

Área: ORG

## Methodology optimization for synthesizing thiols from phenolic compound as potencial AuNPs stabilizers

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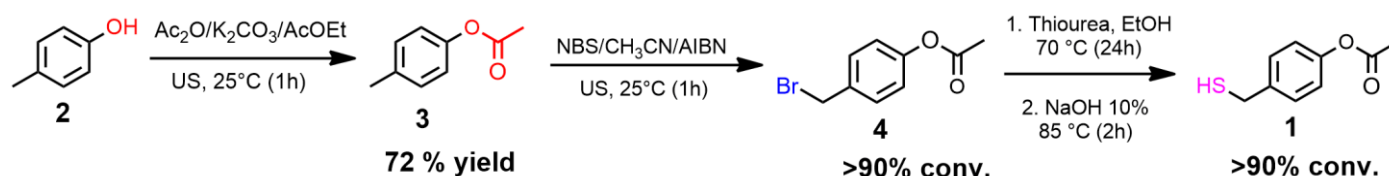
### Highlights

Ultrasound-assisted methodologies enabled the efficient protection of phenolic OH group and Wohl Ziegler bromination with significantly reduced reaction times. Thiol **1** was obtained with 95% conversion.

### Abstract

The modification of natural phenolic compounds represents a promising route for obtaining ligands applicable for the stabilization of gold nanoparticles (AuNPs).<sup>1</sup> In this work, we optimized reaction steps to obtain thiol **1**, as a potential stabilizer for AuNPs. To this end, the phenolic OH group (compound **2**) was initially protected using ultrasound (US)-assisted methodologies, affording the desired product **3** in 72% yield. To obtain compound **4**, different Wohl Ziegler bromination<sup>2</sup> conditions were evaluated, including variations in solvent (CH<sub>3</sub>CN and CH<sub>2</sub>Cl<sub>2</sub>), radical indicators (azobisisobutyronitrile (AIBN) and benzoyl peroxide), and energy sources (conventional heating and US). The synthesis demonstrated efficient radical activation for both initiators, achieving conversions above 90% under conventional heating (90°C, 7h), using CH<sub>3</sub>CN as solvent. Similar results were observed under US irradiation; however, the reaction proceeded in significantly shorter reaction time (1h). Finally, thiol **1** was obtained with 95% conversion by treating compound **4** with thiourea/NaOH (Scheme). This methodology will be applied to the synthesis of target thiols from natural phenolic products, such as carvacrol, thymol, and eugenol.

Scheme: Synthesis of thiol **1** from phenolic compound **2**.



### References:

- 1 WANG, Z. *et al.* Design of polymeric stabilizers for size-controlled synthesis of monodisperse gold nanoparticles in water. 23(2), 885-995, 2007. DOI: 10.1021/la062623h. DOI: 10.1021/la062623h.
- 2 EDDE, F. *et al.* User-friendly and green procedure for a photoinduced Wohl–Ziegler reaction. 28, e202500183, 2025. DOI: 10.1002/ejoc.202500183.

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