

## **Supporting Information**

for

## A new analog of dihydroxybenzoic acid from *Saccharopolyspora* sp. KR21-0001

Rattiya Janthanom, Yuta Kikuchi, Hiroki Kanto, Tomoyasu Hirose, Arisu Tahara, Takahiro Ishii, Arinthip Thamchaipenet and Yuki Inahashi

Beilstein J. Org. Chem. 2024, 20, 497–503. doi:10.3762/bjoc.20.44

## Additional data and NMR spectra

License and Terms: This is a supporting information file under the terms of the Creative Commons Attribution License (<u>https://creativecommons.org/</u> <u>licenses/by/4.0</u>). Please note that the reuse, redistribution and reproduction in particular requires that the author(s) and source are credited and that individual graphics may be subject to special legal provisions.

## Table contents

Figure S1: <sup>1</sup>H NMR spectrum of KR21-0001A (1) in CD<sub>3</sub>OD Figure S2: <sup>13</sup>C NMR spectrum of KR21-0001A (1) in CD<sub>3</sub>OD Figure S3: HMBC spectrum of KR21-0001A (1) in CD<sub>3</sub>OD Figure S4: HSQC spectrum of KR21-0001A (1) in CD<sub>3</sub>OD Figure S5: <sup>1</sup>H,<sup>1</sup>H COSY spectrum of KR21-0001A (1) in CD<sub>3</sub>OD Figure S6: De-sulfurization and hydrolyzation of KR21-0001A (1) Figure S7: LC/MS analyses of the D-FDLA-derivatives Table S1: Physicochemical properties of KR21-0001A (1)



**Figure S1:** <sup>1</sup>H NMR spectrum of KR21-0001A (**1**) in CD<sub>3</sub>OD.



Figure S2: <sup>13</sup>C NMR spectrum of KR21-0001A (1) in CD<sub>3</sub>OD.



Figure S3: HMBC spectrum of KR21-0001A (1) in CD<sub>3</sub>OD.



Figure S4: HMQC spectrum of KR21-0001A (1) in CD<sub>3</sub>OD.



**Figure S5:** <sup>1</sup>H,<sup>1</sup>H COSY spectrum of KR21-0001A (**1**) in CD<sub>3</sub>OD.



Figure S6: De-sulfurization and hydrolyzation of KR21-0001A (1).



Figure S7: LC/MS analyses of the D-FDLA-derivatives.

Properties	KR21-0001A
Appearance	Yellow oil
Molecular formula	C <sub>12</sub> H <sub>13</sub> NO <sub>7</sub> S
Molecular weight	315
HR-ESI-MS ( <i>m/z</i> )	
Calcd.	316.0485 [M+H]⁺
Found	316.0484 [M+H]⁺
$UV_{max}^{MeOH} \lambda nm (\epsilon)$	215 (21389), 286 (10238)
$IR v cm^{-1}$	3247, 2920, 2847, 2520, 1720, 1652, 1605, 1543, 1450, 1428, 1373, 1291, 1223, 1170, 1147, 1044, 1024, 982, 964, 905, 823, 750
[α] <sub>D</sub> <sup>23</sup> ( <i>c</i> 0.1, MeOH)	-11.9
Soluble	MeOH, DMSO

 Table S1: Physicochemical properties of KR21-0001A (1).