# Iodination of aromatic and heteroaromatic compounds in the presence of iodine and hydrogen peroxide in water: A balance between atom economy and high yields.

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## INTRODUCTION

Recently we published a work involving the efficient and selective diiodination of phenols using $I_2$ and $H_2O_2$ 30% in water.[1] Afterwards, we decided to subject aromatic and heteroaromatic compounds to the same reaction conditions, performing a balance between the amounts of the reagents and the yields obtained, aiming to the formation of interesting iodinated molecules in high yields.

## RESULTS AND DISCUSSION

We treated phenol (**1a**) with 1.5 equiv. of $I_2$ and 3 equiv. of $H_2O_2$ 30% in water at 50 °C for 24 h and obtained 2,4,6-triiodophenol (**2a**) in a moderate yield of 65% (Table 1, entry 1). In the attempt of increasing this yield, we used 2 equiv. of $I_2$ and 4 equiv. of $H_2O_2$ 30% producing the triiodinated phenol **2a** in a yield of 83% (entry 2). The aromatic compound **1b** and the heteroaromatic compound **1c** were subjected to the reaction with 2 equiv. of $I_2$ and 4 equiv. of $H_2O_2$ 30% resulting in the triiodinated products **2b** and **2c**, respectively, in good yields (entries 3 and 4). The balance between amounts of the reagents and yields obtained was extended for reactions of diiodination (entries 6 to 9) and for reactions of monoiodination (entries 10 to 15). In general, diiodinated and monoiodinated aromatic and heteroaromatic compounds were produced in considerable yields.

## CONCLUSION

A balance between amounts of the reagents and the yields obtained was carried out for the reaction of iodination of aromatic organic compounds using $I_2$ and $H_2O_2$ 30% in water at 50 °C and interesting iodinated molecules were produced in good yields.

## ACKNOWLEDGEMENTS

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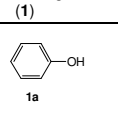
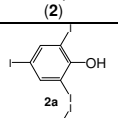
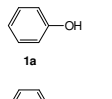
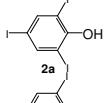
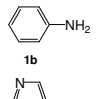
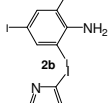
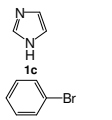
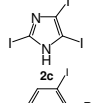
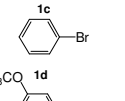
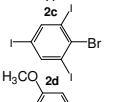
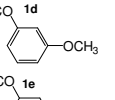
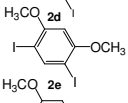
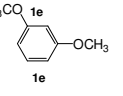
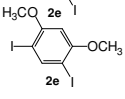
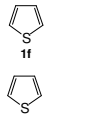
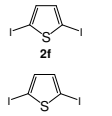
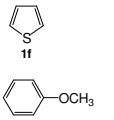
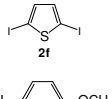
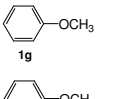
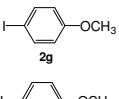
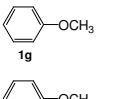
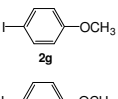
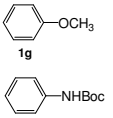
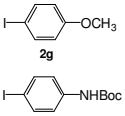
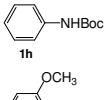
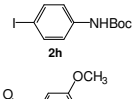
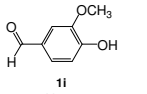
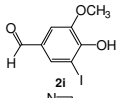
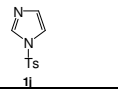
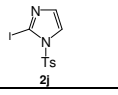
## REFERENCES

[1] Gallo, R. D. C.; Gebara, K. S.; Muzzi, R. M.; Raminelli, C. *J. Braz. Chem. Soc.* **2010**, *21*, 770-774.

**Table 1.** Synthesis of iodinated aromatic and heteroaromatic compounds (**2**).[a]

| Entry | Aromatic reagent (**1**) | Iodinated product (**2**) | Equivs. of $I_2$ / $H_2O_2$ | Isolated yield (%) |
|---|---|---|---|---|
| 1 |  **1a** |  **2a** | 1.5 / 3 | 65 |
| 2 |  **1a** |  **2a** | 2 / 4 | 83 |
| 3 |  **1b** |  **2b** | 2 / 4 | 80 |
| 4 |  **1c** |  **2c** | 2 / 4 | 97 |
| 5 |  **1d** |  **2d** | 2 / 4 | 0 |
| 6 |  **1e** |  **2e** | 1 / 2 | 93 |
| 7 |  **1e** |  **2e** | 2 / 4 | 96 |
| 8 |  **1f** |  **2f** | 1 / 2 | 32 |
| 9 |  **1f** |  **2f** | 2 / 4 | 90 |
| 10 |  **1g** |  **2g** | 0.5 / 1 | traces |
| 11 |  **1g** |  **2g** | 1 / 2 | 50 |
| 12 |  **1g** |  **2g** | 2 / 4 | 97 |
| 13 |  **1h** |  **2h** | 2 / 4 | 82 |
| 14 |  **1i** |  **2i** | 2 / 4 | 90 |
| 15 |  **1j** |  **2j** | 2 / 4 | 70 |

[a] Reaction conditions: 2 mmol of **1**, the indicated amount of $I_2$, the indicated amount of $H_2O_2$ 30% and 10 mL of $H_2O$ were stirred at 50 °C for 24 h.