1st International Conference on Multidisciplinary Engagement

Developing a Local AI Cabot for Real-Time Detection of Captopril Drug-Drug Interactions in Cardiovascular Therapy

Afriza Pujiati[1*], Ikhwan Yuda Kusuma[2], Khamdiyah Indah Kurniasih[3], Siti Setianingsih[4]

[1,2,3,4]*Pharmacy Study Program, Faculty of Health, Universitas Harapan Bangsa, Purwokerto, 53182, Indonesia*

Corresponding Author.
**Email*: afrizapujiati407@gmail.com

Abstract: *Cardiovascular diseases (CVDs), including hypertension and heart failure, are major contributors to global morbidity and mortality, with polypharmacy being a common approach to managing these conditions. However, polypharmacy increases the risk of drug-drug interactions (DDIs), which can result in decreased efficacy, toxicity, and adverse drug reactions. This study aimed to develop and evaluate a local Cabot based on a Large Language Model (LLM) to detect Captopril drug interactions with high accuracy and specificity, ensuring data privacy and computational efficiency. The Cabot was developed using Python, LangChain, FastAPI, and a local LLM for Captopril interaction detection, with 5-fold cross-validation used to evaluate its performance using secondary data from DrugBank and Drugs.com. The system was integrated with PowerShell and ngrok to enable secure, local deployment. The Cabot achieved 100% accuracy and 100% specificity in Cycle 1, with a slight decrease in Cycle 3 to 96.7% accuracy and 92.9% specificity due to one false positive, but no false negatives were observed. The system showed an average 5-fold accuracy of 98.7% and specificity of 98.0%, confirming its potential for real-time DDI detection. The local model ensured data privacy and computational efficiency, offering a robust alternative to cloud-based systems. The Cabot developed in this study shows promise in detecting Captopril DDIs with high accuracy and specificity in cardiovascular therapy, and future improvements should focus on expanding the model's capabilities to handle a broader range of medications and refine its detection algorithms.*
Keywords: *Captopril, Drug Interactions, Polypharmacy, Large Language Models, Artificial Intelligence*

1. INTRODUCTION

Cardiovascular diseases (CVDs), accounting for over 17.9 million deaths annually [1], with hypertension affecting 31.1% of adults in Indonesia [2]. Polypharmacy commonly used to manage these conditions, increases the risk of drug-drug interactions (DDIs) that can reduce efficacy [3], increase toxicity [4], and cause adverse drug reactions [5], leading to treatment failure and mortality [6]. DDIs contribute to over 74,000 emergency department visits and 195,000 hospitalizations annually in the United States [7], and a study Kusuma et al. (2018) [8], revealed that 68.35% of prescriptions for hypertensive patients involved polypharmacy with significant DDIs, predominantly through pharmacodynamic mechanisms (58.89%) and moderate severity (65.74%). The high prevalence of Captopril, angiotensin-converting enzyme inhibitor (ACEI) used for treating hypertension [9], heart failure [10], and diabetic nephropathy [11], increases the risk of DDIs, especially when co-prescribed with other medications [12]. Recent advancements in Artificial Intelligence (AI), particularly Large Language Models (LLMs), have shown promise in detecting DDIs through large-scale text processing [13]. Study in Indonesia demonstrate that integrating LLMs with frameworks like LangChain can improve DDI detection by linking models to verified drug databases such as DrugBank and Drugs.com [14], but challenges such as data privacy, costs, internet dependency, and limitations in local language support remain [15], [16].

This study aimed to address these challenges by developing a Cabot using a Local LLM to detect Captopril monotherapy and combination drug interactions. The Cabot was designed to run locally using PowerShell and ngrok, ensuring data privacy and computational efficiency.

2. METHOD

This research is designed as a development and validation study to create and evaluate a Cabot for detecting DDIs involving Captopril using a Local LLM. The Cabot focuses on identifying interactions in both monotherapy and combination therapy. The study was carried out in five stages: 1) system development, 2) data preprocessing, 3) model integration, 4) system testing, and 5) system validation.

During the system development phase, the dataset was selected, data was preprocessed, the Cabot architecture was designed, and the system was integrated with the LangChain framework. The system validation phase involved comparing the chabot results against DrugBank and Drugs.com to evaluate performance metrics, specifically accuracy and specificity.

The drug interaction detection system was developed using Python 3.8, implemented via PowerShell, and accessed remotely using ngrok for secure internet access. The system runs locally on a high-performance server equipped with a Graphics Processing Unit (GPU) to support inference from large language models The dataset used in this study consists of 50 drug interaction pairs sourced from DrugBank and Drugs.com, with a balanced distribution of interactions and non-interactions. Of the 50 drug pairs, 50% (25 pairs) were interactions (1) and 50% (25 pairs) were non-interactions (0). The dataset was initially downloaded in Excel format, curated, and then converted into a local knowledge base for the Cabot's inference process. LangChain integrates the model with the local database, enabling the Cabot to query and process drug interaction data efficiently [17]. FastAPI facilitates stable data exchange between the user interface and the inference module, with an API endpoint designed to accept a list of medications and return detected interactions along with their severity, interaction mechanism, and references to source data [18].

Data preprocessing involved quality checks to ensure the inclusion of only valid drug interaction pairs, normalization of drug names to their generic forms to avoid discrepancies, and removal of non-relevant attributes such as dosage and formulation details. The LLaMA-3 model was selected for processing drug interaction text in Indonesian and was implemented locally to ensure data privacy and improve computational efficiency [19]. 5-fold cross-validation was employed to evaluate the system's performance using accuracy and specificity as key metrics, ensuring the model's robustness and generalizability across various datasets [20].

The Cabot's performance was evaluated based on accuracy and specificity. Accuracy was calculated as the percentage of correct predictions (true positives and true negatives) out of all test cases, with a threshold of ≥ 85% set for accuracy [21]. Specificity was calculated as the proportion of true negatives correctly identified by the system, with a threshold of ≥ 80% set for specificity [21]. These metrics were used to assess the Cabot's ability to detect DDIs and correctly identify non-interacting drug pairs.

Should be noted that this study focuses on detecting DDIs involving Captopril, which limits the generalizability of the findings to other drug classes or therapeutic areas. Additionally, the dataset used in this study is limited, which may lead to overfitting and high accuracy.

3. RESULTS AND DISCUSSION

To the best of our knowledge, this is the first study to develop and evaluate a Cabot for detecting DDIs involving Captopril using a Local LLM. The Cabot's performance in detecting DDIs involving Captopril was evaluated using 5-fold cross-validation, with a focus on accuracy and specificity.

Figure 1 shows that in the first cycle, the Cabot achieved 100% accuracy and 100% specificity, with no false positives (FP) or false negatives (FN). While these results indicate that the system is highly effective in identifying both genuine drug interactions and non-interactions, the perfect accuracy should be interpreted with caution. Given the limited size of the dataset, there is a possibility of overfitting, which may explain the high accuracy in the first cycle. These results indicate that the system is highly effective in identifying both genuine drug interactions and non-interactions, indicating its potential as a tool for detecting drug interactions in controlled settings. Meanwhile, the third cycle showed a slight decline in performance with an accuracy of 96.7% and a specificity of 92.9%, primarily due to a single false positive (FP).

Each fold of the 5-fold cross-validation was assigned an equal number of drug pairs, with each fold containing 10 drug pairs (50 drug pairs ÷ 5 folds). The dataset was split randomly to ensure a balanced distribution of drug interactions and non-interactions across each fold.

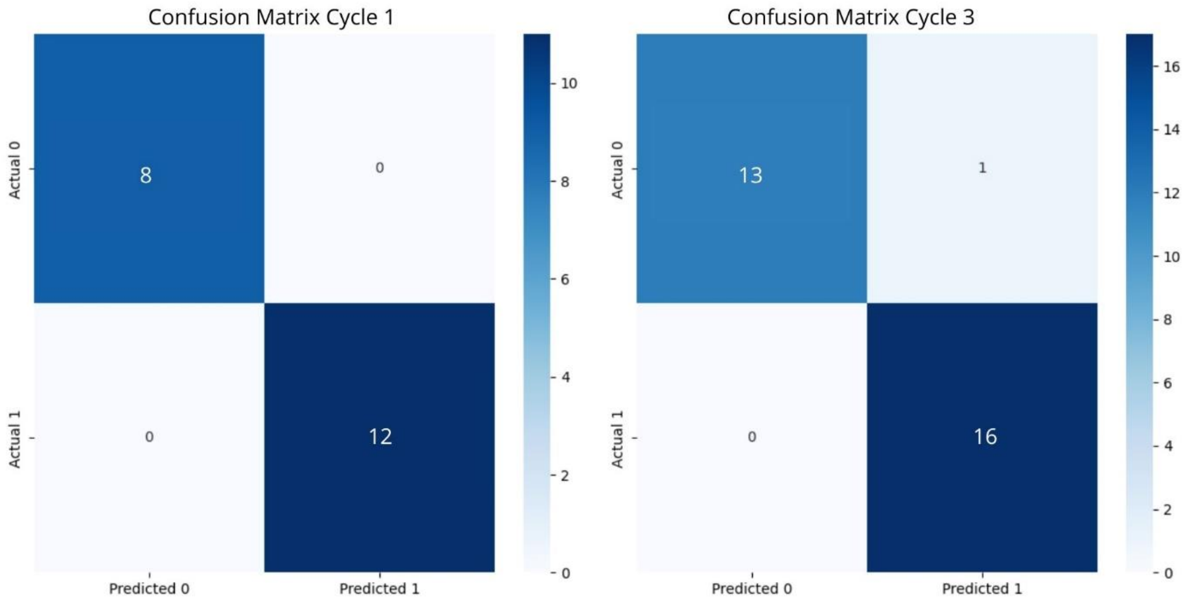

Figure 1. Confusion matrix showing the Cabot's performance in detecting Captopril drug-drug interactions.

The performance of the Cabot in detecting Captopril DDIs was evaluated across five phases: initial testing, model fine-tuning, advanced testing, complex testing, and model finalization. The Cabot demonstrated 100% accuracy and 100% specificity in initial testing with 20 drug pairs, followed by robust performance in the advanced testing phase, which involved 30 drug pairs, maintaining high reliability. The final performance after all stages showed an average 5-fold accuracy of 98.7% and specificity of 98.0%, highlighting its effectiveness in identifying Captopril-related DDIs. The comparison with previous studies is made to provide context to the performance of our model, but it is important to note that differences in the models' datasets, training, and evaluation protocols must be considered. Our study primarily focuses on detecting DDIs for Captopril, whereas the studies referenced in Yemen [22]. Study in Turkey targeted broader or different drug sets, which may account for some of the performance differences [23].

The high performance of the Cabot is particularly significant given the potential consequences of undetected DDIs in clinical settings [24]. Captopril (ACEI), is often prescribed in combination with other medicines [9]. The ability to detect interactions involving such a commonly prescribed drug is crucial for improving patient safety and ensuring effective medication management [25]. The Cabot's capacity to accurately identify both positive interactions (true positives) and non-interactions (true negatives) without producing false alarms (false positives) is critical for ensuring that clinicians can make timely, informed decisions. Study in India [21]. AI-driven clinical decision support systems (CDSS) have been shown to enhance personalized drug therapy and optimize treatment [26]. However, limited studies have focused on local AI-based systems that ensure privacy and maintain high accuracy for DDI detection [27]. This study aims to address this gap by developing a local Cabot for detecting Captopril interactions, offering real-time, accurate detection in cardiovascular therapy controlled settings.

There are several limitations that should be acknowledged. The false positive in Cycle 3 reflects the model's current challenges in accurately distinguishing between non-interacting drugs, which may be addressed in future versions by expanding the training dataset, incorporating more complex drug interactions, and refining the model's detection algorithms. The study's reliance on secondary data from DrugBank and Drugs.com limits the Cabot's performance to the interactions included in these databases. Ensure broader applicability, the Cabot may need further validation with real-world data to account for potential variations in drug use, patient demographics, and clinical settings. While the model was evaluated using controlled data, real-world clinical implementation may present challenges such as integration with existing hospital systems and ensuring user adoption by healthcare professionals.

4. CONCLUSION

This study aimed to develop and evaluate a local AI Cabot using a Large Language Model (LLM) to detect Captopril drug-drug interactions (DDIs) in cardiovascular therapy, focusing on achieving high accuracy and specificity while ensuring data privacy and computational efficiency. The output of this research is a local AI Cabot that demonstrated an average 5-fold accuracy of 98.7% and specificity of 98.0%, capable of detecting clinically significant drug interactions and non-interactions in real-time. Future research should focus on expanding the Cabot's capabilities to detect a wider range of drug interactions, refining detection algorithms to reduce false positives, and validating the system in real-world clinical settings to evaluate its broader applicability and integration into healthcare systems.

ACKNOWLEDGEMENTS

The author would like to express their sincere gratitude to the Pharmacy Research Club and Universitas Harapan Bangsa for their invaluable support throughout this research. The guidance, resources, and collaborative environment provided by the club and the university have been essential in the successful completion of this study. Special thanks to the faculty and fellow researchers for their encouragement and constructive feedback.

REFERENCES

[1] WHO, "WHO: Kardiovaskular dan Pembuluh Darah Jadi Penyebab Kematian Utama Secara Global | tempo.co," Tempo. Accessed: Oct. 15, 2025. [Online]. Available: https://www.tempo.co/gaya-hidup/who-kardiovaskular-dan-pembuluh-darah-jadi-penyebab-kematian-utama-secara-global-395070

[2] Kemenkes, "Survei Kesehatan Indonesia (SKI) 2023," Badan Kebijakan Pembangunan Kesehatan | BKPK Kemenkes. Accessed: Oct. 24, 2025. [Online]. Available: https://www.badankebijakan.kemkes.go.id/hasil-ski-2023/

[3] B. Papotti, C. Marchi, M. P. Adorni, and F. Potì, "Drug-drug interactions in polypharmacy patients: The impact of renal impairment," *Curr. Res. Pharmacol. Drug Discov.*, vol. 2, p. 100020, 2021, doi: 10.1016/j.crphar.2021.100020.

[4] R. W. Hoel, R. M. Giddings Connolly, and P. Y. Takahashi, "Polypharmacy Management in Older Patients," *Mayo Clin. Proc.*, vol. 96, no. 1, pp. 242–256, Jan. 2021, doi: 10.1016/j.mayocp.2020.06.012.

[5] M. Molokhia and A. Majeed, "Current and future perspectives on the management of polypharmacy," *BMC Fam. Pract.*, vol. 18, no. 1, p. 70, Dec. 2017, doi: 10.1186/s12875-017-0642-0.

[6] A. G. Roberts and M. E. Gibbs, "Mechanisms and the clinical relevance of complex drug–drug interactions," *Clin. Pharmacol. Adv. Appl.*, vol. Volume 10, pp. 123–134, Sep. 2018, doi: 10.2147/CPAA.S146115.

[7] S. Kim, E. Kim, and H. S. Suh, "Cost-Effectiveness of an Opioid Abuse–Prevention Program Using the Narcotics Information Management System in South Korea," *Value Health*, vol. 24, no. 2, pp. 174–181, 2021, doi: 10.1016/j.jval.2020.12.002.

[8] I. Y. Kusuma, P. O. D. Megasari, and L. Sukiatno, "Identifikasi potensi interaksi obat pada pasien hipertensi: studi retrospektif resep polifarmasi di Apotek Karya Sehat Purwokerto," *Viva Med. J. Kesehat. Kebidanan Dan Keperawatan*, vol. 12, no. 1, pp. 72–80, 2018.

[9] K. Ahmad *et al.*, "Public health supply chain for iron and folic acid supplementation in India: Status, bottlenecks and an agenda for corrective action under Anemia Mukt Bharat strategy," *PLoS ONE*, vol. 18, no. 2 February, 2023, doi: 10.1371/journal.pone.0279827.

[10] S. Bhullar, A. Shah, and N. Dhalla, "Mechanisms for the development of heart failure and improvement of cardiac function by angiotensin-converting enzyme inhibitors," *Scr. Med. (Brno)*, vol. 53, no. 1, pp. 51–76, 2022, doi: 10.5937/scriptamed53-36256.

[11] Y.-H. Du, C.-J. Guan, L.-Y. Li, and P. Gan, "Efficacy and safety of angiotensin converting enzyme inhibitors and angiotensin II receptor blockers in diabetic nephropathy: a systematic review and meta-analysis," *Ann. Palliat. Med.*, vol. 11, no. 3, pp. 1093–1101, Mar. 2022, doi: 10.21037/apm-22-212.

[12] N. Swekwi, "The effects of co-prescription of warfarin and cardiovascular medicines among atrial fibrillation patients and/or deep vein thrombosis patients in Queensland, Australia," Oct. 01, 2020, *Griffith University*. doi: 10.25904/1912/3978.

[13] A. Cesaro, S. C. Hoffman, P. Das, and C. de la Fuente-Nunez, “Challenges and applications of artificial intelligence in infectious diseases and antimicrobial resistance,” *Npj Antimicrob. Resist.*, vol. 3, no. 1, p. 2, 2025.

[14] R. Qardafil, “Peningkatan Efektivitas Kualitas Chatbot Jala Tech Melalui Implementasi Chat GPT, Auto-GPT, Dan Langchain,” PhD Thesis, Universitas Islam Indonesia, 2023.

[15] Y. N. Pratiwi, Z. Shafa, T. Nike, and P. Perawati, “Mengolah Kata, Menyembuhkan Luka:: Pentingnya Bahasa Indonesia dalam hal Komunikasi Praktik Kedokteran,” *Indones. Res. J. Educ.*, vol. 5, no. 1, pp. 757–764, 2025.

[16] S. Yessy Asri *et al.*, *A Large Language Model (Llm) Penerapan Large Language Model (Llm) Dalam Chatbot*. Uwais Inspirasi Indonesia, 2025.

[17] A. Osheba, A. Abou-El-Ela, O. Adel, Y. Maaod, T. Abuhmed, and S. El-Sappagh, “Leveraging Large Language Models for Smart Pharmacy Systems: Enhancing Drug Safety and Operational Efficiency,” in *2025 19th International Conference on Ubiquitous Information Management and Communication (IMCOM)*, Bangkok, Thailand: IEEE, Jan. 2025, pp. 1–8. doi: 10.1109/IMCOM64595.2025.10857582.

[18] P. K. Narayanan, “Engineering Machine Learning and Data REST APIs using FastAPI,” in *Data Engineering for Machine Learning Pipelines*, Berkeley, CA: Apress, 2024, pp. 323–359. doi: 10.1007/979-8-8688-0602-5_10.

[19] E. M. Tosca, L. Aiello, A. De Carlo, and P. Magni, “Pharmacometrics in the Age of Large Language Models: A Vision of the Future,” *Pharmaceutics*, vol. 17, no. 10, p. 1274, Sep. 2025, doi: 10.3390/pharmaceutics17101274.

[20] B. K. Kalita, K. A. Singh, and M. Kalita, “Fivefold Cross-Validation Approach in Evaluating the Robustness of Machine Learning Models for Prediction of Esophageal Cancer,” *Indian J. Community Med.*, vol. 51, no. Suppl 1, pp. S180–S188, Feb. 2026, doi: 10.4103/ijcm.ijcm_454_24.

[21] H. Khude and P. Shende, “AI-driven clinical decision support systems: Revolutionizing medication selection and personalized drug therapy,” *Adv. Integr. Med.*, vol. 12, no. 4, p. 100529, Dec. 2025, doi: 10.1016/j.aimed.2025.100529.

[22] F. Y. Al-Ashwal, M. Zawiah, L. Gharaibeh, R. Abu-Farha, and A. N. Bitar, “Evaluating the Sensitivity, Specificity, and Accuracy of ChatGPT-3.5, ChatGPT-4, Bing AI, and Bard Against Conventional Drug-Drug Interactions Clinical Tools,” *Drug Healthc. Patient Saf.*, vol. Volume 15, pp. 137–147, Sep. 2023, doi: 10.2147/DHPS.S425858.

[23] Z. Ş. Aksoyalp and B. R. Erdoğan, “COMPARATIVE EVALUATION OF ARTIFICIAL INTELLIGENCE AND DRUG INTERACTION TOOLS: A PERSPECTIVE WITH THE EXAMPLE OF CLOPIDOGREL,” *Ank. Univ. Eczacilik Fak. Derg.*, vol. 48, no. 3, pp. 22–22, Aug. 2024, doi: 10.33483/jfpau.1460173.

[24] M. W. Shiferaw, T. Zheng, A. Winter, L. A. Mike, and L.-N. Chan, “Assessing the accuracy and quality of artificial intelligence (AI) chatbot-generated responses in making patient-specific drug-therapy and healthcare-related decisions,” *BMC Med. Inform. Decis. Mak.*, vol. 24, no. 1, p. 404, Dec. 2024, doi: 10.1186/s12911-024-02824-5.

[25] S. M. AlJassas, N. A. Alzaidi, S. M. Algharqan, S. H. Aljawad, B. M. Alsofyani, and F. Ali Hadadi, “Evaluating the Impact of Drug-Drug Interactions in Polypharmacy Strategies for Safe Medication Management,” *J. Healthc. Sci.*, vol. 04, no. 12, pp. 1051–1056, 2024, doi: 10.52533/JOHS.2024.41255.

[26] Rishi Reddy Kothinti, “Deep learning in healthcare: Transforming disease diagnosis, personalized treatment, and clinical decision-making through AI-driven innovations,” *World J. Adv. Res. Rev.*, vol. 24, no. 2, pp. 2841–2856, Nov. 2024, doi: 10.30574/wjarr.2024.24.2.3435.

[27] H.-X. Huang, K.-K. Liu, L. Zhang, Y.-M. Huang, W.-H. Liu, and J. Xiao, “Influencing factors of end-of-dose failure in patients with cancer pain after oral oxycodone sustained-release tablets: A retrospective, case-control study,” *Jpn. J. Clin. Oncol.*, vol. 51, no. 6, pp. 932–941, 2021, doi: 10.1093/jjco/hyab002.