Supplementary Data

α -D-Glucopyranosyl-(1 \rightarrow 2)-[6-O-(L-tryptophanyl)- β -D-fructofuranoside]

Kwaku Kyeremeh ^{1,*}, Samuel Kwain ¹, Gilbert Mawuli Tetevi ¹, Anil Sazak Camas ², Mustafa Camas ², Aboagye Kwarteng Dofuor ³, Hai Deng ⁴ and Marcel Jaspars ⁴

- ¹ Marine and Plant Research Laboratory of Ghana, Department of Chemistry, School of Physical and Mathematical Sciences, University of Ghana, P.O. Box LG 56, Legon-Accra, Ghana; kwainsamuel75@gmail.com (S.K.); gilberttet@gmail.com (G.M.T.)
- ² Department of Bioengineering, Munzur University, 62000 Tunceli, Turkey; anilsazak@gmail.com (A.S.C.); mustafacamas@gmail.com (M.C.)
- ³ Department of Biochemistry, Cell and Molecular Biology, University of Ghana, P. O. Box LG 54, Legon-Accra, Ghana; akdofuor@st.ug.edu.gh
- ⁴ Marine Biodiscovery Centre, Department of Chemistry, University of Aberdeen, Old Aberdeen, AB24 3UE, Scotland, UK; h.deng@abdn.ac.uk (H.D.); m.jaspars@abdn.ac.uk (M.J.)
- * Correspondence: kkyeremeh@ug.edu.gh; Tel.: +2-3320-789-1320

Received: 13 May 2019; Accepted: 14 June 2019; Published: 16 June 2019

Table of Contents

Figure S1. HRESI-LC-MS data for pure Tortomycoglycoside (1) shows [M+H] ⁺ , [M+Na] ⁺ , base peak and less abundant fragments
Figure S2. Proposed plausible structures for low abundance mass spectrometry fragments of Tortomycoglycoside (1)
Figure S3. UV spectrum of Tortomycoglycoside (1) in 30/70 mixture of water and acetonitrile5
Figure S4. ¹³ C-NMR spectrum of Tortomycoglycoside (1) in DMSO-d66
Figure S5. ¹ H-NMR spectrum of Tortomycoglycoside (1) in DMSO-d67
Figure S6. HSQC spectrum of Tortomycoglycoside (1) in DMSO-d6
Figure S7. COSY spectrum of Tortomycoglycoside (1) in DMSO-d69
Figure S8. HMBC spectrum of Tortomycoglycoside (1) in DMSO-d610
Figure S9. TOCSY spectrum of Tortomycoglycoside (1) in DMSO-d611
Figure S10. T-ROESY spectrum of Tortomycoglycoside (1) in DMSO-d612
Figure S11. 1D-TOCSY irradiation of H-1' in DMSO-d613
Figure S12. 1D-TOCSY irradiation of H-3" in DMSO-d614
Table S1. Examples of Pathogenic and Non-pathogenic Mycobacteria species



Figure S1. HRESI-LC-MS data for pure Tortomycoglycoside (1) shows [M+H]⁺, [M+Na]⁺, base peak and less abundant fragments.



Figure S2. Proposed plausible structures for low abundance mass spectrometry fragments of Tortomycoglycoside (1).



Figure S3. UV spectrum of Tortomycoglycoside (1) in 30/70 mixture of water and acetonitrile.



Figure S4. ¹³C-NMR spectrum of Tortomycoglycoside (**1**) in DMSO-d6.



Figure S5. ¹H-NMR spectrum of Tortomycoglycoside (1) in DMSO-d6.



Figure S6. HSQC spectrum of Tortomycoglycoside (1) in DMSO-d6.



Figure S7. COSY spectrum of Tortomycoglycoside (1) in DMSO-d6.



Figure S8. HMBC spectrum of Tortomycoglycoside (1) in DMSO-d6.



Figure S9. TOCSY spectrum of Tortomycoglycoside (1) in DMSO-d6.



Figure S10. T-ROESY spectrum of Tortomycoglycoside (1) in DMSO-d6.

Figure S11. 1D-TOCSY irradiation of H-1' in DMSO-d6.

MYCOBACTERIUM-WB-SF4-FRESH SAMPLE-1Hirr.21.fid MYCOBACTERIUM-WB-SF4-FRESH SAMPLE-1Hirr H1'

5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 f1 (ppm)

M

w

Figure S12. 1D-TOCSY irradiation of H-3" in DMSO-d6.

MYCOBACTERIUM-WB-SF4-FRESH SAMPLE-1Hirr.22.fid MYCOBACTERIUM-WB-SF4-FRESH SAMPLE-1Hirr H3"



4.00 3.95 3.90 3.85 3.80 3.75 3.70 3.65 3.60 3.55 3.50 3.45 3.40 3.35 3.30 3.25 3.20 3.15 3.10 3.05 3.00 f1 (ppm)

Pathogenic	Non-pathogenic	Pathogenic	Non-pathogenic
Mycobacteria	Mycobacteria	Mycobacteria	Mycobacteria
M. tuberculosis	M. smegmatis	M. malmoense	
M. bovis	M. gordonae	M. caprae	
M. leprae	M. vaccae	M. celatum	
M. lepromatosis	M. aurum	M. neoaurum	
M. avium	M. flavescens	M. immunogenum	
M. abscessus	M. gastri	M. porcinum	
M. marinum	M. gilvum	M. interjectum	
M. kansasii	M. parafortuitum	M. indicus pranii	
M. fortuitum		M. senegalense	
M. chelonae		M. thermoresistible	
M. ulcerans		M. arupense	
M. africanum		M. phocaicum	
M. xenopi		M. farcinogenes	
M. scrofulaceum		M. colombiense	
M. phlei		M. obuense	
M. chimaera		M. septicum	
M. terrae		M. aubagnense	
M. simiae		M. intermedium	
M. canetti		M. bohemicum	
M. haemophilum			

Table S1. Examples of Pathogenic and Non-pathogenic Mycobacteria species.