**Ars Pharm**aceutica
https://revistaseug.ugr.es/index.php/ars
E-ISSN: 2340-9894 ISSN: 0004-2927

doi: 10.30827/ars.v66i2.32423
Artículos revisión

# Curcumin and its derivatives as potential antiviral candidates against monkeypox (mpox): a review of computational studies

## La curcumina y sus derivados como posibles candidatos antivirales contra la viruela del mono (mpox): una revisión de estudios computacionales

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**Received:** 29.12.2024
**Accepted:** 04.02.2025
**Published:** 18.03.2025

**Funding**

No specific funding was received for this research.

**Conflict of interest**

The authors declared no conflict of interest.

**Acknowledgment**

We would like to acknowledge that no external assistance or funding was received for this review.

### Resumen

**Introducción:** La viruela del mono (mpox) es una enfermedad infecciosa causada por el virus mpox que es motivo de preocupación sanitaria mundial porque el brote, a mayo de 2023, ha afectado a más de 80.000 personas en cientos de países. Actualmente, no existe un tratamiento específico, incluidos los antivirales, para los pacientes con mpox. Continúa la exploración de compuestos activos para mpox, uno de los cuales es la curcumina y sus derivados. La curcumina es un compuesto polifenólico que se encuentra predominantemente en la cúrcuma y que se ha documentado que tiene efectos antivirales. Por lo tanto, este estudio tiene como objetivo explorar estudios que investiguen el potencial de la curcumina y sus derivados como candidatos antivirales para atacar a la mpox.

**Método:** Se buscó literatura publicada desde su inicio hasta 2024 en ScienceDirect, PubMed, Scopus y Google Scholar. Las palabras clave utilizadas en esta búsqueda incluyeron cúrcuma, curcumina, tetrahidrocurcumina, demetoxicurcumina, bisdemetoxicurcumina, cúrcuma, viruela del mono y mpox.

**Resultados:** Los resultados de la búsqueda bibliográfica encontraron cinco estudios computacionales que involucran el compuesto curcumina y sus derivados, incluida la tetrahidroxicurcumina y la demetoxicurcumina. Todos los estudios demostraron que la curcumina y sus derivados tienen una mejor afinidad de unión con proteínas de mpox en comparación con el control de varios antivirales. La curcumina y sus derivados tienen un gran potencial para inhibir la replicación del virus mpox y modular el sistema inmunológico.

**Conclusiones:** Esta revisión concluye que la curcumina y sus derivados tienen potencial como candidatos antivirales para el mpox. Sin embargo, los estudios relacionados siguen siendo limitados y se limitan a estudios computacionales. Se necesitan más estudios preclínicos, experimentales y clínicos para confirmar su eficacia y mecanismos de acción.


**Palabras clave:** Antiviral; Curcumina; Viruela del mono; Mpox; Cúrcuma


### Abstract

**Introduction:** Monkeypox (mpox) is an infectious disease caused by the mpox virus that is of global health concern because the outbreak, as of May 2023, has affected more than 80,000 people in hundreds of countries. Currently, there is no specific treatment, including antivirals, for mpox patients. Exploration of active compounds for mpox continues, one of which is curcumin and its derivatives. Curcumin is a polyphenol compound predominantly found in turmeric which has been documented to have antiviral effects. Therefore, this study aims to explore studies investigating the potential of curcumin and its derivatives as antiviral candidates in targeting mpox.

**Method:** Literature published from inception to 2024 in ScienceDirect, PubMed, Scopus, and Google Scholar was searched. Keywords used in this search included curcuma, curcumin, tetrahydrocurcumin, demethoxycurcumin, bisdemethoxycurcumin, turmeric, monkeypox, and mpox.

**Results:** The literature search results found five computational studies involving the compound curcumin and its derivatives, including tetrahydroxycurcumin and demethoxycurcumin. All studies showed that curcumin and its derivatives have better binding affinity with mpox proteins compared to control of several antivirals. Curcumin and its derivatives have strong potential in inhibiting mpox virus replication and modulating the immune system.

**Conclusions:** This review concludes that curcumin and its derivatives have potential as antiviral candidates for mpox. However, related studies remain limited and confined to computational studies. Further preclinical experimental and clinical studies are needed to confirm their effectiveness and mechanisms of action.


**Keywords:** Antiviral; Curcumin; Monkeypox; Mpox; Turmeric

## Highlights

Curcumin and its derivatives have documented antiviral effects through mechanisms such as viral replication inhibition and immune system modulation, but their potential against monkeypox (mpox) remains largely unexplored.

This review highlights curcumin and its derivatives as promising antiviral candidates against mpox based on computational evidence, with superior binding affinities to the virus proteins compared to existing antiviral drugs.

The findings support the potential of curcumin and its derivatives as antiviral candidates for mpox, encouraging further preclinical and clinical studies to validate their efficacy and mechanisms for therapeutic development.

# Introduction

Mpox, formerly called monkeypox, is a viral infection caused by a type of zoonotic virus from the genus *Orthopoxvirus* that has a similar clinical presentation to smallpox[1]. Mpox was first discovered in 1958 and the first human case of mpox infection was identified in the Democratic Republic of Congo in 1970. This infection is transmitted through transmission from infected animals or human to human through body fluids, lesions, droplets, and sexual contact[2-4]. The clinical presentation of mpox infection is systemic symptoms caused by the viremia phase that occurs before the skin rash, including fever, myalgia, sore throat, and lymphadenopathy. Following systemic symptoms, a skin rash appears on the face, oral mucosa and lips, perioral, genital, perianal, and anorectal[5-8]. As of May 2023, data from 111 countries reported 87,704 confirmed cases of mpox with 140 deaths globally[9]. As a result, the World Health Organization (WHO) declared the mpox outbreak a global health emergency of concern[10].

As of the writing of this study, there is no specific treatment for patients with mpox, including specific antivirals; however, supportive care can be given because the clinical progression of mpox is usually mild and self-limiting[11]. Because mpox and smallpox share similarities, antiviral drugs may be beneficial for monkeypox, such as tecovirimat, cidofovir, and brincidofovir[12,13]. However, studies on the effectiveness of these antivirals remain very limited. Tecovirimat is considered promising and safe, but controlled clinical trials are not yet available[14]. Meanwhile, cidofovir is reported to be highly nephrotoxic, and brincidofovir has no significant effectiveness in mpox patients[15]. Therefore, antivirus exploration continues to be conducted. One method that is currently being widely used to analyze drug candidates is computational techniques or *in silico* methods, which can overcome the problems of cost, time, and large resources[16].

Curcumin, one of the most important compounds derived from turmeric (*Curcuma longa*), is a traditional herbal medicine that is widely used and studied. To date, curcumin and its derivatives have been reported to be effective for various diseases[17-21]. Furthermore, studies reported the antiviral effects of curcumin and its derivatives which are promising for treating a number of infectious diseases caused by both RNA and DNA viruses[22-24]. Furthermore, curcumin is considered effective in inhibiting poxvirus infections[25].

Evidence suggests that curcumin, in general, is effective against viruses by mechanisms in which viral replication and/or cellular signaling pathways related to viral replication, such as phosphatidylinositol 3-kinase (PI3K)/AKT and nuclear factor-kappa B (NF-κB), are inhibited[26]. Therefore, they suggest that curcumin and its derivatives may have good efficacy as antiviral candidates for mpox infection.

Exploration of curcumin against mpox is still rare and limited to computational methods. In addition, to the best of our knowledge, as of this writing, no study has summarized and reviewed studies on the potential of curcumin and its derivatives on mpox. Therefore, we attempted to review and summarize the published studies. This study is expected to be used as a reference for future studies related to the development of curcumin and its derivatives as an antiviral for mpox.

# Methods

This study is a literature review on the exploration of the potential of curcumin and its derivatives as an antiviral against mpox. A literature search for computational studies published in ScienceDirect, PubMed, Scopus, and Google Scholar was performed. In the literature search, we used the following keyword combinations: "curcuma", "curcumin", "tetrahydrocurcumin", "demethoxycurcumin", "bisdemethoxycurcumin", "turmeric", "monkeypox", and "mpox". All studies discussing the analysis of the effects of curcumin on mpox published from inception to 2024 were considered for inclusion.

We included all articles if they met the inclusion criteria such as computational studies discussing the potential of curcumin and its derivatives for mpox, written in English, peer-reviewed, and full-text. Review articles, editorials, commentaries, letters to editors, short communications, written in languages other than English, and unavailable full-text were exclusion criteria in the study selection. No restriction on the year of publication was applied. Data extraction was performed using a table containing references/authors, curcumin and/or its derivatives compounds, mpox targets, controls (if any), and results. Finally, all results from the included computational studies were reviewed qualitatively.

# Results

We finally included five computational studies that analyzed the effects of curcumin and its derivatives on mpox. Compounds analyzed in eligible studies include curcumin[27-31], tetrahydroxycurcumin[28], and demethoxycurcumin[31]. Four studies compared the potency of curcumin and/or its derivatives with the antiviral controls acyclovir[27], tecovirimat[28,29], and cidofovir[30]. A summary of the included studies is presented in Table 1.

**Table 1.** Summary of effects of curcumin and its derivatives on mpox targets.

| Reference | Compounds | Mpox Targets | Control | Results |
|---|---|---|---|---|
| Akash et al.[27] | Curcumin | 4QWO | Acyclovir | Curcumin had a binding energy of -7.7 kcal/mol to -8.9 kcal/mol with 4QWO. Acyclovir demonstrated a binding energy of -6.4 kcal/mol. |
| Alagarsamy et al.[28] | Curcumin, tetrahydroxy-curcumin | VarTMPK | Tecovirimat | Tetrahydroxy-curcumin had the strongest binding energy, which is -9.7 kcal/mol, and curcumin showed a binding energy of -7.2 kcal/mol. Tecovirimat had a binding energy of -7.2 kcal/mol. |
| Banik et al.[29] | Curcumin | 4QWO | Tecovirimat | Curcumin showed the lowest binding energy with 4QWO which was -37.43 kcal/mol. Tecovirimat had a binding energy of -20.41 kcal/mol. |
| Maurya et al.[30] | Curcumin | 4E90, 4QWO, 8HG1, 8CEQ | Cidofovir | Curcumin showed a strong binding affinity with 8HG1, -8.5 kcal/mol, compared to cidofovir with a binding affinity of -7.2 kcal/mol. |
| Rout et al.[31] | Curcumin, demethoxy-curcumin | F13 | Not available | Demethoxy-curcumin showed the strongest binding energy with F13, which was -64.86±1.30 kJ/mol, while curcumin was -48.53±1.80 kJ/mol. |

# Discussion

Computational methods were performed to determine the binding affinity between curcumin and its derivatives with mpox-related molecular targets, which in this study, included A42R profilin-like protein (4QWO), thymidylate kinase from Variola virus (VarTMPK), envelope protein (F13), DNA polymerase holoenzyme (8HG1), methyltransferase VP39 (8CEQ), and envelope protein E8 (4E9O). The smaller or

lower the binding energy/affinity, the higher the potential of the compound to be a drug candidate. There is agreement that a docking score of less than -6.0 kcal/mol is considered as standard drug[32].

Curcumin is the most abundant component found in turmeric. Curcumin docked with 4QWO showed stronger and better binding affinity (-7.7 to -8.9 kcal/mol) compared to acyclovir (-6.4 kcal/mol)[27]. A similar study exploring several potential compounds for mpox also reported that curcumin had the strongest binding affinity (-37.43 kcal/mol) with 4QWO compared to other compounds such as gedunin, piperine, and coumadin which had binding affinity values of -34.89, -34.58, and -34.14 kcal/mol, respectively. Surprisingly, tecovirimat, which is considered the most promising for use as an antiviral in mpox patients, had a binding energy of -20.41 kcal/mol[29]. In line with previous studies, the findings of this study reported that curcumin has a strong binding affinity when docked with, in order of the strongest, 8HG1, 8CEQ, 4QWO, and 4E9O with docking scores of -8.5, -8.4, -7.9, and -7.3 kcal/mol, respectively. Interestingly, cidofovir as a control showed a binding affinity of -7.2 kcal/mol when docked with 8HG1[30]. The findings concluded that curcumin showed strong binding affinity with the mpox virus protein compared to the antiviral control and other compounds.

There are two studies that tested not only curcumin, but also curcumin derivatives. Alagarsamy and colleagues docked various compounds with the VarTMPK protein and found that tetrahydroxycurcumin, a curcumin derivative, had the lowest binding energy (-9.7 kcal/mol). In this study, curcumin showed a binding energy of -7.2 kcal/mol. Interestingly, the control in this study, tecovirimat, had a binding energy of -7.2 kcal/mol[28]. Another study also reported that demethoxycurcumin, a curcumin derivative, docked with F13 and showed the strongest binding energy (-64.86±1.30 kJ/mol or -15.50±0.31 kcal/mol) followed by curcumin (-48.53±1.80 kJ/mol or -11.60±0.43 kcal/mol)[31]. It can be concluded that both curcumin and its derivatives showed strong binding energy when docked with mpox protein.

The mechanism of action by which antiviral effect of curcumin on mpox remains unclear. However, evidence proposed a mechanism of action of curcumin against mpox, where curcumin blocks the process of attachment and entry of the virus into the host cell. In addition, curcumin inhibits the transcription and translation processes required for viral genome replication.

Three included studies[27,29,30] using the target 4QWO, the A42R profilin-like protein of mpox that plays a critical role in virus replication and assembly, corroborate the statement where curcumin inhibiting the profilin-like protein resulted in inhibition of mpox virus replication. Additionally, one study[30] docked curcumin with DNA polymerase holoenzyme, an enzyme that plays a role in DNA synthesis during viral replication, and methyltransferase VP39, an enzyme that plays a role in the stabilization of viral mRNA and the efficiency of protein translation during mpox infection, resulting in strong binding affinity. The study, again, found that curcumin was more effective at inhibiting DNA polymerase holoenzyme than the antiviral cidofovir, which is currently considered effective against mpox[33]. Based on these findings, curcumin is believed to be effective in inhibiting mpox virus replication and the process of viral infection; as has been described for other viruses[27,34].

Furthermore, curcumin, in general, has the capacity to modulate host cell signaling pathways, including the PI3K/AKT pathway, NF-κB, Jun activation domain-binding protein 1 (Jab-1), and virus-related inflammatory processes[22]. This evidence is supported by one of the included computational study results, in which curcumin regulated the inflammatory pathway associated with mpox infection, including mitogen-activated protein kinase (MAPK) signaling, tumor necrosis factor (TNF), NF-κB, prostaglandin-endoperoxide synthase 2 (PTGS2), and Toll-like receptor 4 (TLR4), as indicated by strong binding affinity[30]. The MAPK signaling pathway is a promising therapeutic target in combating mpox because MAPK signaling plays a critical role in the response to mpox[35]. In addition, a study also stated that therapy targeting immune responses, such as NF-κB, cytokines, and chemokines, demonstrates inhibited mpox virus replication and systemic inflammation[36]. Overall, these proposed mechanisms suggest the potential of curcumin as an antiviral candidate for the treatment of mpox, not only by inhibiting viral function, but also by supporting modulation of the immune system.

Several computational studies have reported that curcumin and its derivatives, tetrahydroxycurcumin and demethoxycurcumin, have good potential as active compounds that can inhibit mpox virus. The limitations of this review are the lack of studies testing the potential of curcumin and its derivatives

against mpox virus and limited to computational studies. Additionally, the exact mechanism of curcumin and its derivatives in inhibiting the mpox virus remains unclear; therefore, preclinical *in vivo* and *in vitro* studies are needed to prove the effectiveness of curcumin and its derivatives against the mpox virus along with the underlying mechanisms. Furthermore, no clinical studies testing the efficacy of curcumin in humans with mpox infection have been conducted; thus, the findings of this literature review may serve as a consideration for further exploration and clinical testing as an antiviral against mpox.

## Conclusion

This study underlines the antiviral effects of curcumin and its derivatives, tetrahydroxycurcumin and demethoxycurcumin, against mpox virus. However, no preclinical or clinical trials have been reported so far. Therefore, this study provides an overview and proposal of curcumin and its derivatives as candidates for active compounds that have the potential to be antiviral for mpox in further preclinical and clinical investigations. In addition, computational studies to explore other active compounds to determine potential candidates as antivirals for mpox may be needed.

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