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Author: Bruno B.C. Holanda Renan B. Guerra Alexandre O. Legendre Débora F. Almeida Thais F.C. Fraga-Silva Ângela C. Finato James Venturini Gilbert Bannach

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### ACCEPTED MANUSCRIPT

# Thermal, spectroscopic and biological studies on solid ibuprofen complexes of heavy trivalent lanthanides and yttrium

Bruno B. C. Holanda<sup>1</sup>, Renan B. Guerra<sup>1</sup>, Alexandre O. Legendre<sup>1</sup>, Débora F. Almeida<sup>2</sup>, Thais F. C. Fraga-Silva<sup>2</sup>, Ângela C. Finato<sup>2</sup>, James Venturini<sup>2</sup>, Gilbert Bannach<sup>1\*</sup>

\*gilbert@fc.unesp.br

## **HIGHLIGHTS**

- •lbuprofen complexes of heavy trivalent lanthanides and yttrium have been synthetized.
- The thermal analysis provided information about the thermal behavior of the samples.
- Analysis of the IR spectra showed two coordination modes for compounds.
- The TG-EGA-MIR showed propane as the gas evolved during the thermal decomposition.
- •Cytotoxicity and anti-inflammatory activity of the compounds were evaluated.

#### **Abstract**

Heavy lanthanide complexes (Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) and yttrium (III) complexes with ibuprofen ligands (Hibu) were synthesized and characterized by simultaneous thermogravimetric and differential thermal analysis (TG-DTA), differential scanning calorimetry (DSC), attenuated total reflection mid-infrared spectroscopy (ATR-MIR), complexometric titration, X-ray powder diffraction (XRD) in order to determine stoichiometry, thermal stability and the ligand coordination modes of the compounds. The volatiles released were also analyzed by online coupled thermogravimetry–infrared spectroscopy evolved gas analysis (TG-EGA-MIR), to identify the main product resulting from the heating of terbium complex. In addition, ibuprofen and the synthesized compounds were tested to assess cytotoxic/proliferative and anti-inflammatory activity. The results of the cytotoxicity assays showed that compounds [Yb(ibu)<sub>3</sub>], [Lu(ibu)<sub>3</sub>] and [Y(ibu)<sub>3</sub>] decreased the cytotoxic activity of ibuprofen. Furthermore, [Yb(ibu)<sub>3</sub>] and [Lu(ibu)<sub>3</sub>] exhibited a significant anti-inflammatory profile, superior to that of ibuprofen. Under the stimulatory effect of lipopolysaccharide, these compounds displayed anti-inflammatory activity characterized by low TNF-α and H<sub>2</sub>O<sub>2</sub> production and high IL-10 production, emerging as interesting alternatives for further biological applications.

Keywords: thermal behavior, middle infrared spectroscopy, TG-EGA-MIR, metallodrug, lanthanides, biological studies

#### 1. Introduction

<sup>&</sup>lt;sup>1</sup> Faculdade de Ciências, Departamento de Química, UNESP — Univ. Estadual Paulista, 17033-360 Bauru, São Paulo, Brasil.

<sup>&</sup>lt;sup>2</sup> Faculdade de Ciências, Departamento de Ciências Biológicas, UNESP — Univ. Estadual Paulista, 17033-360 Bauru, São Paulo, Brasil.

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