STUDIES ON HOMOPIPERAZINE DERIVATIVES: CONFORMATIONAL ANALYSIS OF 2-(4-ACYLHOMOPIPERAZIN-1-YL)-4-AMINO-6,7-DIMETHOXYQUINAZOLINES BY NMR

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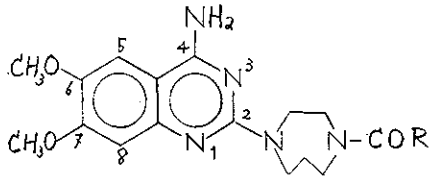
During the course of synthetic studies of the title compounds, we observed unusual behaviors in the n.m.r.spectrum of (1), in which the signals of the terminal CH_3 protons at γ-position appeared as two sets of triplet and one of the aromatic protons showed two different chemical shifts.
Spectroscopic analysis suggested presence of intramolecular interaction in organic solvent such as d_6-DMSO and intermolecular interaction in D_2O.
These intra- and intermolecular interactions might lead to stabilization of specific, at least two, conformations formed through some electrostatic forces between the lone pair electrons of nitrogen at position 1 and the positively charged carbon at the amide function.

The above mentioned unique n.m.r. informations may be explained by the presence of such conformers in the compound.

The conformational structures of (1) and its analogues are proposed.



(1) -R: $-CH_2CH_2CH_3$ (α β γ)