Data in Brief 4 (2015) 66–74

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

# Synthesis of biotinylated probes of artemisinin for affinity labeling

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ARTICLE INFO

*Article history:*
Received 22 April 2015
Received in revised form
26 April 2015
Accepted 27 April 2015
Available online 6 May 2015

*Keywords:*
Synthesis
Biotinylated probes
Artemisinin
Affinity labeling

ABSTRACT

In this data article, we described the synthetic routes to four biotinylated probes (**2**, **3**, **4**, and **5**) of artemisinin and the associated experimental procedures. We also provided the physical data for the synthesized compounds. These synthesized biotinylated probes of artemisinin are useful molecular tools for the affinity-labeling study of target receptor proteins of artemisinin in tropical pathogens such as *Trypanosoma, Leishmania, and Schistosoma*. The data provided herein are related to "Biotinylated probes of artemisinin with labeling affinity toward *Trypanosoma brucei brucei* target proteins", by Konziase (Anal. Biochem. (2015)).



## Specifications table

| | |
|---|---|
| Subject area | Organic chemistry |
| More specific subject area | Organic synthesis |
| Type of data | Synthetic schemes, experimental procedures, physical data |

DOI of original article: http://dx.doi.org/10.1016/j.ab.2015.04.020

*Abbreviations:* *m/z*, mass-to-charge ratio; DPPA, diphenylphosphoryl azide; $Et_2O$, diethyl ether; EtOAc, ethyl acetate; $Et_3N$, triethyl amine; MeOH, methanol; NaOMe, sodium methoxide; THF, tetrahydrofuran

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http://dx.doi.org/10.1016/j.dib.2015.04.017

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|---|---|
| How data was acquired | Chemical reactions; normal phase column chromatography; NMR spectroscopy: JNM-GX-500 (JEOL), Lambda 500 (JEOL), Inova 600 (Varian); mass spectroscopy: JMS SX-102 (JEOL); IR spectroscopy: FT-IR-5300 (JASCO); polarimetry: DIP-370 (JASCO) |
| Data format | Analyzed, text, schemes |
| Experimental factors | N/A |
| Experimental features | Chemical reactions were performed under argon gas unless otherwise indicated; the diazirine-containing probes were synthesized in brown opaque chemical flasks or transparent chemical flasks wrapped with aluminium foil due to photosensitivity. |
| Data source location | Osaka, Japan |
| Data accessibility | Data are available with this article |

## Value of the data

- To reproduce all the experiments described in the research article ref [1].
- To detect and isolate trypanosomal candidate target proteins of artemisinin.
- To study the target receptors of artemisinin in *Leishmania* or *Schistosoma*.

## 1. Materials and methods

### 1.1. General

$^{1}$H-NMR and $^{13}$C-NMR spectra in $CDCl_3$ or $CD_3OD$ with TMS as the internal standard were recorded using a JNM-GX-500 or Lambda 500 (JEOL, Tokyo, Japan) NMR spectrometer operating at 500 MHz and 125 MHz, respectively. 2D NMR data in $CDCl_3$ were recorded using a Varian Inova 600 (Varian, Tokyo, Japan) NMR spectrometer operating at 600 MHz. Chemical shifts ($\delta$) were reported in parts per million (ppm) and the multiplicities were designated as follows: s (singlet), d (doublet), t (triplet), m (multiplet), dd (doublet of doublets), ddd (doublet of doublet of doublets), brd (broad doublet), t-like (triplet like), dt (doublet of triplets). The coupling constants ($J$) were reported in Hz. Fast atom bombardment (FAB) and high-resolution fast atom bombardment (HR-FAB) mass spectra were recorded with a JMS SX-102 (JEOL, Tokyo, Japan) spectrometer in positive ion mode using magic bullet (5:1 dithiothreitol/dithioerythritol; Tokyo Kasei Kogyo) or *m*-nitrobenzyl alcohol as the matrix. Infrared (IR) spectra were recorded by a diffusion-reflection method on KBr powder using an FT-IR-5300 (JASCO, Tokyo, Japan) spectrometer. Shoulder bands in the IR spectra were designated by sh. Optical rotations were measured in a 0.5 dm length cell with a DIP-370 (JASCO, Tokyo, Japan) digital polarimeter. For column chromatography, silica gel (Fuji Sylisia BW-200 or Merck 60–230 mesh) and octadecyl silane ODS (Cosmosil 75$C_{18}$ OPN, Nacalai-Tesque) were used. Chemical reactions were performed under Ar gas unless otherwise indicated. TLC analyses were performed using normal-phase pre-coated plates (Kiesel gel 60$F_{254}$, Merck) and reversed-phase high-performance thin-layer chromatography (HPTLC) plates (RP-18 $WF_{254S}$, Merck). The spots on the thin-layer chromatograms were detected under UV light at 254 and 366 nm and visualized with either *p*-anisaldehyde/$H_2SO_4$ (5 mL of AcOH, 25 mL of *c*-$H_2SO_4$, 425 mL of EtOH, and 25 mL of water) or phosphomolybdic acid (5 g in 100 mL of EtOH) spraying reagents and subsequent heating.

### 1.2. Synthetic methods

By following the synthetic routes described here below, we successfully synthesized four biotinylated probes of artemisinin that were used as molecular tools for the affinity labeling of *Trypanosoma brucei brucei* target proteins [1].