

CHELSIE BLAKE & ANDREAS BAUR, Department of Natural Sciences, Fairmont State University, Fairmont, WV. GC-MS method development for the photochemical copper-mediated decarboxylation of 4-fluorobenzoic acid

Photochemical copper-mediated decarboxylative coupling reactions of benzoic acids have been shown to be useful for the synthesis of substituted arenes. However, in contrast to thermal copper-mediated decarboxylation reactions, there are no mechanistic nor kinetic studies published. This project aimed to develop a sampling methodology for the model reaction of 4-fluorobenzoic acid and copper(II) triflate in acetonitrile under LED irradiation to yield 4-fluorobenzene, with the goal to obtain time-course data through GCMS analysis. The optimized protocol includes the use of an internal standard, trifluoromethylbenzene, filtration through silica gel with ethyl acetate, and a split injection. Derivatization with N-tert-butyldimethylsilyl-N-methyl-trifluoroacetamide gave mixed results due to the loss of volatile fluorine-containing analytes. This research was made possible by WV Higher Education Policy Commission, STaR Division, and Fairmont State University (Falcon Mini-grant 2025/2026).