



48ª
Reunião Anual da
Sociedade
Brasileira de
Química

Emergências Climáticas?
A Química Age e Reage!

ANais

08 a 11 de junho de 2025, Campinas, Expo Dom Pedro

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

Degradation Pathways of Tadalafil: A thermoanalytical investigation

Francisco V.B Nascimento (PG)^{1*}, Ana P.G Ferreira (TC)¹, Caroline Gaglieri (PD)², Aniele de Moura (PD)¹, Éder T.D.G. Cavaleiro (PQ).¹

valdenir.bn@usp.br;

¹ Instituto de Química de São Carlos (IQSC), Universidade de São Paulo; ² Universidade Estadual Paulista (UNESP), Faculdade de Ciências

KEYWORDS: Tadalafil, Thermal Behavior, TGA-FTIR.

Highlights

Tadalafil free base was submitted to thermal analysis

Propyl isocyanate was released followed by 1,3-Benzodioxole, NH₃ and CO₂

The solid intermediate was characterized by LC-MS-MS

Abstract

Tadalafil (TAD, Figure 1), is one of the most marketed drugs for treat erectile dysfunction. Due to its widespread global use, it is interesting to understand different aspects related to this active pharmaceutical ingredient. Thus, in the present study, the thermal behavior of TAD was investigated using thermogravimetry (TGA) and differential thermal analysis (DTA), differential scanning calorimetry (DSC), hot stage microscopy (HSM), and evolved gas analysis using thermogravimetry coupled with vibrational infrared spectroscopy (TGA-FTIR). Furthermore, the solid intermediate formed during the thermal decomposition of the drug was characterized using liquid chromatography coupled to mass spectrometry (LC/MS/MS). TAD decomposed in different ways Under N₂ and air atmospheres. The DSC curves presented an endothermic event related to the melting of the sample at $T_{onset} = 303.3^{\circ}\text{C}$ in the first heating, with no evidence of crystallization under the conditions used in this study. TGA-FTIR revealed that the thermal decomposition of TAD begins with the release of 1,3-benzodioxole, carbon monoxide, and propyl isocyanate. The decomposition of the latter results in carbon dioxide and ammonia, which were identified in the gas phase as by-products of propyl isocyanate thermal degradation. From HSM (Figure 2), allowed the observation of the complete decomposition of TAD at 300°C, corroborating the results from TGA/DTG/DTA and DSC curves. Finally, the results obtained from LC/MS/MS supported the identification of possible intermediates formed during the thermal decomposition of TAD, contributing to the findings from thermal analysis for a deeper understanding of the thermal decomposition of the drug. Based on these results, a thermal decomposition mechanism was proposed.

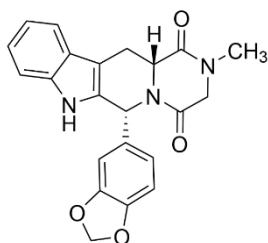


Figure 1 Structural formula of Tadalafil

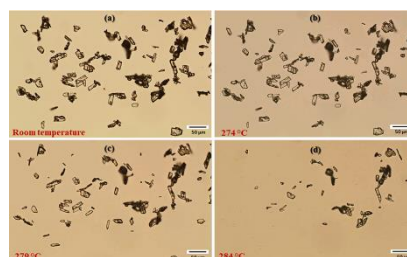


Figure 2. Images from Hot stage microscopy of TAD

Acknowledgments

The authors would like to thank Brazilian Federal Agency for Suport and Evaluation of Graduate Education -CAPES (grant 88887.704933/2022-00), The São Paulo Research Foundation – FAPESP- (grant 24/00779, 23/14645-5, 22/15211-6), and the National Council for Scientific and Technological Development-CNPq, São Carlos Institute of Chemistry (IQSC-USP) for financial support.