Title:	A Primary Amide-Functionalized Heterogeneous Catalyst for the Synthesis of Coumarin-3-carboxylic Acids via a Tandem Reaction
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Abstract:	A crystalline primary amide-based bifunctional heterogeneous catalyst, {[Cd2(2-BPXG)(Fum)2(H2O)2]·2H2O}n (1) (where, 2-BPXG = 2,2′-((1,4-phenylenebis(methylene))bis((pyridin-2-ylmethyl)azanediyl)) diacetamide and Fum = fumarate), has been developed for the one-pot synthesis of a series of potentially biologically active coumarin-3-carboxylic acids at room temperature via a Knoevenagel-intramolecular cyclization tandem reaction. Catalyst 1 is prepared at room temperature from a one-pot self-assembly process in 81% yield and high purity within a few hours and has a ladder-like polymeric architecture based on single-crystal X-ray diffraction. Additional characterization of 1 includes elemental analysis, infrared spectroscopy, thermogravimetric analysis, and powder X-ray diffraction. Based on the optimized conditions, it is determined that 1 is highly efficient (conditions: 2 mol % catalyst, 3 h, and 26–28 °C in methanol) for this reaction. Its recyclability up to five cycles without significant loss of activity and structural integrity is also demonstrated. Using both electron-donating and electron-withdrawing substituents on the salicylaldehyde substrate, seven different derivatives of coumarin-3-carboxylic acid were made. Additionally, the monoamine oxidase (MAO) inhibitor, coumarin-3-phenylcarboxamide, has also been synthesized from coumarin-3-carboxylic acid obtained in the catalysis process. A detailed mechanism of action is also provided.
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