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Development of a Pilot Chatbot to Detect Interactions Between Monotherapy and Combination Therapy with Captopril Using a Local (LLM) in Cardiovascular Therapy

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ABSTRACT

Cardiovascular diseases (CVDs), including hypertension and heart failure, remain major contributors to global morbidity and mortality and frequently require long-term polypharmacy. The concurrent use of multiple medications increases the risk of drug–drug interactions (DDIs), which may reduce therapeutic effectiveness, increase toxicity, and contribute to adverse drug reactions. This study aimed to develop and validate a locally deployed large language model (LLM)-based chatbot for detecting drug–drug interactions involving captopril in both monotherapy and combination therapy settings. A development and validation study was conducted using DDI data obtained from DrugBank and Drugs.com. The chatbot was developed using the LLaMA-3 model integrated with LangChain, Ollama, and FastAPI and was evaluated through iterative testing and 5-fold cross-validation. System performance was assessed using accuracy, sensitivity, specificity, positive predictive value (PPV), and negative predictive value (NPV), while usability was evaluated using the System Usability Scale (SUS) and Single Ease Question (SEQ) questionnaires completed by pharmacists. The chatbot demonstrated progressive performance improvement throughout development and achieved excellent performance during final validation involving 300 drug pairs, with an accuracy of 99.0%, sensitivity of 100.0%, specificity of 98.0%, PPV of 100.0%, and NPV of 92.0%, exceeding all predefined acceptance thresholds. Usability testing indicated only fair to moderate usability, with a mean SUS score of 65.0 and a mean SEQ score of 5.0, suggesting that further refinement of the user interface and workflow may be required. The locally deployed LLM-based chatbot demonstrated satisfactory diagnostic performance and preliminary feasibility for captopril-related DDI screening. Although the system showed promising classification performance, additional usability optimization and evaluation in real-world clinical workflows are needed before broader implementation can be considered as a pharmacist-supportive screening system.

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1. INTRODUCTION

Cardiovascular diseases (CVDs) remain the leading cause of morbidity and mortality worldwide, accounting for more than 17.9 million deaths annually and approximately 32% of all global deaths [1]. Hypertension is one of the most prevalent cardiovascular risk factors, affecting 31.1% of adults in Indonesia [2]. The long-term management of hypertension and other cardiovascular conditions frequently requires multiple medications, resulting in polypharmacy and an increased risk of drug-drug interactions (DDIs) [3]. DDIs may alter drug efficacy and safety through pharmacokinetic or pharmacodynamic mechanisms [4], potentially leading to adverse drug reactions [5], treatment failure [6], hospitalization [7], and mortality [8]. The clinical burden of DDIs is substantial, contributing to more than 74,000 emergency department visits and 195,000 hospitalizations annually in the United States [9]. A study conducted in Indonesia also reported that 68.35% of prescriptions for hypertensive patients receiving polypharmacy contained potential DDIs, with most interactions classified as moderate severity and pharmacodynamic in nature [10]. These findings highlight the importance of accurate and timely DDI detection to improve medication safety in cardiovascular therapy.

Captopril remains one of the most widely prescribed angiotensin-converting enzyme inhibitors (ACEIs) for hypertension [11], heart failure [12], and diabetic nephropathy [13] treatment. The widespread use of captopril increases the likelihood of clinically significant interactions, particularly when co-administered with nonsteroidal anti-inflammatory drugs, potassium-sparing diuretics, potassium supplements, lithium, and other cardiovascular agents [14]. Interactions may result in hyperkalemia [15], renal dysfunction [16], hypotension [17], or reduced antihypertensive efficacy [18]. In addition to its widespread clinical use, captopril was selected as the focus of this study because it is associated with multiple well-characterized and clinically relevant drug–drug interactions across diverse therapeutic classes. Captopril provides an appropriate proof-of-concept model for developing and validating a locally deployed chatbot for DDI detection in cardiovascular pharmacotherapy. healthcare professionals, particularly pharmacists, require reliable tools that can rapidly identify and interpret potential DDIs to support safe prescribing and medication review practices [19].

Recent advances in artificial intelligence (AI) have created new opportunities for enhancing medication safety and clinical decision-making. Machine learning, deep learning, and natural language processing approaches have demonstrated promising capabilities in DDI prediction and detection [20], [21]. Large language models (LLMs) have shown considerable potential for processing complex medical information and providing conversational access to pharmacotherapy knowledge [22]. Several studies in indonesia have reported successful applications of GPT-based chatbots for DDI detection and demonstrated that frameworks such as LangChain can improve information retrieval by integrating LLMs with external knowledge bases [23]. Most existing systems rely on cloud-based infrastructures, raising concerns regarding data privacy, internet dependency, operational costs, and limited support for local languages [24], [25]. Conventional drug interaction databases and commercial DDI checkers typically require users to perform manual searches and independently interpret interaction information from multiple sources. This process may be time-consuming in busy clinical environments and may not provide concise, context-specific explanations tailored to the user's query. Chatbot-based interface has the potential to facilitate more intuitive access to DDI information through conversational interaction while simultaneously presenting interaction severity, mechanisms, clinical implications, and management recommendations in a single response. Evidence regarding locally deployed LLM-based chatbots specifically designed for cardiovascular DDI detection remains limited. The primary novelty of the present study lies in the integration of a locally deployed LLaMA-3 model with a curated retrieval-augmented knowledge base derived from DrugBank and Drugs.com for captopril-related DDI screening. Unlike conventional rule-based interaction checkers and cloud-based AI systems, the proposed approach enables localized DDI screening while leveraging evidence retrieved from validated drug interaction resources. Therefore, this study provides a proof-of-concept for applying locally deployed LLM technology to support captopril-related DDI identification in cardiovascular pharmacotherapy.

This study aimed to develop and validate a locally deployed LLM-based chatbot for detecting captopril-related drug–drug interactions and providing comprehensive interaction information, including interaction status, severity classification, underlying mechanisms, clinical implications, and management recommendations. The chatbot was developed using DrugBank and Drugs.com as reference standards and

evaluated as a proof-of-concept system for supporting captopril-related DDI screening in cardiovascular pharmacotherapy.

2. METHODS

2.1. Study Design

This study was designed as a development and validation study aimed at developing and evaluating a chatbot for detecting DDIs involving captopril using a local LLM. The chatbot was specifically developed to identify potential interactions associated with captopril used either as monotherapy or in combination with other medications commonly prescribed in cardiovascular therapy. The study encompassed the stages of dataset collection, data preprocessing, system development, integration, testing, and validation.

2.2. System Development

The chatbot was developed using Python 3.8 [26] and implemented through Visual Studio Code (*https://code.visualstudio.com*) as the integrated development environment. The system was deployed locally on a high-performance workstation equipped with Graphics Processing Unit (GPU) resources to support large language model inference. A local deployment strategy was selected to enhance data privacy, reduce dependency on cloud-based services, and improve computational efficiency. Language model used in this study was LLaMA-3, executed through the Ollama platform [27]. Ollama served as the runtime environment responsible for model execution, prompt management, and interaction with external system components [28]. Specifically, the chatbot employed the LLaMA-3 8B Instruct model in GGUF quantized format (Q4_K_M), deployed locally through Ollama. The inference temperature was set to 0.1 to promote deterministic and consistent responses for clinical information retrieval. A structured prompt template was implemented to instruct the model to identify the queried drug pair, retrieve relevant interaction information from the knowledge base, summarize the interaction severity and mechanism, and provide management recommendations based exclusively on retrieved evidence.

2.3. Data Preprocessing

Drug interaction data retrieved from DrugBank and Drugs.com were curated and transformed into a local knowledge base. Data preprocessing included removing duplicate and incomplete records, normalizing drug names to their generic nomenclature, and excluding non-essential attributes, such as dosage forms and product-specific information. The curated dataset was organized into a standardized structure containing drug pairs, interaction descriptions, severity classifications, interaction mechanisms, clinical effects, and management recommendations. The knowledge base was integrated with the large language model (LLM) using the LangChain framework. A retrieval-augmented generation (RAG) pipeline was implemented using all-MiniLM-L6-v2 sentence-transformer embeddings stored in a Chroma vector database. Drug interaction records were divided into semantically meaningful chunks containing interaction descriptions, severity classifications, mechanisms, clinical effects, and management recommendations. During inference, the system performed similarity-based retrieval using a top-k value of 3 to identify the most relevant records for each query. LangChain retrieved relevant interaction records before response generation, enabling the chatbot to produce contextually relevant and evidence-based responses. The RAG pipeline was designed to improve response accuracy and reduce the risk of unsupported or hallucinated responses.

2.4. System Integration

The chatbot architecture integrated LangChain, Ollama, FastAPI, and the local knowledge base [29]. FastAPI served as the backend framework to manage communication between the user interface and the inference module [30]. The application programming interface (API) was designed to receive user-entered drug names and return interaction details, including interaction status, severity level, interaction mechanism, clinical implications, and management recommendations. The response pipeline consisted of query preprocessing, vector similarity retrieval, context assembly, LLM inference, and structured response generation. The chatbot was configured to generate responses exclusively from retrieved evidence and to withhold interaction information when no relevant evidence was available in the knowledge base.

2.5. System Testing and Validation

System testing was conducted using predefined captopril-related drug pairs to verify the chatbot's ability to identify drug-drug interactions (DDIs) and generate appropriate responses. To assess the robustness and generalizability of the retrieval pipeline, a five-fold cross-validation procedure was performed [31]. The curated DDI dataset was randomly partitioned into five subsets. During each iteration, one subset was used as

the evaluation set, whereas the remaining subsets served as the reference knowledge base for information retrieval. Because the LLaMA-3 model was neither trained nor fine-tuned in this study, the cross-validation procedure was designed to evaluate the stability and consistency of the retrieval and response generation pipeline across different data partitions rather than model learning performance. Additional validation was performed using captopril-related drug pairs across multiple testing stages. The number of evaluated drug pairs ranged from 100 to 300, depending on the testing stage, with the final evaluation conducted using 300 drug pairs representing a broad range of clinically significant drug-drug interactions.

2.6. Performance Evaluation

System performance was evaluated using accuracy, sensitivity, specificity, positive predictive value (PPV), and negative predictive value (NPV). True positives (TP) were defined as drug interactions correctly identified by the chatbot, true negatives (TN) as correctly identified non-interacting drug pairs, false positives (FP) as non-interacting drug pairs incorrectly classified as interactions, and false negatives (FN) as drug interactions that were not identified by the chatbot. Accuracy was calculated as the proportion of correctly classified interacting and non-interacting drug pairs among all evaluated cases. Sensitivity measured the chatbot's ability to correctly identify existing drug interactions, whereas specificity measured its ability to correctly identify non-interacting drug pairs. Positive predictive value represented the proportion of predicted interactions that were true interactions, whereas negative predictive value represented the proportion of predicted non-interactions that were correctly classified. Performance targets were predefined to facilitate system evaluation. The chatbot was considered to demonstrate satisfactory performance if it achieved an accuracy of at least 85%, sensitivity and specificity of at least 80%, a PPV of at least 75%, and an NPV of at least 90% [32]. These thresholds served as pragmatic evaluation criteria for assessing the retrieval and response-generation performance of the proposed system and were not intended to represent formal diagnostic validation standards.

2.7. Ethics Statement

This study received ethical approval from the Health Research Ethics Committee, Universitas Harapan Bangsa (Approval No. B.LPPM-UHB/1324/12/2025). Participation in the usability evaluation was voluntary, and informed consent was obtained from all pharmacists prior to study participation. No patient data were collected during the study. All participant responses were anonymized and analyzed in aggregate form to ensure confidentiality. The study was conducted in accordance with the ethical principles of the Declaration of Helsinki.

3. RESULTS AND DISCUSSION

To the best of our knowledge, this is the first study to develop and validate a local LLM-based chatbot specifically designed to detect captopril-related DDIs in both monotherapy and combination therapy settings. The chatbot demonstrated excellent diagnostic performance, achieving 99.0% accuracy, 100.0% sensitivity, 98.0% specificity, 100.0% PPV, and 92.0% NPV during final validation. These findings support the potential of locally deployed LLMs as effective clinical decision-support tools for DDI detection while addressing concerns related to data privacy and dependence on cloud-based systems.

3.1. Performance of the captopril drug-drug interaction detection chatbot across validation stages

Performance was observed throughout the chatbot development and validation process. During the initial development cycle (n = 20), all evaluation metrics reached 100.0%, indicating perfect classification of captopril-related drug-drug interactions (DDIs). Following the introduction of a more diverse testing dataset in Cycle 3 (n = 30), a modest decline in performance was observed, with accuracy 91.0%, sensitivity 93.3%, specificity 91.0%, PPV 95.0%, and NPV decreasing to 88.3%. After further system refinement and optimization, performance improved substantially during the final validation phase involving 300 drug pairs. The chatbot achieved an accuracy 99.0%, sensitivity 100.0%, specificity 98.0%, PPV 100.0%, and NPV 92.0%, with all metrics exceeding the predefined acceptance thresholds (Table 1). The confusion matrix for the final validation consisted of 228 true positives (TP), 68 true negatives (TN), 0 false positives (FP), and 4 false negatives (FN). These findings demonstrate the robustness and reliability of the proposed chatbot in identifying clinically relevant captopril-related DDIs across different validation stages.

Table 1. Performance of the captopril drug-drug interaction detection chatbot across validation stages

Metric	Threshold	Cycle 1 (n=20)	Cycle 3 (n=30)	Final Validation (n=300)

Accuracy (%)	≥85	100.0	91.0	99.0
Sensitivity (%)	≥80	100.0	93.3	100.0
Specificity (%)	≥80	100.0	91.0	98.0
PPV (%)	≥75	100.0	95.0	100.0
NPV (%)	≥90	100.0	88.3	92.0

3.2. System Usability Scale (SUS)

The usability evaluation revealed variability in pharmacists' perceptions of the chatbot system (Figure 1). SUS scores ranged from 52.5 to 77.5, with the highest score reported by Pharmacist 2 (77.5) and the lowest score reported by Pharmacist 7 (52.5). Most respondents achieved SUS scores above 60, indicating that the system was generally perceived as usable and acceptable for supporting drug-drug interaction screening activities. The overall mean SUS score was 65.0, which falls within the marginal usability category. This finding suggests that although the chatbot was considered functional and could be used to accomplish the intended tasks, there remains room for improvement in terms of user experience, interface design, and system efficiency. The variation observed among respondents may reflect differences in familiarity with digital health technologies and clinical decision-support systems. The findings suggest that the chatbot demonstrated marginal usability and practical functionality. Further optimization is required to improve usability and support broader adoption in pharmacy practice.

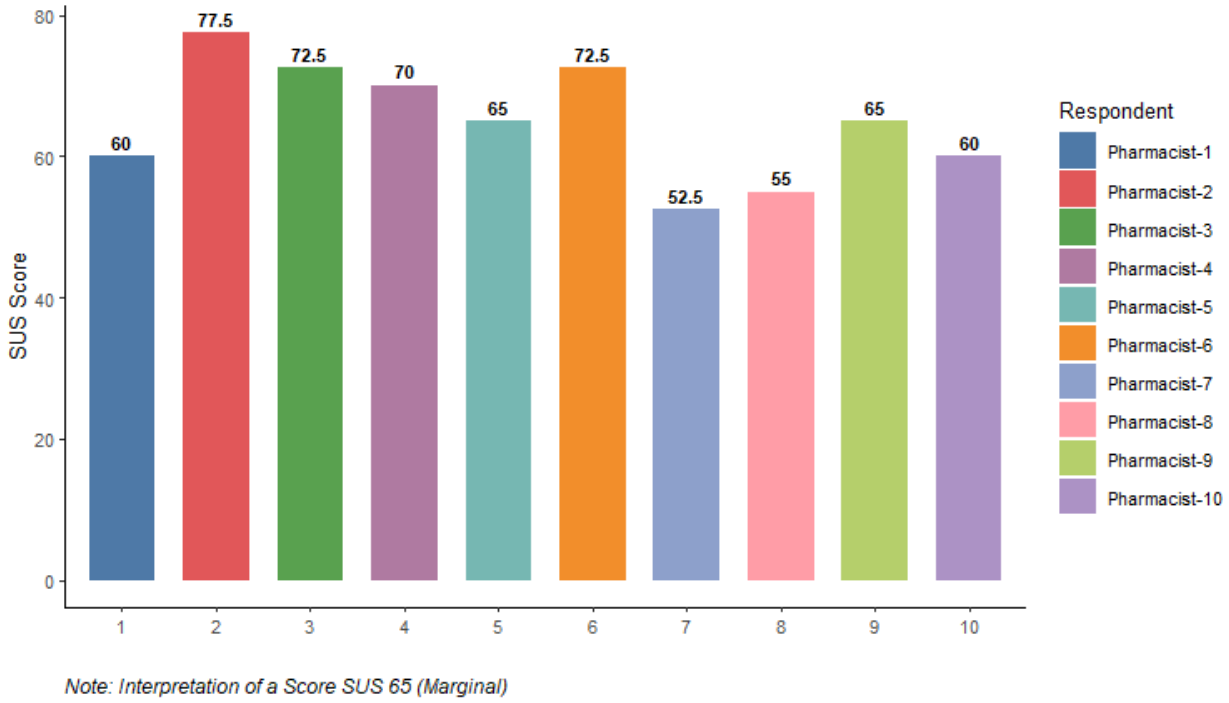

Figure 1. System Usability Scale (SUS) scores reported by participating pharmacists.

3.3. Single Ease Question (SEQ)

Task-based usability was assessed using the Single Ease Question (SEQ) questionnaire. Individual SEQ scores ranged from 2.0 to 6.6, with the highest score reported by Pharmacist 1 (6.6) and the lowest score reported by Pharmacist 9 (2.0) (Figure 2). Most respondents reported SEQ scores above 4.0, indicating that the chatbot was generally perceived as relatively easy to use for completing drug-drug interaction detection tasks. The overall mean SEQ score was 5.0, corresponding to the moderate usability category. Variability in individual scores was observed across respondents, reflecting differences in perceived task difficulty and user experience when interacting with the system. These findings indicate that pharmacists were generally able to complete the intended drug-drug interaction screening tasks using the chatbot, the moderate SEQ score suggests that opportunities remain to improve task efficiency and ease of use.

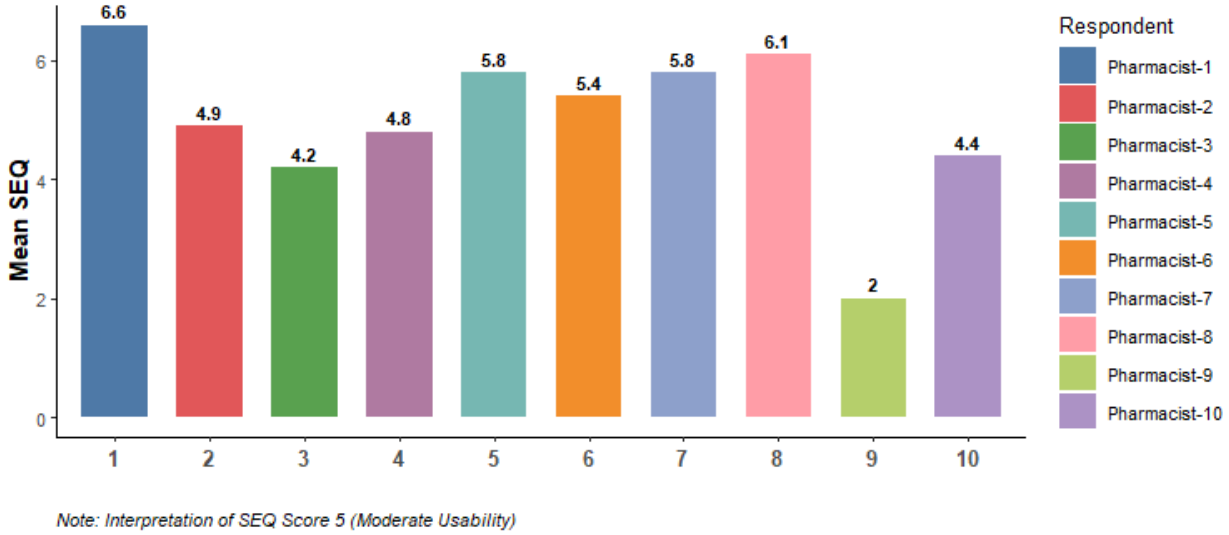

Figure 2. Single Ease Question (SEQ) scores reported by participating pharmacists.

The improvement observed between the development cycles and final validation suggests that iterative optimization contributed substantially to system performance [33]. Although performance decreased slightly during Cycle 3, likely due to the inclusion of more diverse and complex drug pairs, the final validation demonstrated marked improvement across all metrics [34]. These findings suggest that the integration of a local LLaMA-3 model with a curated knowledge base from DrugBank and Drugs.com contributed to the chatbot's overall performance in identifying clinically relevant DDI information [35]. The high sensitivity observed in the final validation is particularly important because missing clinically significant interactions may expose patients to preventable adverse drug events, while the high specificity minimizes unnecessary alerts that could contribute to alert fatigue among healthcare professionals [36].

The strong performance achieved in this study also highlights the potential of local LLM deployment in clinical pharmacy practice. Unlike cloud-based AI systems, locally deployed models offer advantages related to data privacy, reduced internet dependency, and greater control over healthcare information [37]. These characteristics may be beneficial in healthcare settings, where patient confidentiality and data security are important considerations; the present study did not formally evaluate system-level security or data protection mechanisms [38]. The chatbot may serve as a practical decision-support tool for pharmacists during medication review and interaction screening processes [39].

Usability testing demonstrated that pharmacists generally perceived the chatbot as acceptable for practical use. The mean SUS score of 65.0 indicated marginal usability, whereas the mean SEQ score of 5.0 suggested moderate ease of task completion [40]. The difference between these findings may be attributed to the distinct dimensions measured by each instrument [41]. While the SEQ focuses on the ease of performing specific tasks, the SUS evaluates broader aspects of usability, including learnability, consistency, and overall user experience [42]. These findings suggest that pharmacists were generally able to complete DDI screening tasks using the chatbot, although improvements in interface design and workflow optimization may further enhance user satisfaction and usability [43].

This study has several limitations. The chatbot was developed and validated specifically for captopril-related drug-drug interactions (DDIs), which may limit the generalizability of the findings to other medications and therapeutic contexts. System validation relied on DrugBank and Drugs.com as reference knowledge sources and did not include comparisons with commercial drug interaction checkers or cloud-based large language model (LLM) systems. Usability testing involved a relatively small sample of pharmacists, which may have limited the representativeness of user feedback. Future research should evaluate the chatbot using larger datasets, broader therapeutic classes, comparisons with alternative DDI systems, and real-world clinical settings to further establish its effectiveness, robustness, and applicability in pharmacy practice.

4. CONCLUSION

This study successfully developed and validated a locally developed LLM-based chatbot to detect drug interactions associated with captopril, both in monotherapy and combination therapy. The chatbot demonstrated satisfactory diagnostic performance, with high accuracy, sensitivity, specificity, positive predictive value, and negative predictive value, all of which exceeded the established acceptance thresholds. Furthermore, usability evaluations indicated that pharmacists were generally able to use this system effectively for drug interaction screening tasks. These findings demonstrate the preliminary feasibility of a locally deployed LLM-based chatbot for captopril-related DDI screening and support further development and evaluation of the system. The present validation was limited to captopril-related drug pairs and did not include evaluation in real-world pharmacy practice settings. Additional validation using larger datasets, broader therapeutic classes, and real-world clinical settings is required before its applicability in routine pharmacy practice can be established. Future studies should evaluate the system across broader therapeutic classes, larger datasets, and real-world pharmacy practice environments, compare its performance with established DDI checkers, and assess its impact on pharmacist decision-making using real or simulated patient cases.

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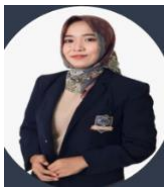	**Khamdiyah Indah Kurniasih** is a lecturer in the Pharmacy Study Program at Universitas Harapan Bangsa, Indonesia. Her research interests focus on community pharmacy, pharmaceutical care, telepharmacy, pharmacy practice, and public health. She has published several scientific articles in national and international journals and actively contributes to research and community engagement activities in the field of pharmacy, Indahaffandy@gmail.com and 0009-0007-5771-410X

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