Abstracts from the Eighth Annual Meeting of the Molecular Graphics Society

The eighth annual meeting of the Molecular Graphics Society was held at the University of St. Andrews, St. Andrews, Scotland, from 29 to 31 March 1989. The abstracts from the meeting are collected below.

Crystal and Molecular Structure of a Potential Anti-oestrogenic Agent and Quantum Mechanical Modeling of Some Related Compounds

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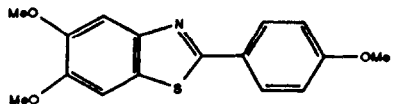
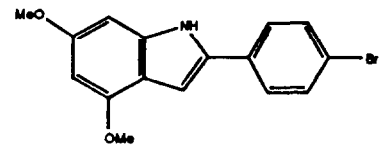
A series of compounds that may show structural and chemical similarities to the flavanoids have been synthesized, with a view to exploring their activity as antioestrogenic agents. These are related to the following benzothiazole compound, (I).



The three-dimensional structure of compound (I) has been determined by X-ray diffraction. Crystals of (I) are monoclinic, space group $P2_1/c$, a = 17.142(1)A, b = 11.165(1)A, c = 7.683(2)A, β = 101.34(1)°. 2 307 reflections have been refined to R = 0.039. The most interesting feature of the structure is a relatively large deviation from planarity. The angle of twist between the two ring systems is 21.3°.

We have performed semiempirical quantum mechanical calculations on this and related compounds. On optimizing all torsion angles, we found that the deviation from planarity increases for (I), giving a new twist angle of 43.9°. However, all the other structures remain planar when optimized.

Similar calculations were performed on the related indole compound shown below.



As with (I), the crystal structure shows a deviation from planarity. The twist angle of −28.6° increases to a value of −111.3° when the torsion angle optimization calculation is performed.

These results are rationalized in terms of steric interactions and crystal packing. The structure of a related benzothiazole and a related indole are predicted.

Graphical Description on the Solute Surface of the Solvation Energy and Solvent Transfer Energy

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The graphical representation of quantum mechanical descriptions of solute properties on the solute molecular surface is attempted with the aid of color-coded surface point models.

The surface is defined in terms of suitably scaled van der Waals spheres, centered on each atom of the solute. For each sphere a set of regular polyhedra is defined. The computed properties, depending on the area of the almost equilateral triangle making up the polyhedron, are displayed as a color-coded point placed in the middle of the related surface.

We have considered a few properties of two solutes: dimethyl ether and propanol. The properties considered are the solvation free energy (its electrostatic and cavi-

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