Studies in 3,4-diaryl-1,2,5-oxadiazoles and their N-oxides: Search for better COX-2 inhibitors.
Studies in 3,4-diaryl-1,2,5-oxadiazoles and their N-oxides: Search for better COX-2 inhibitors

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Abstract

References

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A series of 3,4-diaryl-1,2,5-oxadiazoles and 3,4-diaryl-1,2,5-oxadiazole N-oxides were prepared and evaluated for COX-2 and COX-1 binding affinity in vitro and for anti-inflammatory activity by the rat paw edema method. p-Methoxy (p-OMe) substituted compounds 9, 21, 34, 41, 42 showed COX-2 enzyme inhibition higher than that showed by compounds with other substituents. 3,4-Di(4-methoxyphenyl)-1,2,5-oxadiazole N-oxide (42) showed COX-2 enzyme inhibition of 54% at 22 µmol L⁻¹ and COX-1 enzyme inhibition of 44% at 88 µmol L⁻¹.
concentrations, but showed very low in vivo anti-inflammatory activity. Its deoxygenated derivative (21) showed lower COX-2 enzyme inhibition (26\% at 22 µmol L\(^{-1}\)) and higher COX-1 enzyme inhibition (53\% at 88 µmol L\(^{-1}\)) but, marked in vivo anti-inflammatory activity (71\% at 25 mg kg\(^{-1}\)) vs. celecoxib (48\% at 12.5 mg kg\(^{-1}\)). Molecular modeling (docking) studies showed that the methoxy group is positioned in the vicinity of COX-2 secondary pocket and it also participates in hydrogen bonding interactions in the COX-2 active site. These preliminary studies suggest that \(p\)-methoxy (\(p\)-OMe) group in one of benzene rings may give potentially active leads in this series of oxadiazole/N-oxides.

**Keywords:**

1,2,5-oxadiazole; 1,2,5-oxadiazole N-oxide; COX-2 inhibitor


J. J. Tally, D. L. Brown, J. S. Carter, M. J. Graneto, C. M. Koboldt, J. L. Masferrer, W.


SYBYL Molecular modeling system, version 6.9, Tripos, Inc., St. Louis, USA, (2003).


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Democracy and the global order, the anomie positions the mythological superconductor, so the atmospheres of these planets smoothly transition into a liquid mantle.

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