

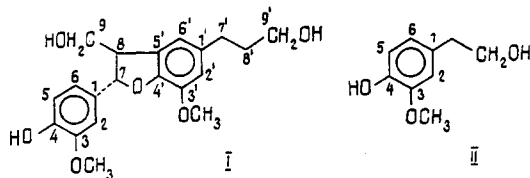
TWO PHENOLIC COMPOUNDS FROM *Aconitum baicalense*Ts. Zhapova N. N. Pogodaeva, A. G. Gorshkov,
and A. A. Semenov

UDC 547.639

When the chloroform fraction of the total alkaloids from the epigeal part of *Aconitum baicalense* was separated, two phenolic compounds were obtained.

To isolate compound (I) we used column chromatography on alumina. The eluent was chloroform–methanol (10:1). After the additional purification of (I) with the aid of HPLC (2.5 × 250 mm column; Nucleosil-5, C₁₈; eluent 45% MeOH; detection at 210 nm) an oily substance was isolated with the composition C₂₀H₂₄O₆, [α]_D²⁰ +6.6 (CHCl₃). Mass spectrum: m/z 360 (M⁺). UV spectrum: λ_{max}^{MeOH} 280 nm. A comparison of this spectral information with the literature permitted compound (I) to be identified as 3β-hydroxymethyl-5-(3-hydroxypropyl)-7-methoxy-2α-(3-methoxy-4-hydroxyphenyl)benzo[b]furan (dihydrodiconiferyl alcohol). Table 1 gives a complete assignment of the signals in the ¹³C and ¹H NMR spectra. The position of the phenolic hydroxyl was established by an analysis of the ¹³C and ¹H chemical shifts observed after the action of trichloroacetyl isocyanate [2], which are given in the Δ column of the table. The relative stereochemistry at the C-7 and C-8 atoms was deduced on the basis of the absence of a nuclear Overhauser effect between the protons attached to them.

Compound (II), with the composition C₉H₁₂O₃ and a molecular mass of 168, was isolated with the aid of column chromatography on silica gel with elution by chloroform. On comparing the physicochemical characteristics of this compound with the literature [3], it was identified as 2-(3-methoxy-4-hydroxyphenyl)ethanol. As in the case of compound (I), the position of the hydroxyl was established by an analysis of the ¹H chemical shifts observed under the action of trichloroacetyl isocyanate. The ¹³C NMR spectrum of compound (II) agrees with the proposed structure.

TABLE 1. Chemical Shifts in the ¹³C and ¹H NMR Spectra of Dihydrodiconiferyl Alcohol

№	C, ppm	ΔC, ppm	H(δ, ppm, J, Hz)	ΔH, Hz	№	C, ppm	ΔC, ppm	H(δ, ppm, J, Hz)	ΔH, Hz
1	133,11	5,4			1'	127,75	-1,8		
2	108,82	1,6	6,93; s		2'	112,42	0,8	6,66; d; 3,3	14
3	146,64	4,8		92	3'	144,19	0,3		
4	146,55	-6,0			4'	145,60	-0,9		
5	115,94	6,8	6,86; d; 8,0		5'	135,41	-0,5		
6	119,42	-1,4	6,88; dd; 8,0	122	6'	114,28	2,2	6,66; d; 3,3	14
			i 1,5						
7	87,88	-0,8	5,53; d; 7,4	46	7'	34,61	-2,8	2,64; m	25
8	53,80	-2,8	3,59; m	33	8'	32,00	-1,9	1,85; m	92
9	63,01	4,9	3,93; q; 5,9;	20	9'	62,29	4,5	3,67; t; 6,3	304
			11,0						
			3,86*	320	OMe	56,00	0,2	3,83; s	
						56,00	0,3	3,85; s	

*Masks the signal of the methoxy group.

Irkutsk Institute of Organic Chemistry, Siberian Branch, Russian Academy of Sciences. Translated from *Khimiya Prirodnikh Soedinenii*, No. 4, pp. 617-618, July-August, 1993. Original article submitted November 16, 1992.

These two compounds have not been isolated from *A. baicalense* previously.

REFERENCES

1. L. N. Lundgren, T. Popoff, and O. Theander, *Phytochemistry*, **20**, No. 8, 1967 (1981); P. K. Argawal, R. P. Rastogi, and B. Q. Osterdahl, *Org. Mag. Reson.*, **21**, No. 2, 119 (1983).
2. A. K. Bose and P. R. Srinivasan, *Tetrahedron*, **31**, 3025 (1975); L. Samek and M. Budesinsky, *Coll. Czech. Chem. Commun.*, **44**, 558 (1979).
3. H. Kodaira, M. Ishikawa, Y. Komoda, and T. Nakajima, *Chem. Pharm. Bull.*, **29**, No. 8, 2391 (1981).