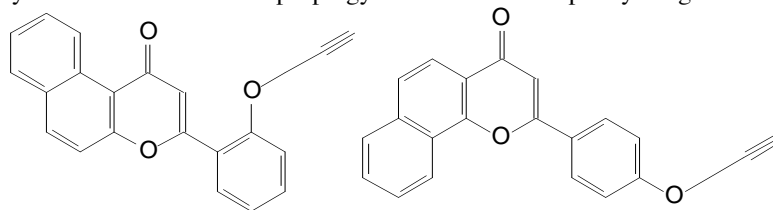


E0004

A Crystallographic Study of Naphthoflavone Inhibitors of Cytochrome P450. Cheryl L. Klein Stevens and Najue Zhu, Dept. of Chemistry, Xavier Univ. of Louisiana, New Orleans, LA 70125.

Cytochrome P450 enzymes oxidize both endogenous compounds (steroids, fatty acids, and vitamins) and xenobiotic compounds (drugs, environmental pollutants, and procarcinogens). These enzymes protect the body from foreign substances through this oxidation mechanism allowing the oxidation products to be more readily eliminated. It has been shown that some naphthoflavones function as substrates of some of the P450 enzymes (specifically P450 1A1 and 1B1) and may also function as enzyme inhibitors. In this study, the X-ray crystal structures of four naphthoflavones have been determined. These include α -naphthoflavone 4'-propargyl ether, β -naphthoflavone 4'-propargyl ether, α -naphthoflavone 2'-propargyl ether, and β -naphthoflavone 2'-propargyl ether. All four molecules crystallized with a planar fused ring system substituted with a propargyl ether substituted phenyl ring.



β -naphthoflavone 2'-propargyl ether α -naphthoflavone 4'-propargyl ether

The 2'-propargyl ether substituted phenyl rings twist significantly out of the plane of the fused ring system (37°) while the 4'-propargyl ether substituted phenyl rings are more coplanar (4°) with the fused ring system.

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