(100 MHz, $CDCl_3$): 38.5 (C-1), 23.9 (C-2), 80.9 (C-3), 39.0 (C-4), 55.5 (C-5), 18.3 (C-6), 34.3 (C-7), 40.9 (C-8), 50.4 (C-9), 37.2 (C-10), 21.0 (C-11), 25.2 (C-12), 38.1 (C-13), 42.9 (C-14), 27.5 (C-15), 35.6 (C-16), 43.0 (C-17), 48.0 (C-18), 48.4 (C-19), 150.9 (C-20), 29.9 (C-21), 34.3 (C-22), 28.1 (C-23), 16.7 (C-24), 16.2 (C-25), 16.0 (C-26), 14.6 (C-27), 18.0 (C-28), 109.3 (C-29), 19.3 (C-30), 127.2 (C-1′), 109.4 (C-2′), 146.8 (C-3′), 147.9 (C-4′), 116.4 (C-5′), 123.0 (C-6′), 144.3 (C-7′), 114.6 (C-8′), 167.1 (C-9′), 56.0 (C−OMe); RABMS m/z (rel. int.): 602 [M^+] (35), 409 (41), 194(13), 177 (95), 154 (64), 136 (55), 105 (52), 77 (100)

Hydrolysis of compound **1**: compound **1** (18 mg) was refluxed with 5% aq. KOH (10 ml) and the reaction mixture was heated at 60 °C for 8 h. The reaction mixture was diluted with H_2O (25 ml) and extracted with Et_2O. The ester extract was purified and yielded lupeol (11 mg). The aq. layer was acidified with 3% HCl and then extracted with CH_2Cl_2 giving ferulic acid (2 mg).

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Two new compounds from the seeds of *Descurainia sophia*

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Two new compounds, descurainin A (**1**) and descurainoside B (**2**), were isolated from the seeds of *Descurainia sophia* (L.) Webb ex Prantl. Their structures were elucidated by spectroscopic methods (MS, ^1H, ^{13}C and 2D NMR).

Descurainia sophia (L.) Webb ex Prantl is widely distributed in the northeast of China, and its seeds are used as a Chinese traditional medicine to relieve cough, prevent asthma, reduce edema, promote urination and have a cardiotonic effect. In some cases the seeds can also be used in the treatment of some cancers (Sun and Li 2002). In previous chemical studies, the isolation of some cardiac glycosides (Chen et al. 1981), flavonoids and phenols (Wang et al. 2004) from the seeds was reported. As our current interest in the medicinal uses of the seeds of *D. sophia*, we also carried out a phytochemical investigation on the seeds of *D. sophia*, which resulted in two new compounds, descurainin A (**1**) and descurainoside B (**2**). This paper deals with the isolation and structural elucidation of the two new constituents (Fig.) on the base of extensive studies of their MS and 1D and 2D NMR.

Compound **1** was obtained as yellow powder from methanol and responded positively to $FeCl_3$ reagent and HCl-Mg reagent which indicated that **1** belong to the flavonoids. The molecular formula of **1** was deduced as $C_{26}H_{24}O_{10}$ from the pseudomolecular ion peaks at m/z 519.3 $[M+Na]^+$ and 495.0 $[M-H]^-$ in ESI-MS and cor-

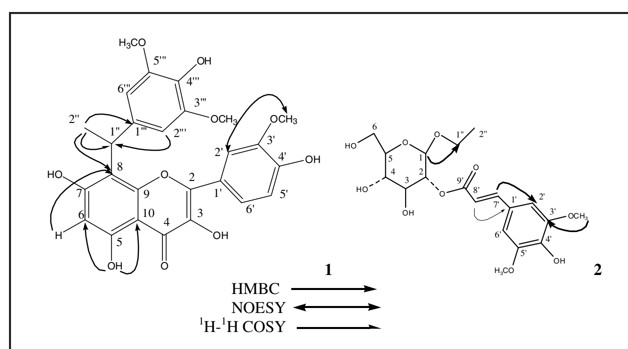

Fig.: Important correlations of compounds **1** and **2**

responding to its NMR spectra. HMQC and NMR spectra of **1** suggested a 4-hydroxy-3,5-dimethoxy-phenyl moiety (Wang et al. 2004) at δ_H 8.10 (1 H, br.s, 4‴-OH), 6.52 (2 H, s, H-2‴, 6‴) and 3.58 (6 H, s, 3‴, 5‴-OCH_3), δ_C 134.9 (C-1‴), 104.8 (C-2‴, 6‴). 147.8 (C-3‴, 5‴), 133.8 (C-4‴) and 56.0 (3‴,5‴-OCH_3), a methyl group connected to one methine group at δ_H 1.72 (3 H, d, J = 7.2 Hz, H-2″) and δ_C 19.1 (C-2″), and a methine substituted by one methyl group at δ_H 4.79 (1 H, q, J = 7.2 Hz, H-1″) and δ_C 32.6 (C-1″) from which the connection of C-1″ and C-2″ could be inferred and was supported by the $^1H-^1H$ COSY spectrum in which the cross peak with H-1″ and H-2″ was observed. Compared with the NMR spectral data of isorhamnetin (Liang et al. 2004; Wang et al. 2004), the moiety of isorhamnetin whose C-8 was substituted could be revealed, and in the NOESY spectrum the cross peak with 3′-OCH_3 and H-2′ confirmed this deduction. In the HMBC experiment, the cross peak with C-6 and 5-OH showed that this carbon was C-6, the cross peaks with C-8 and H-6 and H-2″ confirmed that this carbon was C-8 and C-8 connected with C-1″, and the cross peaks with C-1‴ and H-2″, and C-1″ and H-2‴,6‴ implied the substitution of C-1″ by the 4-hydroxy-3,5-dimethoxy-phenyl moiety. Thus, the structure of **1** was elucidated as 3,5,7-trihydroxy-8-[1″-(4‴-hydroxy-3‴,5‴-dimethoxy-phenyl)-ethyl]-2-(4′-hydroxy-3′-methoxy-phenyl)-chromen-4-one, named descurainin A.

Compound **2** was obtained as white powder from methanol and reacted positive to Molish test and $FeCl_3$ reagent. Acid hydrolysis carried out on TLC yielded only glucose. Its NMR spectra and the pseudomolecular ion peaks at m/z 437.2 $[M+Na]^+$ and 413.1 $[M-H]^-$ in ESI-MS suggested the molecular formula of $C_{19}H_{26}O_{10}$. Combined with HMQC, the ^1H NMR, ^{13}C NMR spectra of **2** exhibited a *trans*-sinapoyl moiety (Wang et al. 2004) at δ_H 8.97 (1 H, br.s, 4′-OH), 7.55 (1 H, d, J = 15.9 Hz, H-7′), 7.04 (2 H, s, H-2′,6′), 6.55 (1 H, d, J = 15.9 Hz, H-8′) and 3.80 (6 H, s, 3′,5′-OCH_3), δ_C 124.5 (C-1′), 106.3 (C-2′,6′), 148.1 (C-3′,5′), 138.3 (C-4′), 145.4 (C-7′), 115.3 (C-8′) and 165.8 (C-9′), an oxyethyl group at δ_H 3.71 (2 H, m, H-6a, 1″a), 3.44 (2 H, m, H-6b, 1″b) and 1.05 (3 H, t, J = 6.9 Hz, H-2″), δ_C 64.0 (C-1″) and 15.2 (C-2″), and a glucose moiety whose anomeric proton signal at δ_H 4.42 (1 H, d, J = 8.1 Hz, H-1) indicated the β orientation of the anomeric center of the glucose and whose anomeric carbon signal at δ_C 100.2 showed that this anomeric carbon was substituted. In the HMBC experiment, the cross peak with C-1″and H-1 revealed that C-1 was substituted by the oxyethyl group, and the cross peaks with C-9′ and H-7′, C-7′ and H-2′, 6′, C-1′ and H-8′, C-2′, 6′ and H-7′, C-3′, 5′ and 3′,5′-OCH_3 and 4′-OH confirmed the presence of a sinapoyl moiety. Compared with kaempferol-3-*O*-β-D-glucopyranosyl-7-*O*-[(2-*O*-*trans*-sinapoyl)-β-D-glucopyranosyl(1→6)]-β-D-glucopyranoside (**3**) (Wang et al. 2004), the carbon signals of **2** were almost identical to those of the (2-*O*-*trans*-sinapoyl)-β-D-glucopyranosyl moiety of **3**, which suggested the substitution of C-2 by the sinapoyl moiety. Therefore the structure of **2** was elucidated as 1-ethyl ether-(2-*O*-*trans*-sinapoyl)-β-D-glucopyranoside, named descurainoside B.

Experimental

1. General procedures

The melting points were measured on a Yamaco micro-hot-stage and are uncorrected. NMR spectra were recorded on a Bruker-ARX-300 spectrometer, using TMS as an internal standard. ESI-MS was performed on a Finnigan LCQ mass spectrometer. Silica gel for chromatography was produced by Qingdao Ocean Chemical Group Co. Ltd., China. Macroporous resin D101 for chromatography was produced by Nankai University. Spots were detected on TLC under UV light or by heating after spraying with 10% H_2SO_4 in C_2H_5OH. Preparative HPLC was carried out using a Shimadzu SPD-6A UV spectrophotometric detector at 254 nm and Shim-pack PREP-ODS reversed phase column (25 mm × 216 mm i.d.).

2. Plant material

The plant material was purchased from Shenyang TCM Corporation (Shenyang), and was identified by Prof. Sun Qishi (Shenyang Pharmaceutical University). A voucher specimen (No.20010321) is deposited in the Research Department of Natural Medicine, Shenyang Pharmaceutical University.

3. Extraction and isolation

The air-dried seeds (10 kg) of *Descurainia sophia* were extracted three times with 70% ethanol for 2 h each. The extract was concentrated *in vacuo*, chromatographed on a D101 macroporous resin column and eluted with H_2O, 20%, 40%, 60% and 95% ethanol successively. The 40% eluate (100 g) was prefractionated by CC on silica gel yielding fraction **1** ($CHCl_3-MeOH$ 200 : 4) and fraction **2** ($CHCl_3-MeOH$ 200 : 7). Fraction **1** was separated by CC on silica gel eluting with petroleum ether-EtOAc-Me_2CO (7 : 1 : 1) to yield fraction **1-1**, which was first chromatographed on Sephadex LH-20 ($CHCl_3-MeOH$ 10 : 1) and then purified by HPLC ($MeOH-H_2O$ 35 : 65) to yield compound 1 (21 mg). Fraction **2** was passed over silica gel (petroleum ether-EtOAc-Me_2CO 5 : 1 : 1) to offer compound **2** (11 mg).

4. Characterization of the compounds

Compound **1**: yellow power, EIS-MS m/z 519.3 $[M+Na]^+$, 495.0 $[M-H]^-$. ^1H NMR (300 MHz, DMSO-d_6): 12.61 (1H, s, 5-OH), 9.78 (3 H, br.s, 3,7,4′-OH), 8.10 (1 H, br.s, 4‴-OH), 7.51 (1 H, br.s, H-2′), 7.44 (1 H, br.d, J = 8.1 Hz, H-6′), 6.88 (1 H,d, J = 8.1 Hz, H-5′), 6.52 (2 H, s, H-2‴,6‴), 6.36 (1 H, s, H-6), 4.79 (1 H, q, J = 7.2 Hz, H-1″), 3.63 (3 H, s, 3′-OCH_3), 3.58 (6 H, s, 3‴,5‴-OCH_3), 1.72 (3 H, d, J = 7.2 Hz, H-2″); ^{13}C NMR (75 MHz, DMSO-d_6): 176.3 (C-4), 161.8 (C-7), 158.7 (C-5), 154.1 (C-9), 148.8 (C-4′), 147.8 (C-3‴,5‴), 147.4 (C-3′), 146.9 (C-2), 135.7 (C-3), 134.9 (C-1‴), 133.8 (C-4‴), 122.1 (C-1′), 121.9 (C-6′), 115.6 (C-5′), 111.6 (C-2′), 109.8 (C-8), 104.8 (C-2‴,6‴), 103.5 (C-10), 98.4 (C-6), 56.0 (3‴,5‴-OCH_3), 55.5 (3′-OCH_3), 32.6 (C-1″), 19.1 (C-2″).

Compound **2**: white power, EIS-MS m/z 437.2 $[M+Na]^+$, 413.1 $[M-H]^-$. ^1H NMR (300 MHz, DMSO-d_6): 8.97 (1 H, br.s, 4′-OH), 7.55 (1 H, d, J = 15.9 Hz, H-7′), 7.04 (2 H, s, H-2′,6′), 6.55 (1 H, d, J = 15.9 Hz, H-8′), 4.62 (2 H, m, H-2,3), 4.42 (1 H, d, J = 8.1 Hz, H-1), 3.80 (6 H, s, 3′,5′-OCH_3), 3.71 (2 H, m, H-6a, 1′a), 3.44 (2 H, m, H-6b, 1′b), 3.19 (2 H, m, H-4,5), 1.05 (3 H, t, J = 6.9 Hz, H-2′); ^{13}C NMR (75 MHz, DMSO-d_6): 165.8 (C-9′), 148.1 (C-3′,5′), 145.4 (C-7′), 138.3 (C-4′), 124.5 (C-1′), 115.3 (C-8′), 106.3 (C-2′,6′), 100.2 (C-1), 77.1 (C-5), 74.4 (C-3), 73.6 (C-2), 70.3 (C-4), 64.0 (C-1″), 60.9 (C-6), 56.2 (3′,5′-OCH_3), 15.2 (C-2″).

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