Crystal and Molecular Structure of Subchrysine - a New Germacranolide from Artemisia subchrysolepis

Arman T. Kulyjasov^b, Irina Yu. Bagryanskaya^a, <u>Yurii V. Gatilov^a</u>, Makhmut M. Shakirov^a, Victor A. Raldugin^a, and Sergazy M. Adekenov^b

^aNovosibirsk Institute of Organic Chemistry, Siberian Branch of the Russian Academy of Sciences, 9 prosp. Acad. Lavrent'eva, 630090 Novosibirsk, Russian Federation. Fax: +7 (383 2) 34 4752. E-mail: raldugin@nioch.nsc.ru ^bInstitute of Phytochemistry MS-AS Republic of Kazakhstan, 470032 Karaganda, Erdzanova av., postbox 19. Fax: +7 (321 2) 51 1023.

A new lactone, named as subshrysine, have been isolated from the aerial part of *Artemisia subchrysolepis* Filat. The structure of this compound is formulated as $\underline{1}$ (¹H and ¹³C NMR spectra, X-ray data). Absolute stereochemistry of ($\underline{1}$) was deduced from CD data for its 1-O-acetate (negative Cotton effect at 258 nm due to $n \rightarrow \pi^*$ - transition in methylenlactone chromophore).



Data of conformational analysis (PM3 and MMX) of subchrysine are presented and discussed also. Semiempirical method PM3 and calculations by method of molecular mechanics (programme of MMX) predict different conformations as the most stable.

NMR spectra ¹H and ¹³C show that molecule of lactone <u>1</u> exists in two conformational states within temperature range between - 20° C to - 60° C. «Crystalline» conformer of subchrysine corresponds to main conformational state of molecule as seen in low-temperature NMR spectra (solvent - CD_2Cl_2).