

MOLECULAR COMPLEXES OF CHOLESTEROL WITH OLEANOLIC ACID AND AESCINE

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Aescine (ES) is the sum of more than 30 triterpene glycosides isolated from the horse chestnut *Aesculus hippocastanum* L. (Sapindaceae Juss.). Among them prevails β -aescine, is a mixture of two glycosides (aescine Ia and aescine Ib). ES has anti-inflammatory, anti-edematous, membranotropic and capillaroprotective properties, improves trophism of tissues with a blood circulation and edema. Oleanolic acid is a 3β -hydroxyolean-12-en-28-oic acid (OleanA). It has hepatoprotective, antimicrobial, antiviral, anti-inflammatory and antitumor activity.

A characteristic feature of saponins is their ability to form molecular complexes with cholesterol (Chol). Investigation of Chol complexation with ES was started a long time ago. In some cases there is no clear evidence of the intermolecular interaction of Chol with saponins by various modern spectral methods.

The synthesis of ES–Chol and OleanA–Chol complexes was carried out in the liquid phase (in a mixture of 70 % aqueous ethanol and chloroform at a ratio of 3:1, v/v). The components ES and Chol (analogically OleanA and Chol) were taken in equimolar ratios. The obtained mixture was incubated at 50 °C for 1.5 h with continuous stirring. The organic solvents were then removed by vacuuming.

The complexation was studied by FTIR spectroscopy. When the ES is complexed with Chol, a low-field shift of the absorption bands of OH bonds stretching vibrations is observed: 3380→3369 cm^{-1} (for ES) and 3401→3369 cm^{-1} (for Chol). The frequency of the absorption band of C=O stretching vibrations in the ES carboxyl group has changed by -12 cm^{-1} . It indicates the formation of a hydrogen bond $-\text{C}=\text{O}\cdots\text{H}-\text{O}-$. In the IR spectra changes in some of the absorption frequencies of CH bonds have been found: $\nu_{\text{C-H}}$ 2930 cm^{-1} in the complex has changed by +5 cm^{-1} (in Chol), and $\nu_{\text{C-H}}$ 2920 cm^{-1} – by -20 cm^{-1} (in ES).

The spectrum of the OleanA–Chol complex exhibited a low-field shift of the absorption bands of OH bonds stretching vibrations in Chol from 3401 to 3379 cm^{-1} , and

in OleanA – from 3458 to 3379 cm^{-1} . The frequency of the absorption band of C=O stretching vibrations in the carboxyl group of OleanA was changed by -3 cm^{-1} . This confirms the formation of a hydrogen bond $-\text{C}=\text{O}\cdots\text{H}-\text{O}-$. By complexation there are some changes in the frequency absorption band of CH bonds: $2936\rightarrow 2929 \text{ cm}^{-1}$, $2870\rightarrow 2865 \text{ cm}^{-1}$ and $1186\rightarrow 1180 \text{ cm}^{-1}$ (OleanA); $2900\rightarrow 2903 \text{ cm}^{-1}$ and $1189\rightarrow 1180 \text{ cm}^{-1}$ (Chol). This fact may indicate the presence of hydrophobic contacts.

Keywords: triterpene glycosides, aescin, oleanolic acid, cholesterol, supramolecular complex, horse chestnut, FTIR spectroscopy.

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