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Data article

Lipase catalyzed synthesis of antimicrobial andrographolide derivatives

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ABSTRACT

In this data article we describe screening of various lipases for the regioselective acylation of Andrographolide. Each lipase was screened with seven acyl donors. Amano lipase AK from *Pseudomonas fluorescens* was used for the synthesis of two new acylated andrographolide derivatives. Two new compounds, andrographolide-14-propionate and andrographolide-14-caproate were characterized by various spectral studies. These two derivatives showed more antimicrobial activity than andrographolide.

Specifications table

Subject area	Chemistry
More specific subject area	Lipase-catalyzed acylation
Type of data	Table, experimental procedure, NMR spectra

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How data was acquired	NMR (Varian spectrometer-400), High Resolution Mass Spectrometry (Thermo Scientific Q Exactive Quadrupole-Orbitrap Mass Spectrometer)
Data format	Analyzed
Experimental factors	Lipase-catalyzed derivatives were purified and analyzed by HPLC, ESI-HRMS, and NMR.
Experimental features	Regio-selective enzymatic acylation of Andrographilide
Data source location	CSIR-National Chemical Laboratory, Pune
Data accessibility	Data is present in this article.
Related research article	*"in press."*

Value of the data

- The data provide screening results for regio-selective acylation of Andrographolide by using various commercial lipases with various acyl donors.
- In this study we optimized the reaction conditions for Andrographolide acylation by using Amano lipase AK *P. fluorescens lipase* with various acyl donors.
- This study yields structural characterization data of two new compounds: andrographolide-14-propionate and andrographolide-14-caproate.
- The synthesized Andrographolide derivatives can be used as antimicrobial agents. Derivatives were more potent antimicrobial agents when compared to Andrographolide (in the related manuscript).

1. Data

Data present in this paper describe the screening of commercially available lipases for the synthesis of 14-acylated andrographolide derivatives (Table 1).

HPLC analysis was performed by using Waters HPLC system with UV–vis detector at 235 nm. Analytical X-Bridge C_{18} column (4.6 × 250 mm, 5 µm) at a flow rate of 1 mL/min. with gradient solvent programme of Acetonitrile (ACN) and water (H_2O). HPLC grade solvents were purchased from Sigma Aldrich (USA). The substrate conversion and initial reaction rate (V_0) were calculated from the HPLC data (Fig. 1).

Characterization of andrographolide-14-propionate (Fig. S1a-d) and andrographolide-14- caproate (Fig. S2a-d): NMR (^1H, ^{13}C, DEPT) spectra were recorded on Varian spectrometer (400 MHz) and chemical shift values were reported in ppm with respect to the residual solvent signal as the reference. HRMS data were collected on Thermo Scientific Q Exactive Quadrupole-Orbitrap Mass Spectrometer. IR spectra were recorded on Perkin Elmer FT-IR spectrophotometer in $CHCl_3$ and optical rotations were determined on JASCO (P-2000), polarimeter using 10 mm cell (*c* in gm/100 ml unit). Acylation position was determined by comparison of the chemical shifts of the acylated product with andrographolide. The structure of products formed was confirmed by comparing with earlier reports [1,2].

Zeiss Axiovert apotome microscope equipped with an AxioCam camera and oil-immersion objective lens (64x) was employed to record the images and were processed with Axiovision 4.7 software. (Fig. 2A in main manuscript) Leica Stereoscan 440 was operated at an accelerating voltage of 15 kV with pressure 5.587E-4 Pa, current 0.14 nA and WD 9.9–10.0 mm det EDT. The pre-scanned samples were sputter coated with 10 nm thick layers of gold nanoparticles by using a Polaron SC 6420 sputter coater. The neat and irradiated samples were sputter coated without any pre-treatment or sample preparation (Fig. 2B in main manuscript).

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