DOI 10.1007/s10600-019-02795-4
Chemistry of Natural Compounds, Vol. 55, No. 4, July, 2019

CHEMICAL CONSTITUENTS OF *Lepidium sativum* SEEDS

A. Kaiyrkulova,[1,2] Jun Li,[1] and H. A. Aisa[1*]

The genus *Lepidium* L. (Brassicaceae) is represented by 234 species worldwide, of which 15 grow in China. It occurs wild everywhere from the Mediterranean and Eastern and Central Asia to North America [1].

L. sativum (garden cress) is an annual herb that is used in folk medicine for various digestive diseases and in culinary arts. Seeds of the plant exhibit anti-inflammatory, antioxidant, antimicrobial, antifungal, and antitumor activity. Alkaloids, flavonoids, terpenes, sterols, and phenylpropanoids were isolated earlier from this plant [2].

Seeds of *L. sativum* were purchased in June 2016 in a medical supermarket in Urumqi (PRC) and were identified by Prof. Ying Feng (Xinjiang Institute of Ecology and Geography, AS, PRC, Urumqi). Specimens of seeds (WY02634) were preserved at the Xinjiang Technical Institute of Chemistry and Physics, AS, PRC.

Dried and milled *L. sativum* seeds (9 kg) were extracted (3×) with EtOH (95%, 1:5). The extract was evaporated to remove the solvent. The EtOH extract (1.328 kg) was suspended in distilled H_2O and extracted successively with petroleum ether, EtOAc, and *n*-BuOH. The BuOH fraction (70 g) was chromatographed over a column of silica gel using a $CHCl_3$–MeOH gradient (100:1, 80:1, 50:1, 30:1, 15:1, 9:1, 4:1, 1:1, 0:1) to produce nine fractions that were rechromatographed over columns of ODS and Sephadex LH-20 and separated by HPLC to isolate **1**–**9** that were identified by comparing mass, PMR, and ^{13}C NMR spectra with literature data. The identified compounds were benzoic acid (**1**), 3-methoxy-4-hydroxybenzoic acid (**2**), niacin (**3**), syringaldehyde (**4**), 2-phenylacetamide (**5**), *β*-sitosterol (**6**), kaempferol-7-*O*-L-rhamnopyranoside (**7**), rutin (**8**), and quercetin-7-*O*-L-rhamnoside (**9**). Compounds **2**–**4** and **7**–**9** were isolated for the first time from this plant.

Benzoic acid (1), $C_7H_6O_2$, mass spectrum, *m*/*z* 121 $[M - H]^-$. PMR and ^{13}C NMR spectra were comparable with those in the literature [3].

3-Methoxy-4-hydroxybenzoic acid (2), $C_8H_8O_4$, mass spectrum, *m*/*z* 167 $[M - H]^-$. PMR and ^{13}C NMR spectra corresponded to those in the literature [4].

Niacin (3), $C_6H_5O_2N$, mass spectrum, *m*/*z* 122 $[M - H]^-$. ^1H NMR spectrum (400 MHz, CD_3OD, δ, ppm, J/Hz): 9.12 (1H, s, H-2), 8.41 (1H, d, J = 7.8, H-4), 7.56 (1H, dd, J = 7.8, 4.8, H-5), 8.73 (1H, d, J = 4.8, H-6). ^{13}C NMR spectrum (100 MHz, CD_3OD, δ, ppm): 167.8 (C=O), 151.3 (C-2), 128.8 (C-3), 139.2 (C-4), 125.2 (C-5), 153.6 (C-6) [4].

Syringaldehyde (4), $C_9H_{10}O_4$, mass spectrum, *m*/*z* 183 $[M + H]^+$. ^1H NMR spectrum (600 MHz, $CDCl_3$, δ, ppm): 9.82 (1H, s, CHO), 7.15 (2H, s, H-2, 6), 6.05 (1H, s, 4-OH), 3.98 (6H, s, 3, 5-OCH_3). ^{13}C NMR spectrum (100 MHz, $CDCl_3$, δ, ppm): 190.8 (CHO), 147.5 (C-3, 5), 128.6 (C-1), 106.5 (C-2, 6), 56.6 (3, 5-OCH_3) [5].

2-Phenylacetamide (5), C_8H_9NO, mass spectrum, *m*/*z* 136 $[M + H]^+$. PMR and ^{13}C NMR spectra were comparable with those in the literature [3].

***β*-Sitosterol (6)**, $C_{29}H_{50}O$, mass spectrum, *m*/*z* 413 $[M - H]^-$. PMR and ^{13}C NMR spectra were comparable with those in the literature [3].

Kaempferol-7-*O*-*α*-L-rhamnopyranoside (7), $C_{21}H_{20}O_{10}$, mass spectrum, *m*/*z* 433 $[M + H]^+$. ^1H NMR spectrum (400 MHz, CD_3OD, δ, ppm, J/Hz): 8.13 (2H, d, J = 8.8, H-2′, 6′), 6.93 (2H, d, J = 8.8, H-3′, 5′), 6.77 (1H, d, J = 2.0, H-8), 6.44 (1H, d, J = 2.0, H-6), 5.58 (1H, s, H-1″), 4.04 (1H, dd, J = 3.2, 1.6, H-2″), 3.86 (1H, dd, J = 9.2, 3.2, H-3″), 3.63 (1H, m, H-5″), 3.51 (1H, t, J = 14.4, H-4″), 1.29 (3H, d, J = 6.0, H-6″). ^{13}C NMR spectrum (100 MHz, CD_3OD, δ, ppm): 177.5 (C-4),

1) The Key Laboratory of Plant Resources and Chemistry of Arid Zone and State Key Laboratory Basis of Xinjiang Indigenous Medicinal Plants Resource Utilization, Xinjiang Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, 830011, Urumqi, P. R. China; 2) University of Chinese Academy of Sciences, 100039, Beijing, P. R. China, e-mail: haji@ms.xjb.ac.cn. Translated from *Khimiya Prirodnykh Soedinenii*, No. 4, July–August, 2019, pp. 629–630. Original article submitted January 26, 2019.

 0009-3130/19/5504-0736

163.3 (C-5), 162.3 (C-7), 160.7 (C-4′), 157.7 (C-9), 148.7 (C-2), 137.5 (C-3), 130.8 (C-2′, 6′), 123.5 (C-1′), 116.3 (C-3′, 5′), 106.2 (C-10), 99.9 (C-6), 99.8 (C-1″), 95.3 (C-8), 73.6 (C-4″), 72.1 (C-3″), 71.7 (C-2″), 71.2 (C-5″), 18.1 (C-6″) [6].

Rutin (8), $C_{27}H_{30}O_{16}$, mass spectrum, *m/z* 633 $[M + Na]^+$. PMR and ^{13}C NMR spectra were comparable with those in the literature [7].

Quercetin-7-*O*-L-rhamnoside (9), $C_{21}H_{20}O_{11}$, mass spectrum, *m/z* 447 $[M - H]^-$. ^1H NMR spectrum (400 MHz, DMSO-d_6, d, ppm, J/Hz): 12.49 (1H, s, 5-OH), 9.68 (1H, s, 4′-OH), 9.57 (1H, s, 3′-OH), 9.35 (1H, s, 3-OH), 7.72 (1H, d, J = 2.4, H-2′), 7.58 (1H, dd, J = 8.4, 2.4, H-6′), 6.88 (1H, d, J = 8.4, H-5′), 6.79 (1H, d, J = 2.0, H-8), 6.41 (1H, d, J = 2.0, H-6), 5.54 (1H, d, J = 1.6, H-1″), 3.83 (1H, m, H-2″), 3.63 (1H, m, H-3″), 3.43 (1H, dd, J = 9.6, 6.4, H-5″), 3.31 (1H, dd, J = 9.2, 5.6, H-4″), 1.12 (3H, d, J = 6.4, H-6″). ^{13}C NMR spectrum (100 MHz, DMSO-d_6, δ, ppm): 176.0 (C-4), 161.4 (C-7), 160.4 (C-5), 155.7 (C-9), 147.9 (C-2), 147.5 (C-4′), 145.1 (C-3′), 136.2 (C-3), 121.8 (C-1′), 120.2 (C-6′), 115.6 (C-2′), 115.2 (C-5), 104.6 (C-10), 98.8 (C-1″), 98.4 (C-6), 94.2 (C-8), 71.6 (C-4″), 70.3 (C-3″), 70.1 (C-2″), 69.9 (C-5″), 18.0 (C-6″) [8].

ACKNOWLEDGMENT

The work was sponsored by the Science and Technology Program of Xinjiang-Uyghur Autonomous Region (Grant No. 2016A03005-3), West Light Foundation, AS, PRC (Grant No. 2015-XBQN-B-08), and Central Asian Center of Drug Discovery and Development, AS, PRC.

REFERENCES

1. *Flora of China*, 8, Flora of China Editorial Committee, Science Press and Missouri Botanical Garden Press, Beijing, 2001, pp. 1–193.
2. V. D. Prajapati, P. M. Maheriya, G. K. Jani, P. D. Patil, and B. N. Patel, *Int. J. Biol. Macromol.*, **65**, 72 (2014).
3. Q. L. Fan, Z. H. Huang, and B. L. Guo, *J. Anhui Agric. Sci.*, **42**, 3533 (2014).
4. Q. Zheng, Q. H. Zhang, D. Lu, L. Leng, P. Y. Li, and J. P. Liu, *Chin. Tradit. Herb. Drugs*, **45**, 2457 (2014).
5. C. Y. Chen, C. L. Kao, W. J. Li, H. C. Chen, and H. T. Li, *Chem. Nat. Compd.*, **54**, 509 (2018).
6. S. K. Chien, L. C. Chen, H. C. Huang, L. C. Chen, J. W. Hsiao, M. J. Cheng, and J. J. Chen, *Chem. Nat. Compd.*, **54**, 1044 (2018).
7. X. J. Wang, X. Luo, J. M. Zhou, Y. L. Song, Y. W. Zhao, W. Z. Huang, Z. Z. Wang, and W. Xiao, *Chin. Tradit. Herb. Drugs*, **47**, 2822 (2016).
8. X. W. Wang, Y. Mao, N. L. Wang, and X. S. Yao, *Molecules*, **13**, 2796 (2008).