuning of LLMs to serve as universal knowledge extraction toolkits. These toolkits can be easily extended for automated extraction from documents and rule-based formatted transformations. Our work lays the groundwork for transformative applications of LLMs in knowledge extraction within the chemical domain.

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Methods

More details will be released after the article is publicly available.

Metrics for Evaluation

Since fine-tuning ChatGPT does not allow for early stopping based on optimal validation loss, we report the performances of all models at the best epoch selected from the evaluation set for fair comparison. Given the task specifics, we use metrics including precision, recall, and F1 score for evaluating entity-level performance. For sentence-level performance assessment, we use Levenshtein similarity, exact match accuracy, partial accuracy, and a modified BLEU score.

Data Availability

All datasets used in this work are available from the authors upon request.

Code Availability

All scrips for training and evaluating can be found on GitHub at https://github.com/zw-SIMM/SFTChatGPT_for_chemtext_mining.

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Contributions

W.Z., J.C.X., Z.Y.F., and M.Y.Z. conceived the idea. M.Y.Z and Z.Y.F designed the research. W.Z., Q.G.W., F.C. implemented the codes. W.Z., Q.G.W., X.T.K, J.C.X, S.K.N., Z.Y.F collected, annotated, and processed training data. D.H.C., B.Y.N., Q.S., and X.T.L. checked the data. M.A.C., R.Z.Z., Y.T.W., L.H.Z benchmarked the models. W.Z. wrote the initial draft. M.Y.Z., Z.Y.F. and Z.P.X. reviewed and refined the article. All authors contributed to the analysis of the results. All authors read and approved the final manuscript.

Competing interests

The authors declare no competing interests.