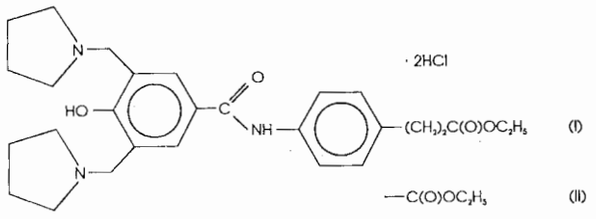
protonated compounds of that type (*J.Med.Chem.* **34**, 2678; *Acta Cryst.* C47, 1038) showed that protonation of the pyrrolidine ring N atom is a key determinant of conformation; hence, we have determined the structures of two diprotonated derivatives to complete the study.

Crystal data: (I) H_2O, 0.5 CH_3OH, C2/c, Z=8, a=20.301, b=11.296, c=24.901Å, β=93.19°, R=0.071. (II) $P2_1/c$, Z=4, a=12.903, b=16.430, c=13.731Å, β=103.64°, R=0.057.

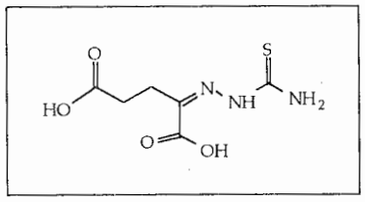


PS-04.01.21 **A STRUCTURAL INVESTIGATION ON THE α-KETOGLUTARIC ACID THIOSEMICARBAZONE IN METAL COMPLEXES** By M. Belicchi Ferrari, G. Gasparri Fava, C. Pelizzi, P. Tarasconi and G. Pelosi, Istituto di Chimica Generale ed Inorganica, Centro di Studio per la Strutturistica Diffrattometrica del CNR, Viale delle Scienze, 43100 Parma, Italy

Thiosemicarbazones present biological and chemical properties which cover a broad spectrum of potentially useful chemotherapeutic properties (antitumoral, antibacterial, as well as antiviral) (S.Padhyè & G.B.Kauffman, Coord.Chem.Rev. ,1985, 63, 127-160).

Our research aims at the understanding of the correlation between the structural features and the biological properties of this class of compounds under different experimental conditions. Many pyruvic acid and pyridoxal thiosemicarbazone complexes have already been synthesised and characterised. Some of them containing copper or cobalt, tested in vitro, have shown an inductive effect on FLC (Friend erythroleukemia cells) erythroid differentiation and a suppressive efficacy on their proliferation (M.Belicchi Ferrari, G.Gasparri Fava, P.Tarasconi, R.Albertini, S.Pinelli & R.Starcich, J.Inorg. Biochem., 1993, accepted for publication).

At present we are studying the behaviour of the α-ketoglutaric acid thiosemicarbazone, a ligand which presents many potential donor



atoms and a variety of potential conformations, in complexes with different co-ordinating ions such as zinc, copper and nickel. All of the cited compounds have been synthesised and characterised spectroscopically and their crystal structures have been determined by X-ray analysis.

PS-04.01.22 **CRYSTAL STRUCTURE OF A QUINOLONE DERIVATIVE WITH ANTIMALARIAL ACTIVITY**. By **Mario V. Capparelli*** (Fac. Ciencias, Univ. Central de Venezuela, Caracas 1050, Venezuela), **Jaime E. Charris** (Fac. Farmacia, Univ. Central de Venezuela, Caracas 1050, Venezuela) and **Duilio Cascio** (Molec. Biology. Inst., UCLA. Los Angeles, CA 90024, USA)

According to the World Health Organization malaria is still the chief cause of human death, aside from natural causes. The antimalarial drugs currently in use, mainly aminoquinolines, pyrimidines, sulfonamides and sulfones, are being rendered increasingly ineffective by the appearance of resistant strains of *Plasmodium*.

A number of new N-methylated quinolones were synthesized as a part of a program to develop more active and less toxic new antimalarial drugs. These compounds were tested *in vitro* for antimalarial activity and seven of them were found to be between 100% and 75% effective in inhibiting the growing of *P. falciparum*.

The crystal structure of one of the active compounds, *viz.* 2,4-diamino-10-methyl-9-methoxypyrimido[4,5-b]5-(10H)-quinolone (activity 89%), was determined. The tricyclic molecule is essentially planar, with both methyl groups out of the plane. Bond lengths and angles are within normal values; the C=O distance, 1.263(2) Å, indicates a weakened double bond. The molecules are stacked along [101], with N-H...O and N-H...N bonds connecting molecules in adjacent piles.

Crystal Data: $C_{13}H_{13}N_5O_2$, M_r = 271.28, monoclinic, $P2_1/n$, a = 10.664(2), b = 10.111(2), c = 11.318(2) Å, β = 99.351(4)°, D_x = 1.50 gcm^{-3}, Z = 4, F(000) = 568, μ(Mo-Kα) = 1.00 cm^{-1}. The structure was solved by direct methods and refined to R = 0.049 for 1941 unique reflections with I > 3 σ(I).

PS-04.01.23 X-RAY CRYSTAL STRUCTURAL ANALYSIS OF TWO NEW POTENTIAL ACTIVE ANTIMALARIAL DRUGS. D. Gómez de Andérez[1], R. Avila[1], J. Domínguez[2], and S. Khan[3]. [1]Universidad de Los Andes, Facultad de Ciencias, Mérida-Venezuela, [2]Universidad Central de Venezuela, Facultad de Farmacia, Caracas-Venezuela, [3]University of California, Chemistry Dept., Los Angeles, CA-USA.

Malaria is distributed widely throughout populated areas where the average temperature is 60°F or higher and some extends to more temperate climates. Because of the acute toxicity of some antimalarial drugs, there is interest in testing new compounds against this disease. Methylthio-4-ciano-5-pyrazolone ($C_5H_5N_3OS$) and 3-amino-5-(2-methoxyanilino)-4-metoxy-carbonylpyrazol ($C_{12}H_{14}N_4O_3$) are compounds with potential antimalarial activity.
X-Ray single crystal analysis shows: (a) C_5H_5OS is monoclinic, $P2_1/c$, a=4.514(1), b=13.536(1), c=11.455(1)A and B=92.82(1), Mo K=O, 7107A. F(000)=320, 2349 unique reflections measured, 1167 with I>3σ(I). The structure was solved by direct methods, the final anisotropic refinement using full matrix least-square gave R=0.047, Rw=, GOF=1.77. (b) $C_{12}H_{14}N_4O_5$ is monoclinic $P2_1/n$, a=13.108(3), b=7.739(2), c=13.224(3)A, B=110.65(1) MoKα=0.7107, F(000)=552. 4053 unique reflections measured, 1890 with I>3σ(I). The final anisotropic refinement gave R=0.049, Rw=0.060, GOF=1.683.

PS-04.01.24 **BETICOLINS, A NEW CLASS OF TOXINS PRODUCED BY CERCOSPORA BETICOLA, A PARASITIC STRAIN OF SUGAR BEETS.** By A. Neuman[1], T. Prangé[1], M.L. Millat[3], J. Einhorn[2], J.P. Blein[3]. . [1]Chimie Biomoléculaire (URA 1430 CNRS) UFR-Biomédicale, 93012-BOBIGNY CEDEX, France ; [2] Laboratoire de Phytopharmacie, I.N.R.A., F-78026 VERSAILLES CEDEX, France ; [3] Laboratoire de Phytopharmacie, I.N.R.A., BV 1540, 21034-DIJON CEDEX, France

Cercospora Beticola is a parasitic fungus responsible for leaf spot disease on sugar beet. The pathogen agent produces, in addition to the red cercosporin, several yellow toxic metabolites with a new

