

Supporting information

Anti-inflammatory, anti-angiogenetic and antiviral activities of dammarane-type triterpenoid saponins from the roots of *Panax notoginseng*

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General experimental procedures

Optical rotations were recorded on a JASCO P-1020 polarimeter (Jasco, Tokyo, Japan). UV spectra were recorded on a JASCO V-550 UV/Vis spectrophotometer (Jasco, Tokyo, Japan). IR spectra were determined on a JASCO FT/IR-480 plus Fourier transform infrared spectrometer (JASCO, Tokyo, Japan) using KBr pellets. HR-ESI-MS data were recorded on an Agilent 6210 MSD TOF mass spectrometer (Agilent technologies, CA, USA) and Waters Xevo G2 QToF (Waters, USA), The NMR spectra were recorded on AV-600/400/300 spectrometers (Bruker, fallanden, Switzerland). Analytical HPLC was performed on Agilent 1260 Infinity with a VWD detector (Agilent technologies, CA, USA) and an analytical column (COSMOSIL 5C18-MS-II, 5 μ m, 4.6 \times 250 mm). Preparative HPLC was performed on Agilent 1260 Infinity equipped with an UV detector (Agilent technologies, CA, USA) and a semi-preparative column (COSMOSIL 5C18-MS-II, 5 μ m, 10 \times 250 mm). Thin-layer chromatography (TLC) was performed using precoated silica gel plates (GF254, Qingdao, P. R. China), ODS (Daisogel, Japan) and Sephadex LH-20 (Pharmacia Biotec AB, Sweden).

Chemicals and Reagents

L-cysteine methyl ester hydrochlorid was purchased from Adamas Reagent Co., Ltd (Shanghai, China). *O*-Tolyl Isothiocyanate and monosaccharide standards were obtained from Macklin Co., Ltd (Shanghai, China). LPS (*E. coli*, 055: B5, L2880) and dimethyl sulphoxide (DMSO) were purchased from Sigma-Aldrich Co., Ltd (St Louis, MO, USA). Tricaine was obtained from Macklin (Shanghai, China). Methylene blue was provided by Meilunbio (Dalian, China). Dexamethasone (Dex) was from Tianxin (Guangzhou, China). RNAiso Plus, the PrimeScript[®] RT Reagent kit and TB Green[™] Premix Ex Taq[™] II were obtained from TaKaRa Biotechnology Co., Ltd (Shiga, Japan).

The crude extract of *P. notoginseng* was provided by Guangxi Wuzhou Pharmaceutical Group Co., Ltd.

Table S1 Primer sequence of qRT-PCR

Primer name	Primer sequence (5'→3')
β -actin –F	ATGGATGAGGAAATCGCTG
β -actin –R	ATGCCAACCATCACTCCCTG
IL-6 –F	AGACCGCTGCCTGTCTAAAA
IL-6 –R	TTTGATGTCGTTACCAGGA
TNF- α –F	GCTGGATCTTCAAAGTCGGGTGTA
TNF- α –R	TGTGAGTCTCAGCACACTTCCATC
NF- κ B –F	GAGCCCTTTGTGCAAGAGAC
NF- κ B –R	TGGGATACGTCCCTCCTGTTT
I κ B α –F	GGTGGAAAGACTCCTGAAAGC
I κ B α –R	TGTAGTTAGGGAAGGTAAGAATG
MyD88 –F	GAGGATGGTGGTGGTCATCT
MyD88 –R	CGACAGGGATTAGCCGTTTA
STAT3 –F	CCCTGGGACTAACTCTGGCA
STAT3 –R	AGAGGTCCTGGATTGGCCTC

Table S2 ¹H NMR data of compound **9** and **10** (pyridine-*d*₅, *J* in Hz)^a

No.	9	10	No.	9	10
1	1.53	1.55, 0.73	28	1.28 s	1.28 s
2	2.21, 1.85	2.21, 1.84	29	1.10 s	1.10 s
3	3.26 dd (11.7,4.6)	3.25 dd (11.9,4.5)	30	0.96 s	0.94 s
5	0.65 (11.3)	0.65 d (11.8)	C-3 sugars		
6	1.48, 1.36	1.59, 1.48	1'	4.92 d (7.5)	4.92 d (7.6)
7	1.46, 1.2	1.47, 1.19	2'	4.25	4.25
9	1.35	1.35	3'	4.16	4.25
11	1.98, 1.59	1.95, 1.52	4'	4.35	4.37
12	4.16	4.13	5'	3.94	3.93
13	1.97	1.97	6'	4.58, 4.49	4.57, 4.48
15	1.48, 1.03	1.52, 1.00	1''	5.37 d (7.6)	5.37 d (7.6)
16	2.21, 1.85	1.84, 1.34	2''	4.13	4.13
17	2.54	2.54	3''	4.33	4.33
18	0.95 s	0.95 s	4''	4.16	4.14
19	0.80 s	0.80 s	5''	3.94	3.93
20	-	-	6''	4.49, 4.35	4.48, 4.36
21	1.56 s	1.57 s	C-20 sugar		
22	2.38, 1.81	2.38, 1.81	1'''	5.07 d (7.5)	5.00 d (7.2)
23	2.51, 2.22	2.53, 2.25	2'''	3.98	4.41
24	5.28 t (7.2)	5.27 t (6.6)	3'''	4.25	4.18
26	1.64 s	1.63 s	4'''	4.16	4.29
27	1.62 s	1.61 s	5'''	4.29, 3.70 t (10.2)	4.28, 3.77 d (12.0)

a: 600 MHz; overlapped signals are reported without designating multiplicity

Table S3 ^{13}C NMR data of compound **9** and **10** (pyridine- d_5 , 600 MHz)

No.	9	10	No.	9	10
1	39.4	39.4	26	26.1	26.1
2	27.0	27.0	27	18.0	18.1
3	89.2	89.2	28	28.4	28.4
4	40.0	40.0	29	16.5	16.5
5	56.6	56.6	30	17.7	17.7
6	18.7	18.7	C-3 sugars		
7	35.4	35.4	1'	105.4	105.4
8	40.3	40.3	2'	83.6	83.6
9	50.4	50.4	3'	79.4	78.6
10	37.1	37.1	4'	71.9	72.0
11	31.1	31.1	5'	78.4	78.2
12	70.4	70.3	6'	63.1	63.1
13	49.7	49.7	1''	106.3	106.3
14	51.7	51.6	2''	77.4	77.4
15	31.0	31.0	3''	78.6	78.4
16	26.9	26.9	4''	71.8	71.8
17	52.0	51.8	5''	78.6	78.6
18	16.9	16.9	6''	62.9	62.9
19	16.2	16.3	C-20 sugars		
20	83.5	83.3	1'''	99.1	99.0
21	22.5	22.5	2'''	75.2	72.8
22	36.3	36.3	3'''	78.2	75.6
23	23.5	23.4	4'''	71.2	69.9
24	126.1	126.1	5'''	67.3	67.2
25	131.4	131.4			

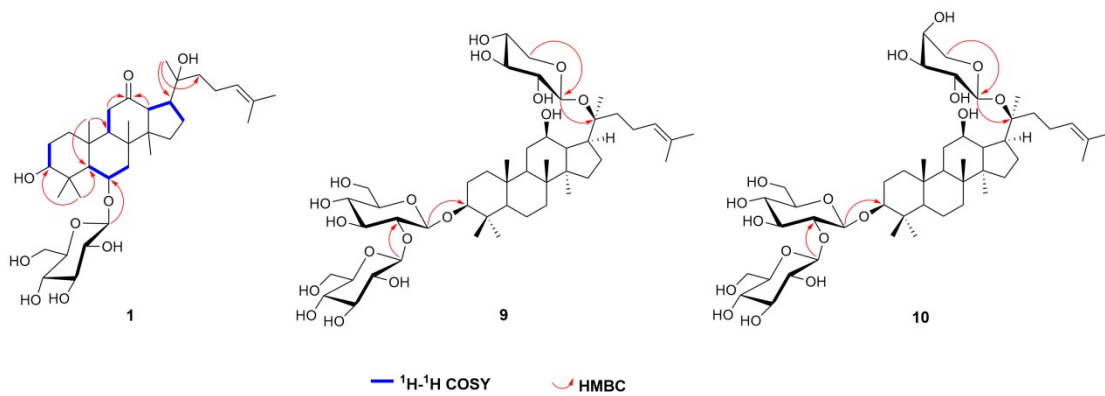


Figure S1. Key ^1H - ^1H COSY and HMBC correlations of **1**, **9** and **10**