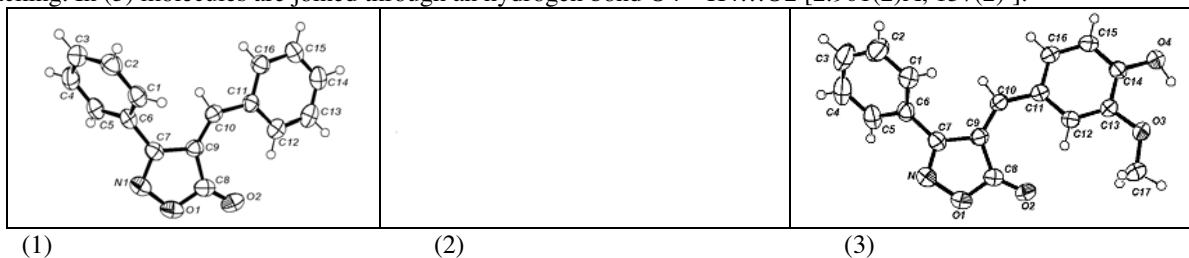


## W0162

**A New Biological Insight for the Organic Compounds  $C_{16}H_{11}O_2N$ ,  $C_{17}H_{13}O_3N$  and  $C_{17}H_{13}O_4N$ .** H.C.A.S. Napolitano<sup>1</sup>, R.H.A. Santos<sup>1</sup>, A.B.F. Silva<sup>1</sup>, L. Silva<sup>2</sup>; R. Borges<sup>2</sup> & C.N. Alves<sup>2</sup>, <sup>1</sup>Instituto de Química de São Carlos, USP & <sup>2</sup>Dept. de Química, CCEN, UFPA.

The combination of different pharmacophoric groups in a single molecule to obtain lead compound is a strategy frequently used to design new compound potentially useful in the management of disease with complex and heterogeneous pathogenesis. Aiming at obtaining this kind of compounds for inflammatory disorders three substituted 3-phenyl-2-isoxazolin-5-one-4-benzilidene were synthesized and their crystal structures were determined:  $C_{16}H_{11}O_2N$  (1),  $C_{17}H_{13}O_3N$  (2) and  $C_{17}H_{13}O_4N$  (3). These compounds showed significant anti-inflammatory activity and their structures were refined to R1-values of 0.0451 (1), 0.0523 (2) and 0.0465 (3). It is interesting to note that the dihedral angle between the sigma bonded phenyl ring and the isoxazolin decreases with substitution [59.0 (1), 54.6 (2), and 33.4° (3)] and they are involved in C—H... $\pi$  interactions: C2—H2...Cg<sup>2</sup> [2.929Å, 130.8°] and C14—H14...Cg<sup>3</sup> [2.955Å, 136.2°] (1); C17—H17...Cg<sup>2</sup> [2.839Å, 147.8°] (2); C2—H2...Cg<sup>3</sup> [3.014Å, 147.3°] (3). It may be postulated that in (1) and (2) these interactions are responsible for the crystal packing. In (3) molecules are joined through an hydrogen bond O4—H4...O2 [2.901(2)Å, 157(2)°].



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