

Regioselective enzymatic hydrolysis of hexa-*O*-acetyl-lactal in a green non-aqueous medium

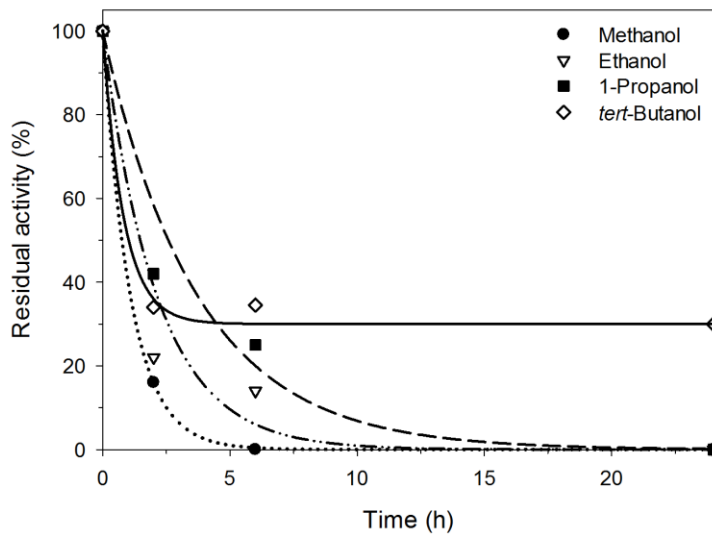
Teodora Bavaro, Pamela Torres-Salas, Daniela Ubiali and Marco Terreni

SUPPLEMENTARY INFORMATION

TABLE OF CONTENTS

1	Stability of RML-OAg in alcohols (7% water v/v)	S3
2	Analytical characterization of penta-<i>O</i>-acetyl-3-hydroxylactal (2)	S4

1. Stability of RML-OAg in alcohols (7% water v/v)



Stability of immobilized RML on octyl-agarose (RML-OAg) in alcohols (7% water v/v). For experimental details, see stability assay procedure in the main text.

2. Analytical characterization of penta-*O*-acetyl-3-hydroxylactal (2)

General methods

Nuclear Magnetic Resonance (NMR): ^1H spectra was recorded in CDCl_3 at 400.1 MHz on a Bruker AVANCE 400 Spectrometer (Bruker, Karlsruhe, Germany) equipped with a Topspin software package on a workstation running Windows operating system. Chemical shifts (δ) are given in ppm, and were referenced to the solvent signals (δ_{H} 7.26, δ_{C} 77.00). Signal multiplicities are abbreviated as follows: s, singlet; d, doublet; t, triplet; m, multiplet. Spectra analyses were carried out using iNMR reader software (www.inmr.net) on an Apple computer.

Mass Spectrometry (MS): Mass spectra were recorded on a LCQ-DECA Thermo Finnigan Spectrometer according to the method of ionization ESI (Electron Spray Ionization) with an ionic source by the software Xcalibur 1.3 (Thermo-Finnigan, St. Jose, CA, USA). For sample injection, a flow of 5 μs l/min was used. Analyses were run under positive modality and the experimental conditions are: voltage of the source 5.0 kVs, voltage of the capillary 14 V, flow of the gas 35 (arbitrary unity), temperature 200 °C.

6,2',3',4',6'-Penta-*O*-acetyl-3-hydroxylactal (2): ^1H NMR (400 MHz, CDCl_3): δ = 6.40 (d, J = 6.00 Hz, 1 H, 1-H), 5.37 (d, J = 3.32 Hz, 1 H, 4'-H), 5.23 (t, J = 8.00 Hz, 1 H, 2'-H), 5.02 (dd, 1 H, 3'-H), 4.78 (dd, 1 H, 2-H), 4.59 (d, J = 7.9 Hz, 1 H, 1'-H), 4.50 (m, 1 H, 3-H), 4.18–4.15 (m, 2 H, 6a-, 6'b-H), 4.10–4.02 (m, 2 H, 6'a-, 6b-H), 4.00 (m, 1 H, 5'-H), 3.98 (m, 1 H, 5-H), 3.65 (m, 1 H, 4-H), 2.00-2.18 (5 s, 15 H, COCH_3) ppm.

MS (ESI) calcd for $[\text{C}_{22}\text{H}_{30}\text{O}_{14} + \text{Na}]^+$ 541.45, found 541.20.