

SOCIEDADE BRASILEIRA DE QUÍMICA

Anais da 48^a Reunião Anual da SBQ



48^a
Reunião Anual da
Sociedade
Brasileira de
Química

Campinas-SP
2025

Copyright © 2025 para os autores

Revisão textual e gramatical: Resposanbilidade dos respectivos autores.

Todos os direitos reservados 2025

A reprodução não autorizada desta publicação, no todo ou em parte,
constitui violação de direitos autorais (Lei 9.610/98).

Dados Internacionais de Catalogação na Publicação (CIP)
(Câmara Brasileira do Livro, SP, Brasil)

Reunião Anual da SBQ (48. : 2025 : Campinas, SP)
Anais da 48ª Reunião Anual da SBQ [livro
eletrônico] / Sociedade Brasileira de Química. --
1. ed. -- Campinas, SP : Aptor Software, 2025.
PDF

Vários autores.
Vários colaboradores.
Bibliografia.
ISBN 978-85-63273-70-3

1. Química I. Sociedade Brasileira de Química.
II. Título.

25-282696

CDD-540

Índices para catálogo sistemático:

1. Química 540

Eliete Marques da Silva - Bibliotecária - CRB-8/9380

Structure and Leishmanicidal activity of a new organometallic Ru(*p*-cym) complex containing a β -diketonate and 3-Chloropyridine

Eduardo M. F. Amaral (PG),^{1,2*} Kamila A. Fontoura (PG),³ Kelly A.G. Yoneyama (PQ),³ Javier A. Ellena (PQ),⁴ Gustavo Von Poelhsitz (PQ).¹

eduardo.amaral@uftm.edu.br

¹Instituto de Química, Universidade Federal de Uberlândia, Uberlândia-MG, Brazil; ²Câmpus Universitário de Iturama, Universidade Federal do Triângulo Mineiro, Iturama-MG, Brazil; ³Instituto de Biotecnologia, Universidade Federal de Uberlândia, Uberlândia-MG, Brazil; ⁴Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos-SP, Brazil.

Keywords: Organometallic complex, Leishmanicidal activity, β -diketonate.

Highlights

A new organoruthenium complex was synthesized and characterized, showing activity against *L.L. amazonensis* and cytotoxic potential due to structural changes from ligand exchange.

Resumo/Abstract

Leishmaniasis is a neglected tropical disease with a significant global health impact. Current treatments face challenges related to resistance, safety, efficacy, and cost. New strategies to address these limitations are under investigation, and Ru(II) complexes based on *p*-cymene, which have shown promising biological activity, are considered potential alternatives. In this study, a new organoruthenium complex with the formula [Ru(η^6 -*p*-cymene)(HBTA)(3-ClPy)]PF₆ (HBTA = 4,4,4-trifluoro-1-phenyl-1,3-butanedionate; 3-ClPy = 3-chloropyridine) was synthesized, characterized, and evaluated for its potential to inhibit *Leishmania amazonensis* growth using well-established methods. FTIR analysis revealed characteristic bands for $\nu(\text{C=O})$ and $\nu(\text{C=C})$ stretching modes of the bidentate O,O-donor diketonate ligand within the range of 1595–1531 cm⁻¹. The ¹H NMR spectrum displayed all expected signals for the coordinated *p*-cymene, β -diketonate, and pyridine derivative ligands, with a singlet near 6.2 ppm corresponding to the methylenic hydrogen of the diketonate ligand. X-ray diffraction analysis, performed on single crystals obtained from complex recrystallization, confirmed that the compound crystallizes in the P2₁/c space group of the monoclinic system, and the molecular structure clearly exhibits a “piano-stool” pseudo-octahedral geometry. While the precursor complex is inactive, the newly synthesized complex demonstrated higher activity than uncoordinated β -diketonate against *L. amazonensis* promastigotes. Moreover, the substitution of the chloride ligand with a pyridine-derived ligand significantly influenced the cytotoxic potential, demonstrating that structural modifications can substantially impact biological activity.

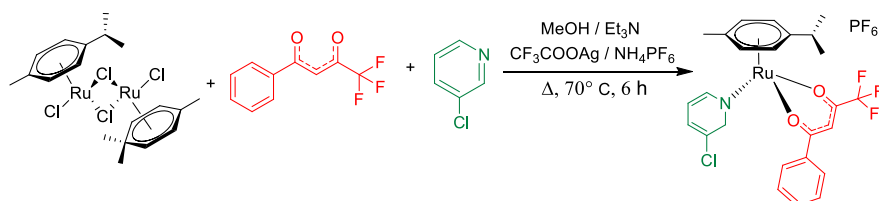


Figure 1. General scheme for synthesis and general structure of complex.

Ru complexes	IC ₅₀ (95% CI), μM^a
[RuCl ₂ (<i>p</i> -cim)] ₂	> 200
(HBTA)	57.8
[Ru(<i>p</i> -cim)(HBTA)(Cl)]PF ₆	90.5
[Ru(<i>p</i> -cim)(HBTA)(3-ClPy)]PF ₆	27.10

Table 1. IC₅₀ (95% CI) of ruthenium complexes and β -diketonates on *Leishmania amazonensis* promastigotes.

Agradecimentos/Acknowledgments



APQ-1820-21



311424/2021-0



www.lafotcm.org

