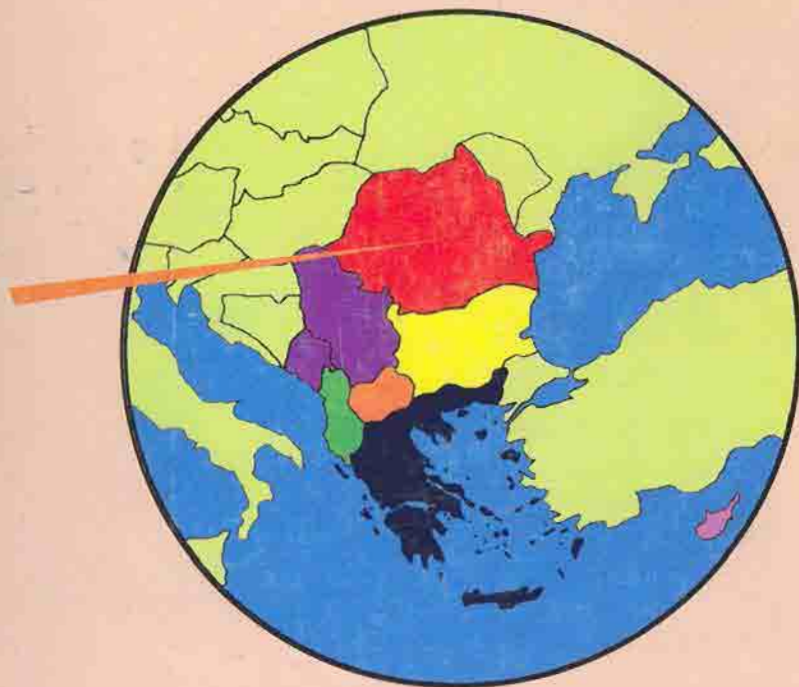


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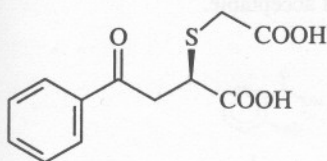
ROMANIA

CRYSTAL STRUCTURE OF 2-CARBOXYMETHYLSULFANYL-4-OXO-4-PHENYLBUTYRIC ACID

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We have synthesized a series of 2-carboxymethylsulfanyl-4-oxo-4-arylbutyric acids. Compounds having fragment $-S-CH_2-COOH$ in their structure, exert a potent antyrheumatic [1], hypolipidemic [2], immunomodulative [2] and antibacterial [3] activities.



Scheme 1

The crystal structure of (*R*)-(-)-2-carboxymethylsulfanyl-4-oxo-4-phenylbutyric (Scheme 1) acid was determined. This compound has been characterized by single crystal X-ray analysis. It crystallizes in the triclinic system, space group $P1$ -, with unit-cell parameters: $a = 8.116(3) \text{ \AA}$, $b = 9.435(2) \text{ \AA}$, $c = 10.377(2) \text{ \AA}$, $\alpha = 96.40(2)^\circ$, $\beta = 107.32(2)^\circ$, $\gamma = 112.52(3)^\circ$. The X-ray diffraction data were collected on an Enraf-Nonius CAD-4 diffractometer using $Mo-K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$).

In crystal lattice, the organic molecules and water are linked together by a network of intermolecular hydrogen bonds. Some of H-bonds are fairly strong with distance between H atom and H-acceptor less than 2.0 \AA . All non-hydrogen atoms, except those in carboxylic groups, are approximately coplanar. Two $COOH$ groups are oriented to the opposite sides of the plane defined by other non-hydrogen atoms.

In the crystal lattice the molecules are oriented in such way that between sp^2 hybridized atoms exists $\pi \dots \pi$ stacking interaction with interatomic distance of about 3.5 \AA .

[1] K. Kameo, K. Ogawa, K. Takeshita, S. Nakaike, K. Tomisava:

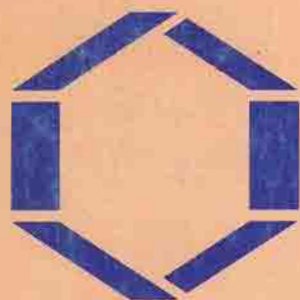
Chem. Pharm. Bull. 36(6) 2050 (1988) and reference cited therein

[2] K. Tomisava, K. Kameo, T. Matsunaga, S. Saito, K. Sohoda, T. Asami, K. Sota

Chem. Pharm. Bull. 33 2386 (1985)

[3] Branko Drakulić, Marina Soković and Ivan Juranić: To be published (submitted to the same congress).

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