

DESIGN, SYNTHESIS, AND PHYSICOCHEMICAL CHARACTERIZATION OF QUERCETIN DERIVATIVES AS NEW SUBSTRATES IN CHEMICAL REACTIVITY WITH METAL IONS

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Abstract: The project focuses on the structural modification of flavonoids in order to achieve highly soluble and bioavailable species. The first step in that investigation was the synthesis of the 5'-sulfonic derivative of quercetin, with the ultimate goal being the increase in flavonoid solubility in aqueous media. The product was initially characterized by Infrared Spectroscopy (FT-IR), while its molecular structure was determined by X-ray crystallography. Subsequently, quercetin 5'-sulfonic acid was used in the synthesis of ternary complexes with lanthanide ions.

• Introduction

The main causes of morbidity and mortality worldwide are chronic diseases, such as cancer, cardiovascular diseases, Diabetes mellitus, as well as neurodegenerative disorders. These diseases are inextricably linked to oxidative stress, namely the imbalance between reactive oxygen species and antioxidant defense, ultimately resulting in cellular damage [1]. Consequently, the need for search of potent antioxidant compounds becomes imperative. Flavonoids, and especially quercetin, attract intense research interest as they possess both antioxidant and anti-inflammatory properties [2].

• Materials and methods

The flavonoid Quercetin (**Fig. 1**) in this study was used without further purification.

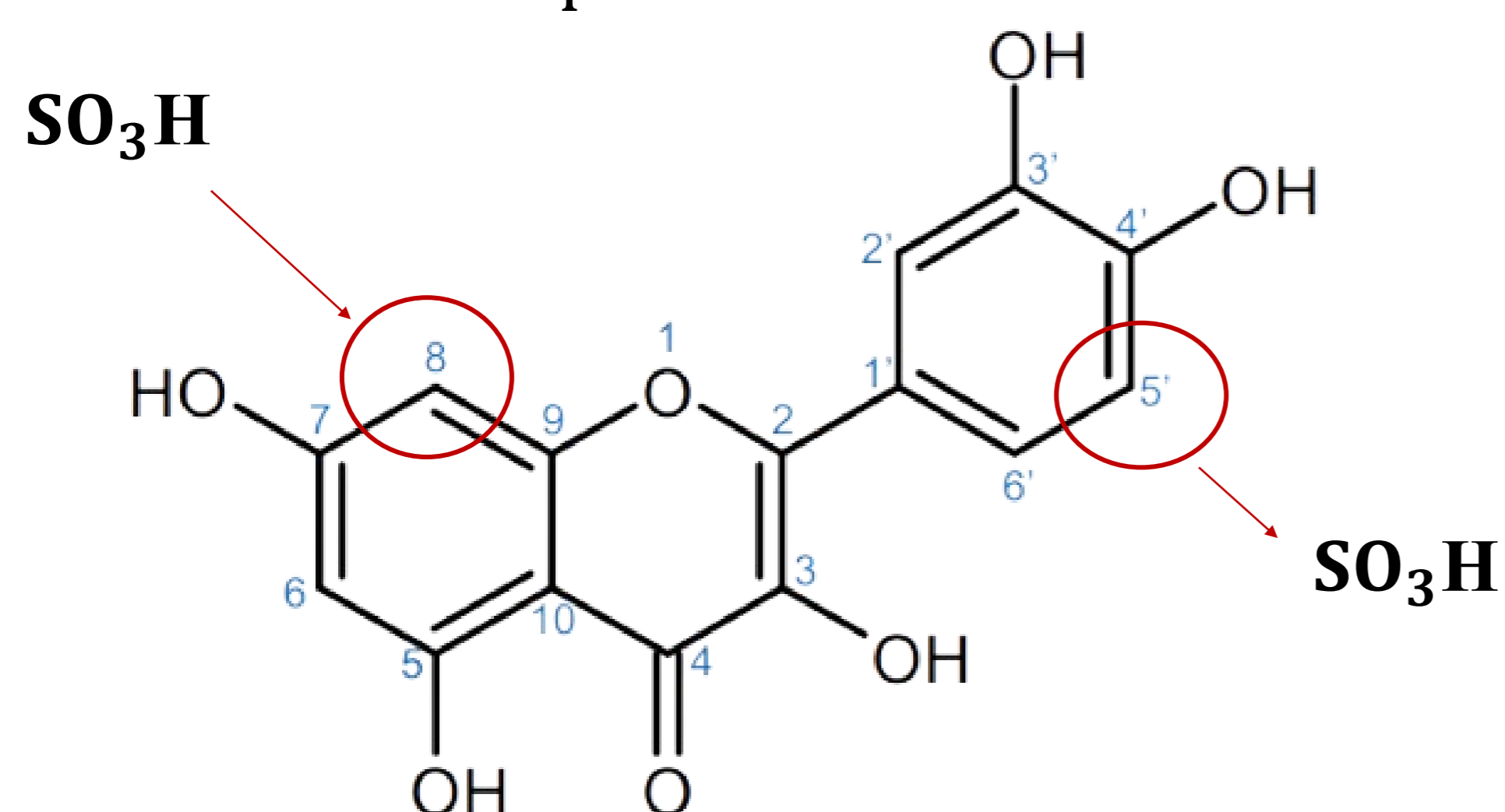
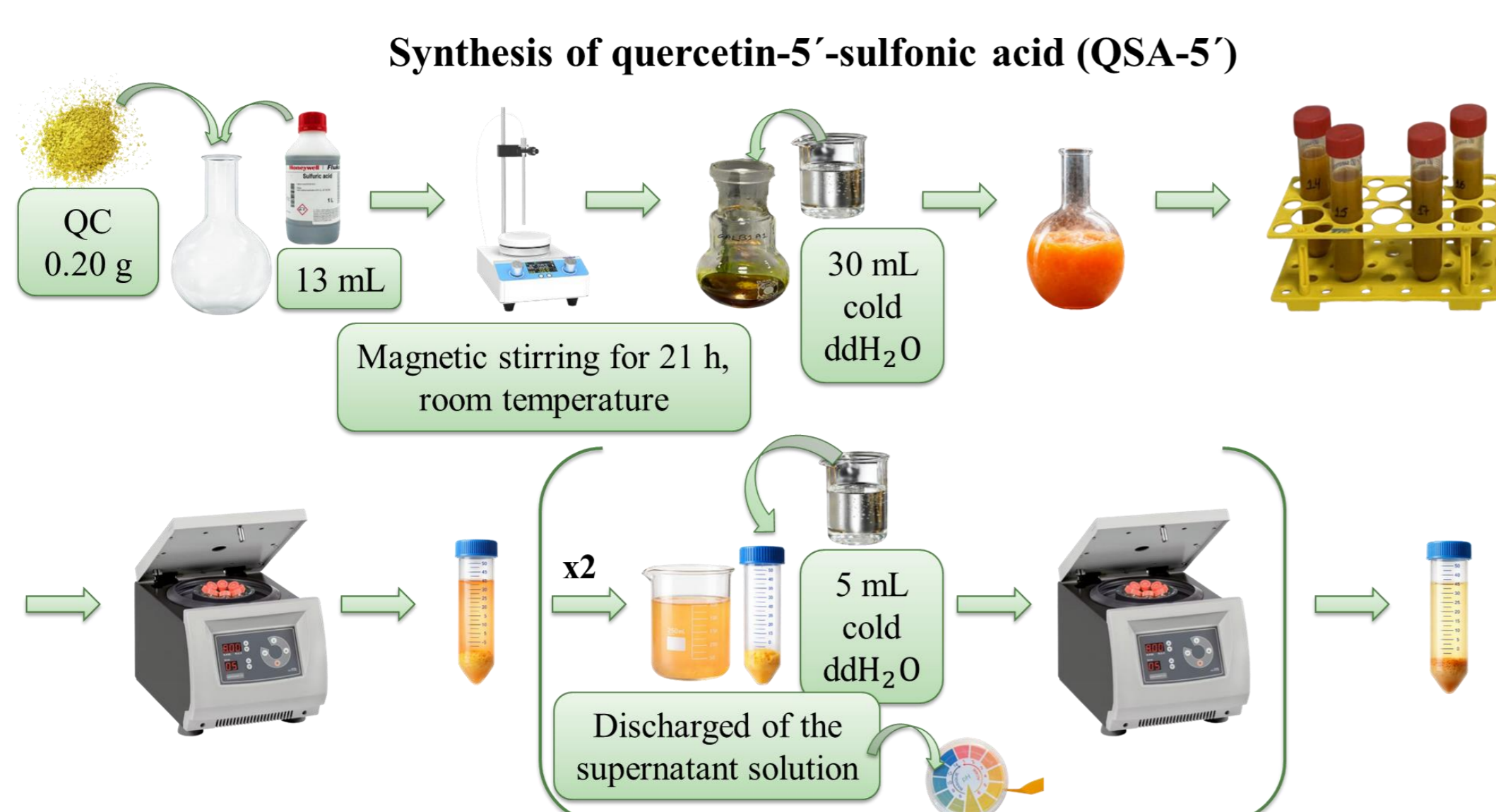


Fig. 1: Targeted Quercetin sites for modification through sulfonation



• Results and discussions

Sulfonation of quercetin (QC) was achieved through the reaction shown in **Fig. 2** and the isolated material was characterized by elemental analysis and FT-IR.

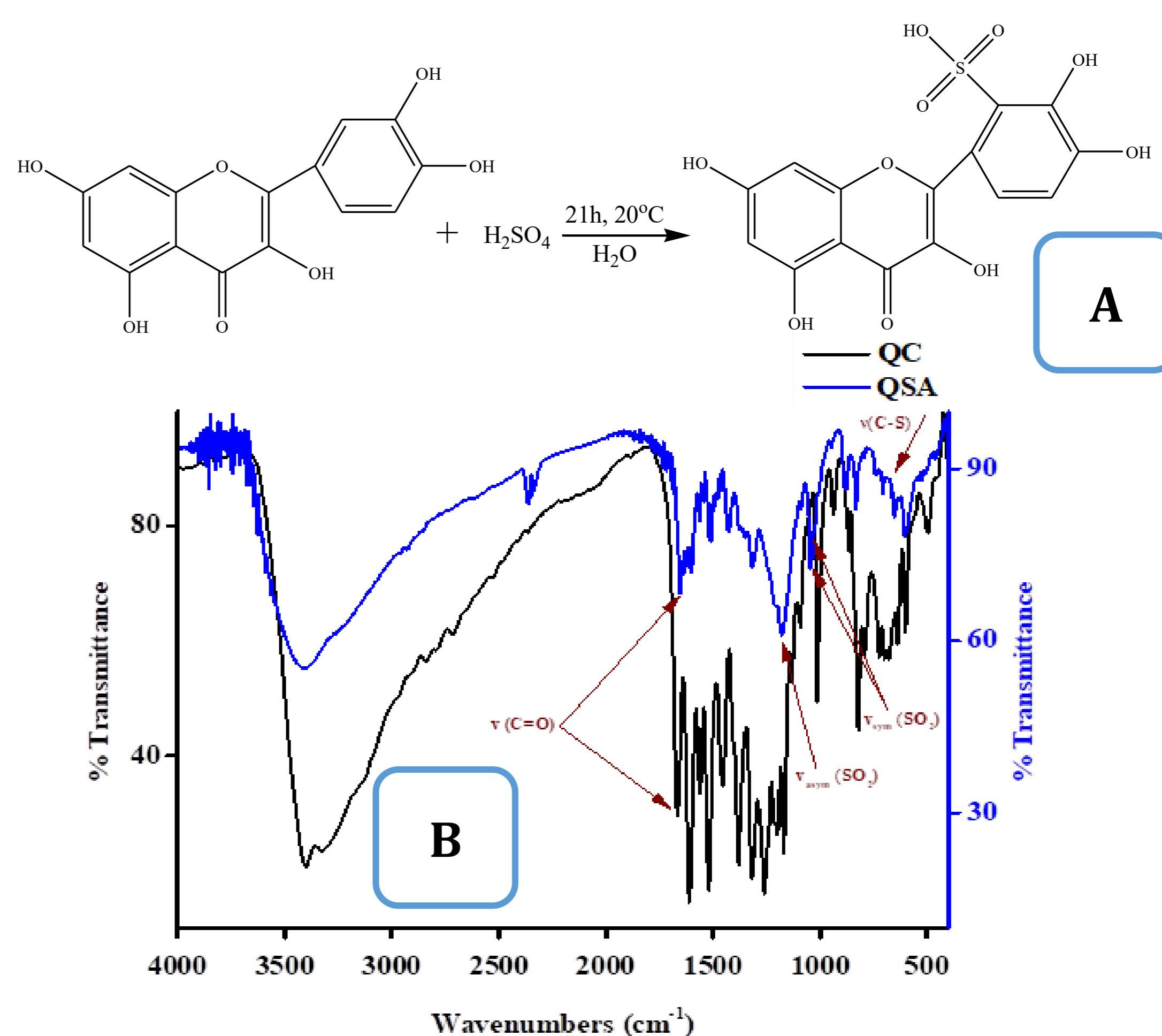


Fig. 2: A. Synthesis of sulfonated quercetin B. FT-IR spectrum

• Conclusions

Sulfonated Quercetin was isolated by precipitation with hot water and, following characterization, it was further used to react with lanthanide metal ions, thus leading to ternary complexes.

Complete characterization of sulfonated Quercetin, in its pure form, took place through elemental analysis, FT-IR, ESI-MS, and NMR.

References:

- [1] Rodríguez-Arce E., Saldías M., *Biomedicine & Pharmacotherapy* 143 (2021) 112236.
- [2] Xu D., Hu M.J., Wang Y.-Q., Cui Y.-Q., *Molecules* 24(6) (2019) 1123.