

## COMPONENTS OF THE AERIAL PART OF *Peganum harmala*

M. T. Agedilova,<sup>1</sup> A. Zh. Turmukhambetov,<sup>1</sup> E. E. Schultz,<sup>2</sup>  
M. M. Shakirov,<sup>2</sup> and S. M. Adekenov<sup>1</sup>

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The genus *Peganum* (Peganaceae) is represented in the flora of the CIS by the two species *P. harmala* L. (wild rue) and *P. nigellastrum* Bge. This genus is broadly represented by wild rue in Kazakhstan [1-3]. Various parts of the plant are used in folk medicine to treat several illnesses [4]. Researchers from various countries have been studying the chemical composition of this plant since 1841 because of its therapeutic importance [5-13]. Mainly the alkaloid composition is studied. Herein we report experimental results from a study of the component composition of the petroleum-ether extract of the aerial part of wild rue.

Extraction with petroleum ether of the air-dried aerial part of *P. harmala* collected near Karaganda during flowering-fruiting produced the total extracted substances (0.96%, 7.0 g).

Extract (1 g) was dissolved in diethylether (15 mL) and left overnight in a refrigerator. The resulting precipitate was filtered off and washed with cold (-20°C) ether to produce a substance (0.22 g) that was a mixture of alkaloids (by PMR, mainly peganine and vasicinone). The mother liquor was evaporated. The residue was separated by the standard method [boiled for 10 min in KOH solution (10%) in MeOH. MeOH was evaporated, and the residue was separated between CHCl<sub>3</sub> and H<sub>2</sub>O] into acidic and neutral parts. The acidic part (0.3 g) was methylated and analyzed using GC—MS. The neutral part was evaporated (0.45 g), dissolved in CHCl<sub>3</sub> (10 mL), passed over a silica-gel column (5 g), and eluted with CHCl<sub>3</sub> (20 mL). The combined effluents were evaporated to afford an oil (0.4 g) that was analyzed by GC—MS.

GC—MS was performed on a Hewlett—Packard 5890/II MSD gas chromatograph with a quadrupole mass spectrometer (HP MSD 5971) as a detector, a quartz column (30-m, HP-5 MS, copolymer 5%-diphenyl-95%-dimethylenesiloxane) with internal diameter 0.25 mm and thick layer of stationary phase (0.25 μm), temperature 50-280°C, heating rate 4°C/min, 280°C temperature change over 15 min. The percent composition of the components was calculated from peak areas in the plots using correction coefficients. The qualitative analysis was based on comparison of retention times and full mass spectra with those of pure compounds and a library of mass spectrometric data Wiley 275 (275,000 mass spectra) and catalogs [14, 15].

Melting points were determined on a Boetius instrument. IR spectra were recorded on a Vektor 22 spectrometer in KBr disks.

Table 1 gives the contents of fatty acids and high-molecular-weight alcohols from *P. harmala*.

The results showed that the acidic part contained a significant amount of high-molecular-weight (C<sub>28</sub>-C<sub>30</sub>) and a few unsaturated acids (principal ones linoleic and linolenic). The principal fatty acids of *P. harmala* were hexadecanoic (palmitic), octacosanoic, nonacosanoic, and triacontanoic (melissic).

The components of the neutral part were high-molecular-weight alcohols (32.183% of the neutral part mass) C<sub>26</sub>H<sub>53</sub>OH, mp 84-85°C (0.053% yield) and C<sub>29</sub>H<sub>59</sub>OH, mp 79-81°C (0.065% yield of air-dried raw material mass) that were identified as 1-hexacosanol and 1-nonacosanol.

In addition to the alcohols and fatty acids, GC—MS showed that the extract contained saturated hydrocarbons *n*-hexadecane (0.602%), *n*-octadecane (0.344%), *n*-heptacosane (0.847%), *n*-octacosane (0.343%), *n*-nonacosane (15.736%), *n*-hentriacontane (0.458%), and 2-nonacosane (2.206%). Furan derivatives were also detected in the extract. These were 2,2-diethoxyfuran (1.723%), 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuran (0.189%), and hexadecanal (0.987%), 4,8,12-trimethyltridecan-4-olide (0.456%), and β-sitosterol (4.753%).

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1) Institute of Phytochemistry, Ministry of Education and Science of the Republic of Kazakhstan, Karaganda, ul. Gazaliev, 4, Kazakhstan; 2) Novosibirsk Institute of Organic Chemistry, Siberian Division, Russian Academy of Sciences, Novosibirsk, Russia. Translated from *Khimiya Prirodnikh Soedinenii*, No. 2, pp. 186-187, March-April, 2006. Original article submitted April 3, 2006.

TABLE 1. Fatty Acids and Alcohols from *Peganum harmala* L.

Acid	RT, min	Content, %	Alcohol	RT, min	Content, %
16:0	37.12	0.840	Eicosanol-1	45.457	0.49
18:2	41.012	0.126	Docosanol-1	56.904	0.68
18:3	41.177	0.238	Decacosanol	58.544	0.118
18:0	41.774	0.223	Tetracosanol	58.739	1.786
22:0	50.00	0.187	Hexacosanol	59.99	6.184
24:0	53.677	0.184	Heptacosanol	60.631	0.348
26:0	57.11	0.397	Octacosanol	61.595	0.312
28:0	60.34	1.872	Nonacosanol	63.083	4.18
29:0	61.896	0.101	Triacosanol	63.659	0.36
30:0	63.411	1.613	1-Hentetracontanol	85.877	0.874

RT is retention time, min.

## REFERENCES

1. *Flora of Kazakhstan*, Vol. 6 [in Russian], Alma-Ata (1963), p. 32.
2. M. V. Telezhenetskaya, in: *Progress in Research on Alkaloid-Bearing Plants*, Kh. N. Aripov, ed. [in Russian], Fan, Tashkent (1993), p. 221.
3. *Atlas of Areal and Resources of Medicinal Plants of Kazakhstan* [in Russian], Gylym, Almaty (1994), p. 18.
4. R. N. Chopra, S. L. Nayar, and I. C. Chopra, *Glossary of Indian Medicinal Plants*, C.S.I.R., New Delhi (1956), 187.
5. S. Siddiqui, *Pak. J. Sci. Ind. Res.*, **5**, 207 (1962).
6. Kh. N. Khashimov, M. V. Telezhenetskaya, Ya. V. Rashkes, and S. Yu. Yunusov, *Khim. Prir. Soedin.*, 453 (1970).
7. B. Kh. Zharekeev, M. V. Telezhenetskaya, and S. Yu. Yunusov, *Khim. Prir. Soedin.*, 279 (1973).
8. A. I. Botbaev, N. V. Plekhanova, and E. V. Nikitina, *Izv. Akad. Nauk Kirg. SSR*, **2**, 52 (1974).
9. E. McKenzie, L. Nettleship, and M. Slaytor, *Phytochemistry*, **14**, 273 (1975).
10. W. Barz, H. Herzbeck, W. Husemann, G. Schneiders, and H. K. Mangold, *Planta Med.*, **40**, 137 (1980).
11. F. Goebell, *Justus Liebig's Ann. Chem.*, **38**, 363 (1841).
12. S. Siddiqui, O. Y. Khan, B. S. Siddiqui, and S. Faizi, *Heterocycles*, **26**, No. 6, 1563 (1987).
13. S. Siddiqui, O. Y. Khan, B. S. Siddiqui, and S. Faizi, *Phytochemistry*, **26**, No. 5, 1548 (1987).
14. F. V. McLafferty and D. B. Stauffer, *The Wiley NBS Registry of Mass Spectra*, Wiley Interscience, New York (1989), 1-7.
15. *Eight Peak Index of Mass Spectra*, Royal Society of Chemistry, University of Nottingham, England (1983), 3rd Ed., 1-2.