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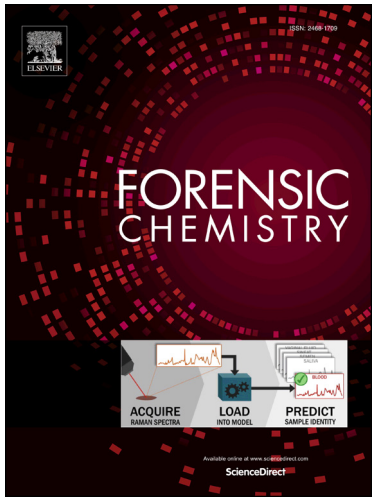

The Synthesis and Investigation of Impurities found in Clandestine Laboratories: Baeyer-Villiger Route Part II; Synthesis of Phenyl-2-propanone (P2P) analogues from Substituted Benzaldehydes

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The Synthesis and Investigation of Impurities found in Clandestine Laboratories: Baeyer-Villiger Route Part II; Synthesis of Phenyl-2-propanone (P2P) analogues from Substituted Benzaldehydes

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Abstract

We have previously reported phenylpropan-2-one (most commonly known as phenyl-2-propanone, P2P) and methamphetamine derived by-products formed in the Baeyer-Villiger route starting from benzaldehyde. This route is a three step synthesis to P2P; an aldol condensation of benzaldehyde and methyl ethyl ketone (MEK), a Baeyer-Villiger reaction and a subsequent ester hydrolysis. We now report on our investigations into the synthesis of P2P analogues from substituted benzaldehydes via the Baeyer-Villiger route. When strong electron donating substituents are present in the three position of a substituted benzaldehyde (e.g. 3-methoxy and 3,4-methylenedioxy), the resulting aldol reaction is very sensitive to the amount of hydrogen chloride present due to the occurrence of a competing cyclization side reaction yielding various indenes by-products. In contrast, substrates bearing electron-withdrawing substituents react poorly under the Baeyer-Villiger reaction conditions described in this paper. Several new compounds were identified, namely esters **4c**, **f** and **g**, amongst the known P2P precursors and derivatives. In addition, this work identifies several new by-products in the Baeyer-Villiger route namely **6**, **10**, **13**, **14**, **15** and **21**; we also report the analytical data for various analogues prepared by this method and this is of value to forensic analysts.

Keywords

Baeyer-Villiger, aldol, amphetamine type stimulants, P2P.

Introduction

Phenylpropan-2-one (most commonly known as phenyl-2-propanone, P2P) **5a** is a key intermediate molecule synthesized *en route* in the clandestine production of amphetamine type stimulants (ATS) [1-3]. P2P **5a** may be manufactured using: hydrolysis of α-