Extraction and Characterization of Bioactive Compounds from *Cucumeropsis mannii* Seed Oil

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Introduction: Bioactive compounds are naturally occurring molecules with therapeutic potential, playing a crucial role in pharmaceutical, biomedical, and environmental research. These compounds exhibit antioxidant, anti-inflammatory, and anticancer properties, making them valuable for drug development [1]. However, extracting and characterizing these compounds from natural sources is challenging due to their complex structures and physicochemical properties. Conventional extraction methods often rely on hazardous solvents and suffer from limitations in selectivity, efficiency, and sustainability [2]. Cucumeropsis mannii seed oil (CMSO) has been identified as a promising source of bioactive compounds with medicinal potential. Previous in vivo study highlights its antioxidant and anti-inflammatory activities, suggesting a role in mitigating oxidative stress-related diseases [3]. However, the specific bioactive constituents remain largely uncharacterized, and traditional extraction methods can lead to their degradation or loss. Optimized extraction strategies are essential to harness CMSO's therapeutic potential. Recent advancements in liquid-liquid interface extraction (LLIE) provide an alternative for selective and sustainable extraction [4]. LLIE enhances separation efficiency while minimizing toxic solvent use, aligning with green chemistry principles [5]. Novel solvents, such as deep eutectic solvents and ionic liquids, further improve environmental sustainability [6]. Accurate characterization of bioactive compounds is also critical, with advanced analytical techniques such as Raman spectroscopy and self-assembly sensors offering molecular-level insights [7]. Additionally, machine learning (ML) enhances bioactive compound research by optimizing data analysis and predictive modeling [8]. This study focuses on the phytochemical composition and GC-MS analysis of CMSO.

Main Part: Peeled *Cucumeropsis mannii* seeds were manually ground and mechanically pressed using a mortar and pestle to extract oil. The composition of CMSO was analyzed using gas chromatography-mass spectrometry (GC-MS) and phytochemical screening. Phytochemical screening, based on Trease and Evans [9], confirmed the presence of flavonoids, alkaloids, phenols, and saponins. GC-MS analysis, following Adams (2007), identified key bioactive compounds, including oleic acid (30.6%), octadec-9-enoic acid (23.1%), and cyclopentadecanone, 2-hydroxy (14.5%), along with various alkanes, fatty acid esters, and terpenoids. The oil contained significant levels of tannins (444.99 ± 8.24 mg/100 g), phenols (682.88 ± 4.83 mg/100 g), alkaloids (345.72 ± 4.27 mg/100 g), flavonoids (1109.09 ± 48.11 mg/100 g), hydrogen cyanide (HCN) (0.24 ± 0.01 mg/100 g), glycosides (83.33 ± 1.12 mg/100 g), terpenoids (206.17 ± 4.75 mg/100 g), saponins (0.27 ± 0.01 mg/g), and steroids (0.26 ± 0.01 mg/g). These compounds may contribute to the renoprotective effects observed in previous *in vivo* studies [3].

Conclusion: The present study provides a foundation for understanding the phytochemical composition and GC-MS profile of CMSO. It highlights CMSO's potential as a rich source of nutraceuticals. Future research will focus on applying LLIE to enhance selectivity and sustainability. The strategy will leverage deep eutectic solvents, self-assembly sensors, and AI-driven modeling to optimize extraction conditions. These advancements aim to improve efficiency and promote environmentally friendly practices in bioactive compound research.

List of References

1. Atanasov, A.G., Zotchev, S.B., & Dirsch, V.M. Natural products in drug discovery: advances and opportunities. *National Review Drug Discovery* **20**, 200–216 (2021). https://doi.org/10.1038/s41573-020-00114-z

2. Chemat, F., Vian, M. A., Fabiano-Tixier, A.S., Nutrizio, M., Jambrak, A. R., Munekata, P.E., & Cravotto, G. (2020). A review of sustainable and intensified techniques for extraction of food and natural products. *Green Chemistry*, 22 (8): 2325-2353

3. Ale, B. A., Aja, P.M., Okoro, I.J. Nwite, F.E., Agu, P.C., Eze, E.D., Nnamani, I.V., & Ogugua, V.N (2024). Renoprotective effects of Cucumeropsis mannii seed oil on cisplatin-induced nephrotoxicity in Wistar rats. *Phtomedicine Plus*, 4(2): 100536. https://doi.org/10.1016/j.phyplu.2024.100536

4. Jiafu, L., Wenshan, S., Yuting, L., Junlin, L., Jingsi, C., Chengzhi, & H., Huiyu, D. (2024). Revealing the impact of sample enrichment method on concentration and cytotoxicity of volatile disinfection byproducts in drinking water: *A quantitative study for liquid-liquid extraction*, *Water Research*, 266: 0043-1354. <u>https://doi.org/10.1016/j.watres.2024.122370</u>.

5. Mehdi, A., & Rezvan, T. (2025). Examining an essential factor in liquid-liquid extraction columns: Evaluating the mass transfer coefficients critically. *International Communications in Heat and Mass Transfer*, 161: 0735-1933, https://doi.org/10.1016/j.icheatmasstransfer.2024.108446.

6. Junmiao, L., Xiaoxia, L., & Kyung, H. (2022). Development of deep eutectic solvents for sustainable chemistry, Journal of Molecular Liquids 362: 0167-7322, https://doi.org/10.1016/j.molliq.2022.119654

7. Gupta, A., Roy, A, Pandit, S, Pandey, N., & Rustagi, S. (2023). Evaluation of Bioactive Compounds Obtained from Ginkgo Biloba Again,st Crystal Structure of Myelin Oligodendrocyte Glycoprotein (MOG). *OBM Neurobiology* 7(4):186. doi:10.21926/obm.neurobiol.2304186.

8. Wang, C., Ye, C., Bi, Y., Wang, J., & Han, Y. (2023). "Application of Mechanical Product Design Parameter Optimization Based on Machine Learning in Identification." *Production Planning & Control* 1–15. <u>https://doi.org/10.1080/09537287.2022.2160388</u>

9. Trease, G.E., & Evans, W.C. (2002). Phytochemicals. In: Pharmacognosy. 15th ed. Saunders Publishers, London. 42-44, 221- 229, 246- 249, 304-306,331-332, 391-393.

10. Adams, R.P. (2007). Identification of Essential Oil Components by Gas Chromatography/Mass Spectrometry. 4th Edition Allured Publishing Corporation, Carol Stream