PS05.07.06 CRYSTAL STRUCTURES OF SOME ACRIDINE DIONES - LASER ACTIVE COMPOUNDS. K. Gunasekaran, V.K. Ganesh, D. Velmurugan. Department of Crystallography and Biophysics, University of Madras, Madras 600 025, India; S. Ramasubbu, Department of Oral Biology, SUNY, Buffalo, USA; K. Panneerselvam and Manuel Soriano-Garcia, Instituto de quimica UNAM, circuito Exterior, cd. Univ, Mexico D.F. 04510, Mexico; V.T. Ramakrishnan, Department of Organic Chemistry, University of Madras, Madras -25

DNA intercalating property is considered as one of the potent factor for DNA binding drugs. Acridine orange and 9-amino acridine are widely studied towards underdstanding their intercalating behaviour. Here three acridine diones which are showing laser activity are taken for crystallographic study as the first phase of work for their binding nature studies with DNA. (1)9-vinyl-10-methyl, (2)9-phenyl, 3,4,6,9,10 hexahydro 2,2,8,8 tetramethyl 1,8 acridine dione and (3) 9-(4-methoxyphenyl)-10- phenyl 3,4,6,9,10 hexahydro 1,8 acridine dione. Preliminary results:

	a	b	c	α	β	γ
1	14.578(1)	15.398(2)	8.646(1)	90	90	90
2	17.618(2)	17.618(2)	10.121(2)	90	90	90
3	8.670(1)	11.140(1)	21.198(1)	90	92.5(1)	90

The space groups are Pnma, P42/n and P21/n respectively. The final R factor for the three are 0.061, 0.049 and 0.051 respectively. In all the three cases the compound itself folded into different extents and the substituents are in cis type orientations. The conformational details will be presented.

PS05.07.07 CRYSTAL STRUCTURE OF TRANS[1,5-BENZOTHIAZEPINE-4(5H)-ONE-1OXIDE-2,3-DIHYDRO-3-HYDROXY-2(4-METHOXYPHENYL)](+). P.Kumaradhas and K.A.Nirmala, Department of Physics, Bangalore University, Bangalore-560 056, INDIA

The title compound is a drug intermediates of diltiazem. Diltazem belongs to the family of drugs commonly named as calcium channel blockers or calcium antagonist and is useful for the treatment of cardiac and coronary diseases. The structure of title compound, is takenup to understand the effect of the molecular geometry, conformation of the seven membered ring and the crystal packing. The colourless crystals were grown from ethonal at room temperature, and x-ray diffraction data was collected at All India Institute of Medical Sciences, New Delhi. Crystal Data: $C_{16}H_{15}NO_4S$, Space group P-1, Triclinic, a=7.721(4), b=8.695(2), c=11.347(9)Å, α=83.38(2)° ß=79.79(6)°, γ=81.38(2)°, V=737.7(8)Å^3, Z=2, λ=1.5418Å, D_c=1.429 mg/^{3}

The structure has been solved by direct method SHELXS-86 and refined by full matrix least-squares method to the final value of R=0.058 and wR=0.140. The seven membered ring is distorted showing twist boat conformation. The methoxy and hydroxy groups has torsion angle 61.5(4)Å that is gauche orientation. The carbonyl oxygen is pseudo-equatorial and methoxyphenyl group is axial to the seven membered ring. There are two intermolecular hydrogen bonding forming the dimers in the crystal. On the whole the crystal packing is stabilized by hydrogen bonding.

PS05.07.08 STRUCTURE OF N'[BIS(METHYLTHIO)-METHYLEN] CYANO-ACETAHYDRAZIDE. Ariel Gómez González *, Ramón Pomés Hernández and Aristides Rosado Pérez, National Center for Scientific Research. P.O.Box 6990. Havana. Cuba, Basilia M. Nápoles Frías., Pedagogical University, Havana, Cuba, Raúl Alfredo Toscano, Institute of Chemistry, UNAM. 04510, México, D.F.

In the course of a project for finding possible bioactive products attention has been focused on the use of cyanoacetahydrazide derivatives as drugs (Negwer, 1987); in this light the title compound, $C_6H_9N_3OS_2$, has been synthesized. It was obtained from the cyanoacetahydrazide by adding, at room temperature, carbon disulfide and methyl iodide. The title compound has shown biological activities against fungus and parasites of bovine cattle.

Crystals suitable for X-ray analysis were obtained by evaporation from ethanol solution. The compound crystallize in the orthorhombic system with space group $P2_12_12_1$, Z=4, a = 4.634 (1) , b = 13.069 (4), c = 15.832 (5) Å, 680 F(hkl), R=3.9, wR=5.0 %. The structure was solved by direct method using *SHELXTL-Plus.*

The crystal packing includes infinite chains of hydrogen bonded molecules along the [100] direction. The amine N(1) atom of a molecule is hydrogen bonded to the carbonyl O(1) atom of the molecule of the adjacent cell, the length of the N...O bond is 2.813 (6) Å. The chains are held in the crystal by means of van der Waals forces. The bond lengths and angles are in good agreement with the average literatute values.

Negwer, M. (1987). Organical-Chemical Drugs and Their Synonyms, Akademie Verlag, Berlin.