Supporting Information

for:

**Nostochopcerol, a new antibacterial monoacylglycerol from the edible cyanobacterium *Nostochopsis lobatus***

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**Preparation of linoleic acid from methyl linoleate**



Methyl linoleate (1.00 g) was dissolved in a 1:1 mixture of *t*-BuOH (5 mL) and 2N KOH (3 mL) and the solution was stirred for 3 h at an ambient temperature. After removing *t*-BuOH by a reduced pressure, the resulting residue was partitioned between EtOAc (20 mL) and 2N HCl (20 mL). The EtOAc layer was successively washed with water and brine and then slowly passed through anhydrous Na2SO4 to give linoleic acid (1.04 g), which was used for the next step without further purification.

**Chiral -linoleyl-**'**,-*O-*isopropylidene glycerols 2a and 2b**



To the solution of linoleic acid (112.8 mg, 0.402 mmol for **2a**; 122.2 mg, 0.436 mmol for **2b**) in CH2Cl2 (3 mL) was added (*R*)- or (*S*)-solketal (=2,2-dimethyl-1,3-dioxolane-4-methanol: 59 mg, 0.45 mmol; 1.1 eq.), 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (86.9 mg, 0.45 mmol: 1.1 eq.), and one crystal of *N*,*N*-dimethyl-4-aminopyridine (=DMAP: ~5 mg), and the reaction mixture was stirred for 2.5 h at an ambient temperature. After removing the solvent under reduced pressure, the resulting concentrate was passed through a short column of silica gel to remove DMAP and 1-(3-(dimethylamino)propyl)-3-ethylurea. The eluate was concentrated and purified by ODS-HPLC (solvent: 95%MeCN) to give 1-linoleoyl 2,3-*O*-isopropylidene-*sn*-glycerol **2a** (90.6 mg, 57.5%) and 3-linoleoyl 1,2-*O*-isopropylidene-*sn*-glycerol **2b** (125.0 mg, 72.7%), respectively.

1-Linoleoyl-2,3-*O*-isopropylidene-*sn*-glycerol (**2a**): []23.7D 0.69 (c 1.0, MeOH); HRESIMS: *m/z* 417.2969 [M+Na]+ (calcd. for C24H42NaO4, 417.2975). IR (ATR) max 3010, 2987, 2929, 2856, 1743, 1458, 1381, 1372, 1254sh, 1215,1161, 1087, 1059, 976, 844, 726 cm-1. 1H and 13C NMR data are essentially the same as **2b**.

3-Linoleoyl-1,2-*O*-isopropylidene-*sn*-glycerol (**2b**): []23.7D –0.64 (c 1.0, MeOH); HRESIMS: *m/z* 417.2961 [M+Na]+ (calcd. for C24H42NaO4, 417.2975). IR (ATR) max 3010, 2987, 2929, 2857, 1743, 1458, 1381, 1372, 1254sh, 1215,1161, 1085, 1058, 977, 844, 727 cm-1; 1H and 13C NMR, see Table S1.

**Chiral -linoleoylglycerols 3a and 3b**



-Linoleoyl-',-*O*-isopropylideneglycerol **2a** (5.9 mg, 15.0 mol) or **2b** (6.2 mg, 15.7 mol) was dissolved in 80% aqueous acetic acid (2 mL) and the solution was stirred occasionally in a sealed 6-mL screw-capped vial at 58–59 oC for 30 min. After removing the solvents by a stream of N2 gas, the resulting concentrate was purified by silica gel-HPLC (Cosmosil SL-II ** 1 x 25 cm) eluted with *n*-hexane-EtOAc (1:1) (4 mL/min) monitored at 210 nm to give 1-linoleoyl-*sn*-glycerol **3a** (4.3 mg, 81.1%) or 3-linoleoyl-*sn*-glycerol **3b** (5.1 mg, 91.6%). respectively.

1-Linoleoyl-*sn*-glycerol (**3a**): []22.2D +5.5 (c 0.30, MeOH); HRESIMS: *m/z* 377.2652 [M+Na]+ (calcd. for C21H38NaO4, 377.2662). IR (ATR) max 3404, 3010, 2927, 2856, 1740, 1458, 1378, 1243, 1177,1118, 1052, 726 cm-1; 1H and 13C NMR, see Table S1.

3-Linoleoyl-*sn*-glycerol (**3b**): []22.7D –5.5 (c 0.30, MeOH); HRESIMS: *m/z* 377.2642 [M+Na]+ (calcd. for C21H38NaO4, 417.2662). IR (ATR) max 3407, 3010, 2926, 2856, 1739, 1458, 1379, 1242, 1177,1120, 1053, 723 cm-1. 1H and 13C NMR data are essentially the same as **3a**.

**Table S1:** 1H (500 MHz) and 13C (125 MHz) NMR data for compounds **2b** and **3a** in CDCl3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **2b** | | **3a** | |
| Position | C | H*a* | C | H*a* |
| 1 | 173.6 |  | 173.4 |  |
| 2 | 34.1 | 2.34, t (7.6), 2H | 34.1 | 2.35, t (7.6), 2H |
| 3 | 24.9 | 1.62, brqui (7.3), 2H | 24.9 | 1.63, brqui (7.2), 2H |
| 4 | 29.081*b* | 1.30, ovl | 29.12 | 1.3068, ovl |
| 5 | 29.087*b* | 1.30, ovl | 29.06 | 1.3076, ovl |
| 6 | 29.1 | 1.30, ovl | 29.06 | 1.3076, ovl |
| 7 | 29.3*c* | 1.32, ovl, 2H | 29.3*i* | 1.31, ovl, 2H |
| 8 | 27.19*d* | 2.05, ovl, 2H | 27.18*j* | 2.05, ovl, 2H |
| 9 | 130.2*e* | 5.38*f*, m, 1H | 130.2*k* | 5.38*l*, m, 1H |
| 10 | 128.1*g* | 5.323*h*, m, 1H | 128.1*m* | 5.348*n*, m, 1H |
| 11 | 25.6 | 2.77, brt (6.6), 2H | 25.6 | 2.77, brt (6.6), 2H |
| 12 | 127.9*g* | 5.316*h*, m, 1H | 127.9*m* | 5.32*n*, m, 1H |
| 13 | 130.0*e* | 5.36*f*, ovl, 1H | 130.0*k* | 5.355*l*, ovl, 1H |
| 14 | 27.18*d* | 2.05, ovl, 2H | 27.15*j* | 2.05, ovl, 2H |
| 15 | 29.6*c* | 1.33, ovl, 2H | 29.6*i* | 1.34, ovl, 2H |
| 16 | 31.5 | 1.29, ovl, 2H | 31.5 | 1.29, ovl, 2H |
| 17 | 22.6 | 1.30, ovl, 2H | 22.5 | 1.302, ovl, 2H |
| 18 | 14.1 | 0.89, t (7.0), 3H | 14.0 | 0.89, t (6.9), 3H |
| *sn*-1 | 66.4 | 3.74, dd (6.2, 8.4), 1H | 63.3 | 3.60, dd (5.8, 11.4), 1H |
|  |  | 4.07, dd (6.4, 8.6), 1H |  | 3.70, dd (4.0, 11.5), 1H |
| *sn*-2 | 73.7 | 4.31, m, 1H | 70.3 | 3.93, m, 1H |
| *sn*-3 | 64.5 | 4.09, dd (6.0, 11.5), 1H | 65.2 | 4.15, dd (6.2, 11.7), 1H |
|  |  | 4.16, dd (4.7, 11.5), 1H |  | 4.21, dd (4.7, 11.7), 1H |
| acetonide-O*C*O | 109.8 |  |  |  |
| acetonide-CH3-1 | 26.7 | 1.43, s, 3H |  |  |
| acetonide-CH3-2 | 25.4 | 1.37, s, 3H |  |  |

*a*Chemical shift in ppm, multiplicity (*J* in Hz), integral. *b-u*Interchangeable.



1H NMR spectrum of nostochopcerol (**1**) (500 MHz, CD3OH)



13C NMR spectrum of nostochopcerol (**1**) (125 MHz, CD3OD)



COSY spectrum of nostochopcerol (**1**) (500 MHz, CD3OD)



HSQC spectrum of nostochopcerol (**1**) (500 MHz, CD3OD)



HMBC spectrum of nostochopcerol (**1**) (500 MHz, CD3OD)

1H NMR spectrum of 3-linoleoyl-1,2-*O*-isopropylidene-*sn*-glycerol (**2b**) (500 MHz, CDCl3)



13C NMR spectrum of 3-linoleoyl-1,2-*O*-isopropylidene-*sn*-glycerol (**2b**) (500 MHz, CDCl3)



COSY45 spectrum of 3-linoleoyl-1,2-*O*-isopropylidene-*sn*-glycerol (**2b**) (500 MHz, CDCl3)

HSQC spectrum of 3-linoleoyl-1,2-*O*-isopropylidene-*sn*-glycerol (**2b**) (500 MHz, CDCl3)



HMBC spectrum of 3-linoleoyl-1,2-*O*-isopropylidene-*sn*-glycerol (**2b**) (500 MHz, CDCl3)



1H NMR spectrum of 1-linoleoyl-*sn*-glycerol (**3a**) (500 MHz, CDCl3)



13C NMR spectrum of 1-linoleoyl-*sn*-glycerol (**3a**) (500 MHz, CDCl3)



COSY45 spectrum of 1-linoleoyl-*sn*-glycerol (**3a**) (500 MHz, CDCl3)



HSQC spectrum of 1-linoleoyl-*sn*-glycerol (**3a**) (500 MHz, CDCl3)



HMBC spectrum of 1-linoleoyl-*sn*-glycerol (**3a**) (500 MHz, CDCl3)