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Abstract

Late-Stage Oxygenation towards the Preparation of Metabolites of Agrochemical Active Ingredients †

Duarte B. Clemente [1,2,*], Carlos M. Monteiro [3] and Jaime A. S. Coelho [1]

[1] Centro de Química Estrutural, Institute of Molecular Sciences, Universidade de Lisboa, 1049-001 Lisbon, Portugal
[2] Department of Chemistry and Biochemistry, Faculdade de Ciências, Universidade de Lisboa, 1049-001 Lisbon, Portugal
[3] ASCENZA Agro, S.A., Screening and Synthesis Laboratory, 2910-440 Setúbal, Portugal
* Correspondence: duarteclemente@alunos.fc.ul.pt
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Abstract: The development of plant protection products requires the safety profile analysis of active ingredients (AIs). This includes the toxicity determination of AI metabolites. A very common phase-one metabolism reaction is C-oxygenation catalyzed by cytochrome P450 enzymes. Thus, the synthesis of oxygenated AI metabolites is of great importance to agrochemical producing companies, namely ASCENZA Agro, for safety evaluation purposes. Herein, we describe the progress towards the synthesis of hydroxylated aromatic metabolites of several AIs using methods described by Tobias Ritter and co-workers. These methods allow the late-stage oxygenation of the aromatic and benzylic positions by generating mesylate derivatives with bis(methanesulfonyl) peroxide as an oxidant, followed by conversion to the corresponding phenols.

Keywords: late-stage; oxygenation; metabolites; agrochemical active ingredients

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