Green Mechanochemical One-Pot Isoxazoline Synthesis With TPGS-750-M Micelle

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Isoxazolines are important heterocycles often found in various pharmaceuticals, but many reactions that produce them are inefficient and use chlorinated solvents, which are potent pollutants. However, a micelle, TPGS-750-M, can be used in an aqueous solvent to dissolve reactants and more efficiently produce a specific isoxazoline derivative from methyl acrylate and 4-methoxybenzaldehyde (p-anisaldehyde.) This micelle can be extracted from solution and recycled due to its specific head/tail structure, which saves resources and aligns with the principles of green chemistry. The reaction of focus is a two-step reaction with an oxime intermediate. It is also a one-pot synthesis, which simplifies subsequent isolation and purification. Mechanochemical methods show promise in optimizing the first step of the reaction to around ~83% efficiency. The primary oxidant, Oxone™, was specifically used alongside other benign salts to minimize environmental impact. HNMR analysis reveals that this reaction has an efficiency of ~42% relative to a baseline of 0-20%.

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