

THE STRUCTURE OF GLUCOTHEASAPONIN

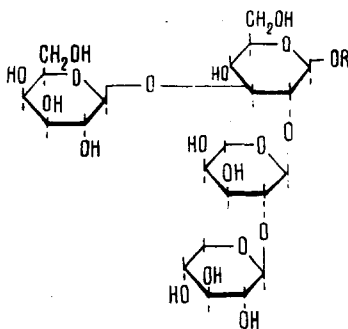
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We have previously reported [1] that the mother liquor obtained from the crystallization of a butanolic extract in the isolation of theasaponin from the seeds of Chinese tea contained a glycoside differing from theasaponin by the presence of glucose as a component. The chromatographic mobilities of the two glycosides are similar, and we separated theasaponin from the accompanying glycoside only by repeated recrystallization.

The substance mentioned was dissolved in water, the insoluble matter was separated by centrifuging, and the centrifugate was passed through a column of Dow-3 ion-exchange resin. After evaporation of the aqueous eluate and crystallization, a chromatographically homogeneous substance was obtained: $C_{59}H_{92}O_{26}$, mp 250-254°C, $[\alpha]_D^{21} +23.0^\circ$ (c 1.5; ethanol), which we have called *glucotheasaponin* and which, in contrast to theasaponin, is readily soluble in water.

After acid and then alkaline hydrolysis it was found that it contained the same aglycones and fatty acids as theasaponin [2]. In the acid hydrolyzate by chromatography on paper and in a thin layer of silica gel we identified D-glucose, D-galactose, L-arabinose, and D-xylose. In the products of the acid hydrolysis of completely methylated glucotheasaponin by gas-liquid chromatography in the presence of markers we identified 2,3,4,6-tetra-O-methyl-D-galactose, 2,3,4-tri-O-methyl-D-xylose, 3,4-di-O-methyl-L-arabinose, and 4,6-di-O-methyl-D-glucose in a ratio of 1:1:1:1, i.e., the same set of methylated monosaccharides as from reduced theasaponin [2]. Partial hydrolysis of glucotheasaponin yielded a fragment of the glycoside with the composition $C_{42}H_{70}O_{16} \cdot H_2O$, mp 240-246°C; its carbohydrate moiety was represented solely by glucose and galactose. The substance was similar to the fragment isolated from reduced theasaponin [2]. These results, and also those of methylation, give grounds for assuming a carbohydrate chain of the following structure for glucotheasaponin:



Thus, the triterpene glycoside glucotheasaponin that we have isolated for the first time differs from theasaponin by the structure of the carbohydrate chain, which contains glucose in place of glucuronic acid.

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2. I. N. Sokol'skii, É. P. Zinkevich, A. I. Ban'kovskii, and M. M. Molodozhnikov, *Khim. Prirodn. Soedin.*, 654 (1972).