THE CONFIGURATION OF THE ACID RESIDUE IN THE MOLECULES OF FLOROSELIN, SESELIRIN, AND SESELIFLORIN

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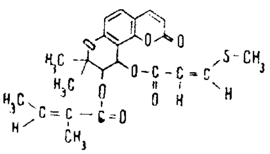
We have previously reported the trans configuration of the olefinic protons of the 3-methylthioacryloyloxy group in the molecules of the dihydrofurocoumarin floroselin, the dihydrofurocoumarin seseliflorin, and the chromone seselirin [1-3].

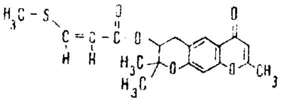
The trans configuration of the olefinic protons was deduced by a comparison of the melting points of the 3-methylthioacrylic acid (121.5-122°C) obtained by the saponification of floroselin with literature data [4] for the trans form of this acid (mp of cis-3-methylthioacrylic acid 99-100°C, and that of the trans-3-methylthioacrylic acid 124°C).

However, the results of a comparison of the spin-spin coupling constants of the olefinic protons of the 3-methylthioacryloyloxy group in the molecules of floroselin, seseliflorin, and seselirin, and also in the molecule of the free acid isolated by the saponification of floroselin (10.0 Hz) with the new literature figures for trans-3-methylthioacrylic acid (J=15.0 Hz, mp 141°C) [5] shows the cis configuration of the 3-methylthioacryloyl group in these compounds. As Dr. L. Novotny has kindly informed us, he and his colleagues [4] had in both cases a mixture of the cis and trans forms of 3-methylthioacrylic acid.

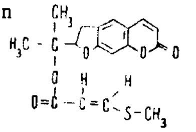
Thus, floroselin, seselirin, and seseliflorin have the following structures:



Floroselin



Seselirin



Seseliflorin

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