2P-56

New Aromatic Compounds from the Stem Bark of *Bombax ceiba*

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Introduction

Bombax ceiba L. (Syn: *Bombax malabaricum* DC.), (Family: Bombacaceae), is a deciduous tree about 40 m tall. It is locally called as “Simal” in Nepal and distributed throughout Nepal, India, West China and Malaysia between 22-900 m.

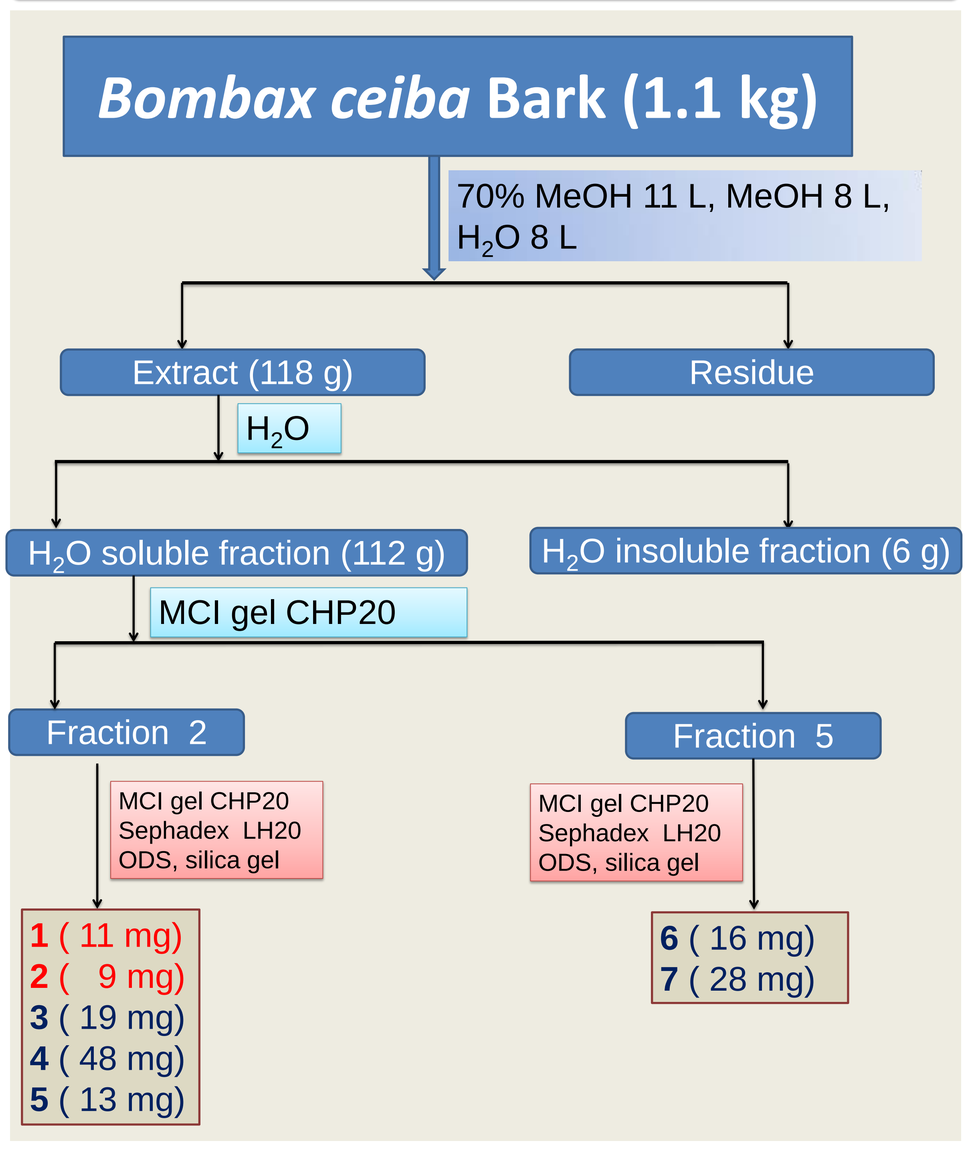
Traditionally in Nepal, barks are used in wound healing. Gum from bark is used as remedy for diarrhea, dysentery, influenza, blood vomiting and menorrhagia.

We have previously reported the phenolic compounds from the flowers of this plant.[1,2)] In present, we report the constituents from the bark. The shade dried stem bark of *B. ceiba* were extracted successively with 70% MeOH, MeOH and water. The combined extract was then subjected to repeated column chromatography on MCI gel CHP20P, ODS, Sephadex LH20 and silica gel to isolate compounds **1-7**.

Bombax ceiba plant

Bombax ceiba bark

Extraction and Isolation



Results and Discussion

The structures of two new aromatic compounds; simalin A (**1**) and simalin B (**2**) together with five known compounds; shamiminol (**3**), (-)-epicatechin-7-O-β-xylopyranoside (**4**), (-)-catechin-7-O-β-xylopyranoside (**5**), (+)-isolarisiresinol-9’-O-β-glucopyranoside (**6**) and (+)-lyoniresinol-9’-O-β-glucopyranoside (**7**) were elucidated on the basis of chemical and spectroscopic methods. Compounds **6** and **7** were isolated for the first time from *B. ceiba*. Compounds **4**, **5**, **6** and **7** showed potent antioxidant activity in the 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging test.

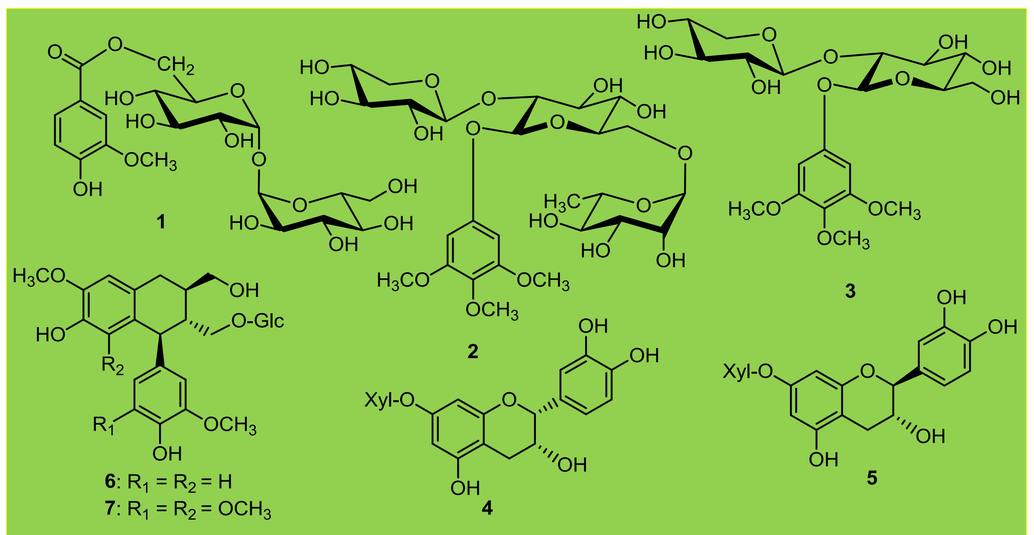


Figure 1. Structures of isolated compounds from *Bombx ceiba* bark.

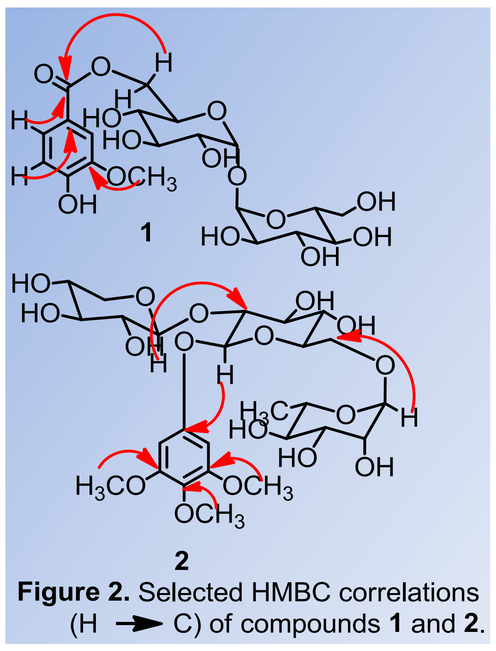


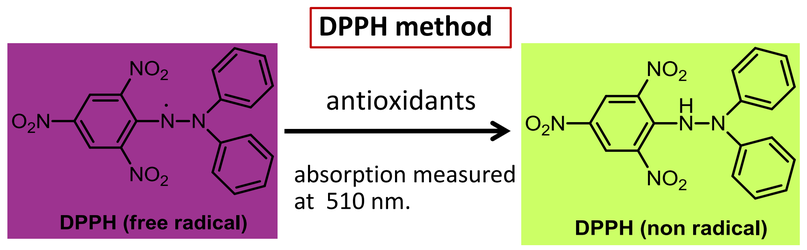
Figure 2. Selected HMBC correlations (H ➔ C) of compounds **1** and **2**.

***Simalin A* (1):** Colorless gum; $[\alpha]_D^{20}$ +80.4° (c 0.61, MeOH); HR-FAB-MS (positive mode) $[M+Na]^+$ at 515.1380 (Calcd. for $C_{20}H_{28}O_{14}$ Na, 515.1377).

***Simalin B* (2):** Colorless gum; $[\alpha]_D^{20}$ -47.1° (c 0.81, MeOH); HR-FAB-MS (positive mode) peak of $[M+Na]^+$ at 647.2181 (Calcd. for $C_{26}H_{40}O_{17}Na$, 647.2163).

Antioxidative activity

The antioxidant activity of compounds **1—7** was evaluated by DPPH free radical scavenging assay. Trolox was used as positive control with IC_{50} 121 μM. Among the tested compounds **4, 5, 6** and **7** showed significant scavenging activity (Table 2, Figure 2).



$$\text{Scavenging Effect (\%)} = \frac{(\text{Control absorbance} - \text{Test absorbance})}{\text{Control absorbance}} \times 100$$

Table 2. Free Radical Scavenging Effects on DPPH of Compounds **1—7.**

Compounds	IC_{50} (μM)
simalin A (**1**)	>1500
simalin B (**2**)	>1500
shamiminol (**3**)	>1500
(-)-epicatechin-7-*O*-β-xylopyranoside (**4**)	171
(-)-catechin-7-*O*-β-xylopyranoside (**5**)	158
(+)-isolarisiresinol-9`-*O*-β-glucopyranoside(**6**)	140
(+)-lyoniresinol-9`-*O*-β-glucopyranoside (**7**)	144
Trolox	121

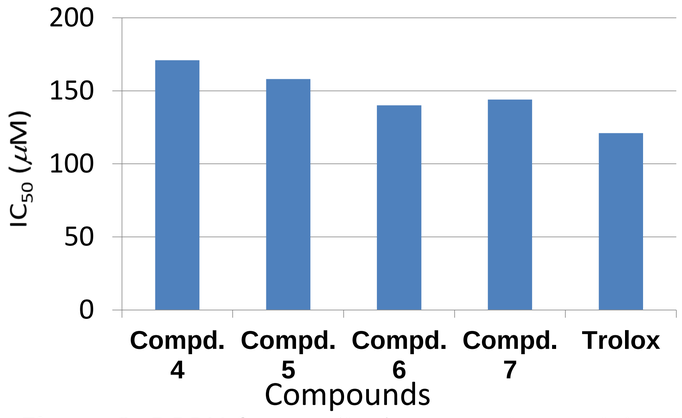


Figure 3. DPPH free radical scavenging activity of compounds **4**-**7** and Trolox.

Table 1. ^{1}H and ^{13}C NMR data of compounds **1** and **2** in CD_3OD

Position	Compound 1		Position	Compound 2	
	δ^1H (J in Hz)	δ^{13}C		δ^1H (J in Hz)	δ^{13}C
1		122.6	1		155.8
2	7.75, d (2.1)	113.7	2	6.42, s	97.3
3		148.8	3		154.8
4		152.9	4		134.9
5	6.85, d (7.9)	116.0	5		154.8
6	7.58, dd (2.1, 7.9)	125.2	6	6.42, s	97.3
7		168.1	3-OCH_3	3.81, s	56.8
3-OCH_3	3.90, s	56.5	4-OCH_3	3.70, s	61.2
Glc 1	5.12, d (3.7)	95.1[a]	5-OCH_3	3.81, s	56.8
Glc 2	3.53, dd (3.7, 9.8)	72.2	Glc 1	4.93, d (7.3)	102.0[a]
Glc 3	3.81-3.84	73.3[b]	Glc 2	3.57-3.59	83.7
Glc 4	3.40-3.47	71.6[c]	Glc 3	3.30-3.36	77.4[d]
Glc 5	4.15-4.18	74.6[d]	Glc 4	3.24-3.28	74.0
Glc 6	4.52, dd (2.1, 11.9)	65.0	Glc 5	3.30-3.36	77.7[d]
	4.40, dd (5.8, 11.9)		Glc 6	4.02, brd (9.5)	67.7
Glc 1’	5.12, d (3.7)	95.2[a]		3.63, brd (9.5)	
Glc 2’	3.53, dd (3.7, 9.8)	73.2[b]	Xyl 1	4.63, d (7.3)	106.3
Glc 3’	3.77-3.80	73.9	Xyl 2	4.49-4.50	75.7
Glc 4’	3.40-3.47	71.9[c]	Xyl 3	3.30-3.36	77.4
Glc 5’	3.82, ddd (3.9, 5.2, 9.8)	74.8[d]	Xyl 4	3.30-3.39	72.4[b]
Glc 6’	3.66, dd (5.2, 11.9)	62.6	Xyl 5	3.85, dd (5.2, 11.5)	67.2
	3.77-3.84			3.24-3.28	
			Rha 1	4.69, d (1.5)	101.9[a]
			Rha 2	3.57-3.59	70.1[c]
			Rha 3	3.57-3.59	70.2[c]
			Rha 4	3.30-3.39	72.1[b]
			Rha 5	3.57-3.59	69.8
			Rha 6	1.19, d (6.4)	17.9

[a, b, c, d] assignments may be reversed in the same column.

Acknowledgement

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References

1) Joshi, K.R., Devkota, H.P., Yahara, S., 2013. Chemical Analysis of Flowers of *Bombax ceiba* from Nepal. *Natural Product Communication*, **8**, 583-584.

2) Joshi, K.R., Devkota, H.P., Yahara, S., 2012. . Chemical Analysis on Flowers of *Bombax ceiba*. *The 59th Annual Meeting of the Japanese Society of Pharmacognosy*, September 17-18, Chiba, Japan.