

Supporting Information

for

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

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Additional data and NMR spectra

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

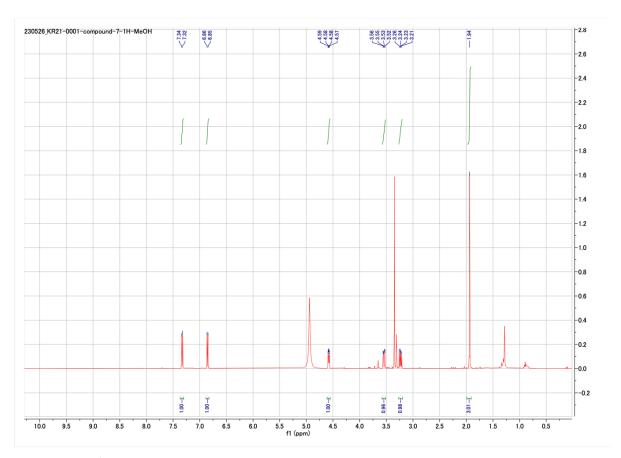


Figure S1: ¹H NMR spectrum of KR21-0001A (**1**) in CD₃OD.

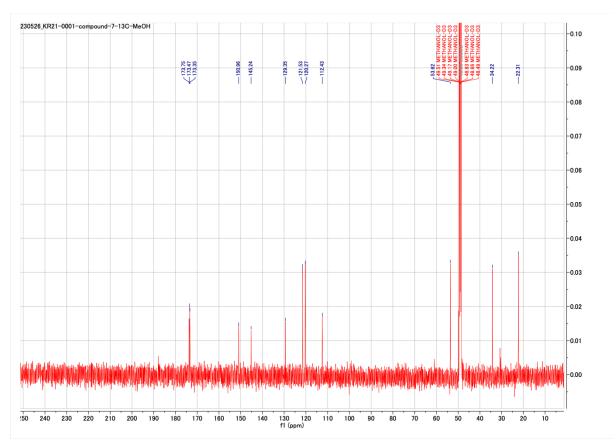


Figure S2: ¹³C NMR spectrum of KR21-0001A (1) in CD₃OD.

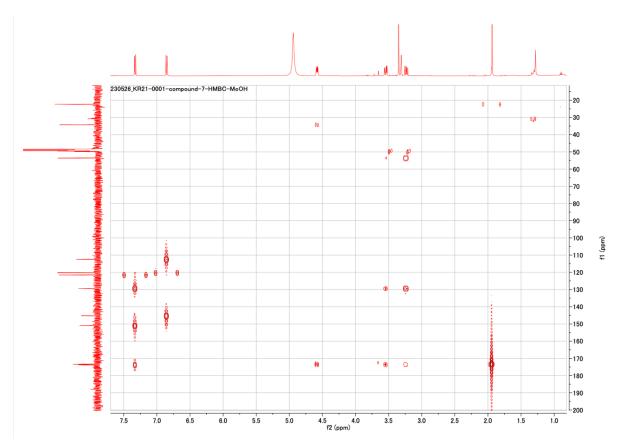


Figure S3: HMBC spectrum of KR21-0001A (1) in CD₃OD.

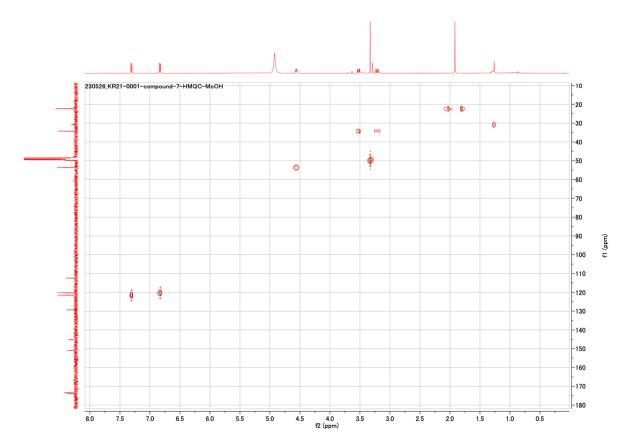


Figure S4: HMQC spectrum of KR21-0001A (1) in CD₃OD.

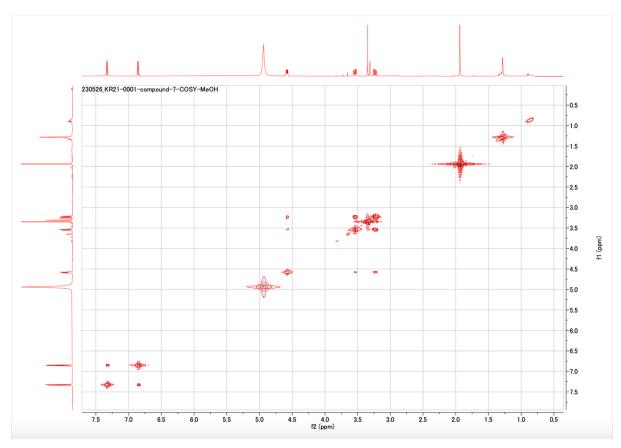


Figure S5: ¹H,¹H COSY spectrum of KR21-0001A (1) in CD₃OD.

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

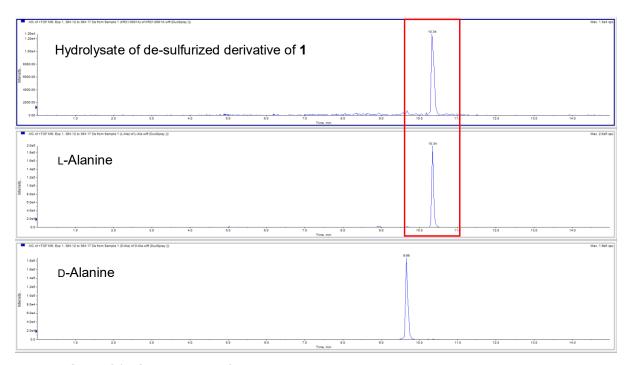


Figure S7: LC/MS analyses of the D-FDLA-derivatives.

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

Properties	KR21-0001A
Appearance	Yellow oil
Molecular formula	$C_{12}H_{13}NO_7S$
Molecular weight	315
HR-ESI-MS (m/z)	
Calcd.	316.0485 [M+H] ⁺
Found	316.0484 [M+H] ⁺
UV^{MeOH}_{max} λ nm (ϵ)	215 (21389), 286 (10238)
IR <i>v</i> cm ⁻¹	3247, 2920, 2847, 2520, 1720, 1652, 1605, 1543, 1450, 1428, 1373, 1291, 1223, 1170, 1147, 1044, 1024, 982, 964, 905, 823, 750
$[\alpha]_D^{23}$ (c 0.1, MeOH)	-11.9
Soluble	MeOH, DMSO