Supporting Information

General Experimental Procedures. NMR spectra were recorded on a Varian 300 spectrometer operating at 300 MHz for ^{1}H and at 75 MHz for ^{13}C NMR spectra, respectively. COSY and NOESY spectra were recorded with standard pulse set up in the Varian program. Chloroform-d_1 and methanol-d_4 were used as solvent and TMS as internal standard. The optical rotation was determined on a Perkin-Elmer 241 polaritmeter. *n*-Hexane, MeOH, MeCN, CH_2Cl_2, $CHCl_3$ and DMSO were all of HPLC grade from Merck (Darmstadt, Germany). D-Galactose and glycerol were of highest quality from Fluka (Buchs, Switzerland) and aqueous NaOH (50%) was obtained from J.T. Baker (Netherlands). Open-column chromatography was performed with silica gel 60 (63–200 μm, Merck). TLC: silica gel 60 F_{254} Al sheets (0.1 mm) (Merck), developed using 10% H_2SO_4 in MeOH followed by heating. Preparative HPLC was carried out using a Merck L-6200 intelligent pump equipped with a Merck L-4200 UV detector. Separations were performed on a RP-C_{18} column (particle size 5 μm; 250 × 20 mm i.d., Develosil ODS-HG-5, Nomura Chemical Co., Japan) protected with a guard cartridge (50 × 20 mm i.d.) packed with the same material as the column. Analytical HPLC was carried out on a SUMMIT/Dionex HPLC system (Dionex Denmark A/S, Denmark) equipped with a diode array detector (DAD) operating between 200–650 nm. Separations were performed on a LiChrospher 100 RP- C_{18} (particle size 5 μm; 244 × 4 mm i.d., Merck) column. High performance anion exchange chromatography coupled with pulsed amperometric detection (HPAEC-PAD) was carried out on a Dionex series 300DX ion chromatograph system using a CarboPac PA10 column (250 × 4 mm i.d., Dionex Denmark A/S, Denmark). Eluant 52 mM NaOH and flow rate 1.5 mL/min.

Extraction and Isolation: Dried and milled fruits of dog rose (1 kg) were sequentially extracted with *n*-hexane, CH_2Cl_2, MeOH and water. The dog rose powder was first submerged in *n*-hexane (2 L) overnight at room temperature, filtered and the powder washed with *n*-hexane (2 × 500 mL). The combined *n*-hexane solutions were evaporated to dryness under reduced pressure at below 40 °C. The powder was then submerged in CH_2Cl_2, MeOH and water, subsequently, following the same procedure as described above for extraction with *n*-hexane. The resulting *n*-hexane (30 g), CH_2Cl_2 (10 g), MeOH (35 g) and water extracts (125 g) were tested for inhibition of chemotaxis of human peripheral blood neutrophils *in vitro*. The activity was confined to the CH_2Cl_2 extract which was subjected to silica gel (400 g) open-column chromatography (column dimensions, 5 × 50 cm), eluting with a stepwise gradient of CH_2Cl_2–MeOH mixtures (100 mL 100:0, 100 mL 99:1, 100 mL 98:2, 150 mL 95:5, 150 mL 90:10, 450 mL 80:20, 950 mL 0:100) to give 20 fractions (fr. 1 to fr. 20, each fraction 100 mL). The individual fractions were concentrated *in vacuo* (below 40 °C) and tested for inhibition of chemotaxis of human peripheral blood neutrophils *in vitro*. The activity appeared to be confined to one major constituent in fr. 10–12 as shown by TLC (CH_2Cl_2–MeOH–H_2O, 70:30:3, R_f 0.46) and HPLC-DAD (see below). Fr. 10–12 (850 mg) was further separated by preparative HPLC on a RP-C_{18} column eluting with a stepwise MeCN–H_2O gradient (150 mL 25:75; 150 mL 50:50; 200 mL 60:40; 200 mL 70:30; 200 mL 80:20; 350 mL 90:10 and 400 mL 100:0, column temperature 35 °C, flow rate = 7 mL/min, UV detection at 203 nm, injection volume = 5 mL) to give 14 fractions (fr. 10–12.1 to fr. 10–12.14) of which only fr. 10–12.11 (t_R ~ 163–179 min, 1145–1255 mL, fraction volume = 110 mL) showed high activity. The active principle in fr. 10–12.11 was found to be confined to one compound that was obtained as a colorless oil (250 mg) and identified as (2*S*)-1,2-di-*O*-[(9*Z*,12*Z*,15*Z*)-octadeca-9,12,15-

trienoyl]-3-*O*-*β*-D-galactopyranosyl glycerol (**1**). The purity of the galactolipid **1** (> 98%) was determined by analytical HPLC-DAD using a LiChrospher RP-C_{18} column and eluting with a MeCN–20% MeCN (aq) gradient (0–10 min (0:100), 10–25 min (from 0:100 to 50:50), 25–55 min (from 50:50 to 100:0), 55–64 min (100:0), gradient linear programmed, column temperature 35 °C, flow rate = 1 mL/min, injection volume = 20 μl, UV detection at 203 nm, t_R (compound **1**) = 54 min). The structure of **1** was identified from the ^{1}H- and ^{13}C-NMR data (see Table I and Table II) and $[\alpha]_D$ ($[\alpha]_D^{26}$ –3.0° (*c* 0.4 $CHCl_3$)) and by comparison with literature data.[1–3] The structure of **1** was further confirmed by basic methanolysis and acidic hydrolysis. Basic methanolysis[2] yielded methyl linolenate as the only methyl ester as shown by GC-MS, whereas acid hydrolysis in 4 N HCl afforded D-galactose and glycerol as shown by HPAEC-PAD.

Table I. ^{1}H-NMR spectral data (300 MHz, $CDCl_3$ and CD_3OD, δ-values in ppm) for compound **1**.

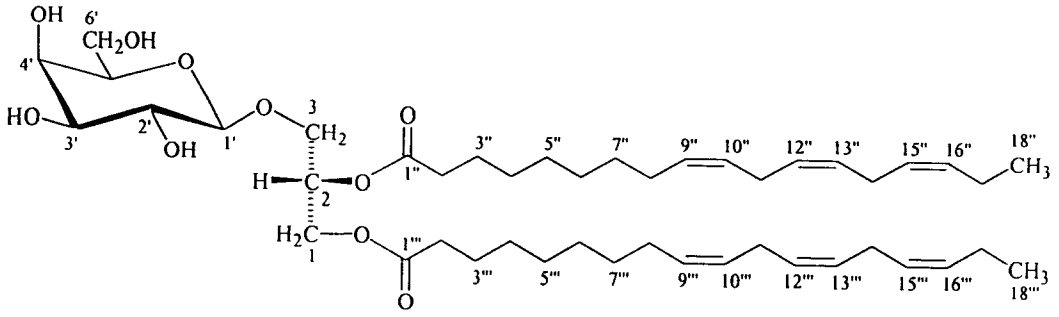
H	δ_H (multiplicity, *J* in Hz) in $CDCl_3$	δ_H (multiplicity, *J* in Hz) in CD_3OD
1'	4.24 (*d*, 6.8)	4.23 (*d*, 6.6)
2'	3.63 (*m*)	3.51 (*dd*, 6.6, 9.7)
3'	3.54 (*m*)	3.45 (*dd*, 2.1, 9.7)
4'	3.91 (*m*)	3.84 (*dd*, 0.5, 2.1)
5'	3.58 (*m*)	3.48 (*m*)
6'a	3.88 (*m*)	3.73 (*dd*, 6.6, 12.0)
6'b		3.75 (*dd*, 4.4, 12.0)
1a	4.22 (*dd*, 6.8, 12.0)	4.22 (*dd*, 6.9, 12.0)
1b	4.40 (*dd*, 2.0, 12,0)	4.43 (*br d*, 12.0)
2	5.28 (*m*)	5.27 (*m*)
3a	3.72 (*dd*, 6.0, 11.0)	3.71 (*dd*, 5.4, 11.0)
3b	3.99 (*m*)	3.98 (*dd*, 5.4, 10.8)
2",2'''	2.32 (*br t*, 7.0)	2.32 (*br t*, 7.0)
3",3'''	1.60 (*m*)	1.60 (*m*)
4"–7", 4'''–7'''	1.32 (*m*)	1.35 (*m*)
8",17'',8''',17'''	2.08 (*m*)	2.08 (*m*)
9",10",12",13'',15'',16'' 9''',10''',12''',13''',15''',16'''	5.36 (*m*)	5.35 (*m*)
11",14'', 11''', 14'''	2.81 (*br t*, 6.8)	2.82 (*br t*, 6.8)
18", 18'''	0.97 (*t*, 7.5)	0.98 (*t*, 7.5)

Abbreviations for multiplicity: *d* = doublet, *dd* = double doublet, *m* = multiplet, *t* = triplet. *br* = broad. Assignments based on ^{1}H-^{1}H-COSY and ^{1}H-^{1}H-NOESY NMR experiments.

Table II. ^{13}C-NMR spectral data (75 MHz, $CDCl_3$ and CD_3OD, δ-values in ppm) for compound **1**.

Assignments	Multiplicity*	δ_C ($CDCl_3$)	δ_C (CD_3OD)
C-1'	*d*	104.3	106.3
C-2'	*d*	71.6	73.3
C-3'	*d*	73.7	75.7
C-4'	*d*	69.5	71.1
C-5'	*d*	74.8	77.7
C-6'	*t*	62.4	63.3
C-1	*t*	63.1	64.9
C-2	*d*	70.4	72.7
C-3	*t*	68.4	69.6
C-1'', C-1'''	*s*	174.1, 173.7	176.1, 175.8
C-2'', C-2'''	*t*	34.5, 34.3	36.0, 35.8
C-3'', C-3'''	*t*	25.1[a]	26.8[a]
C-4'', C-4'''	*t*	29.8[b]	31.6[b]
C-5'', C-5'''	*t*	29.5[b]	31.2[b]
C-6'', C-6'''	*t*	29.4[b]	31.1[b]
C-7'', C-7'''	*t*	29.3[b]	31.0[b]
C-8'', C-8'''	*t*	27.4	29.0
C-9'', C-9'''	*d*	132.2[c]	133.8[c]
C-10'', C-10'''	*d*	130.4[c]	132.1[c]
C-11'', C-11'''	*t*	25.9[a]	27.4[a]
C-12'', C-12'''	*d*	128.6[c]	130.2[c]
C-13'', C-13'''	*d*	128.5[c]	130.2[c]
C-14'', C-14'''	*t*	25.8[a]	27.3[a]
C-15'', C-15'''	*d*	128.0[c]	129.9[c]
C-16'', C-16'''	*d*	127.3[c]	129.2[c]
C-17'', C-17'''	*t*	20.8	22.3
C-18'', C-18'''	*q*	14.5	15.5

*Multiplicity determined by DEPT and HETCOR-NMR experiments. Abbreviations for multiplicity: *s* = singlet, *d* = doublet, *t* = triplet, *q* = quartet. [a, b, c] In the same column: These assignments may be interchanged.



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References

1. Wegner, C.; Hamburger, M.; Kunert, O.; Haslinger, E. *Helv. Chim. Acta* **2000**, *83*, 1454–1464.
2. Murakami, A.; Nakamura, Y.; Koshimizu, K.; Ohigashi, H. *J. Agric. Food Chem.* **1995**, *43*, 2779–2783.
3. Olugbade, T. A.; Adesanya, S. A. *Phytochemistry* **2000**, *54*, 867–870.