

SUMMARY

Alloxazines are closely related to flavins and lumazine. Compared to flavins, however, alloxazines gained little attention until discovering their ingenious ability of undergoing catalytical excited-state proton transfer reactions.

The work provides spectral and photophysical characteristics of three groups of derivatives: - a series of alloxazines substituted in N(1) and N(3) positions with a methyl group, that cannot undergo proton-transfer reactions, - four - ring alloxazines (1,3-dimethylbenzo[g]alloxazine, benzo[g]alloxazine), and - mono- and dimethyl- derivatives represented by 6-methylalloxazine and 8,9-dimethylalloxazine. Majority of experiments was followed by quantum – mechanical calculations at the level of DFT and TD-DFT theory for ground state and excited states, respectively. The main part of the work is a discussion concerning the acid-catalized phototautomerization of model derivatives, 6-methylalloxazine and 8,9-dimethylalloxazine. It was concluded that the phototautomerization occurs in a different way in each case. The position of methyl substituent in the C-ring of alloxazine molecule influences the reaction especially due to electron density changes, rather than steric interaction.