One-pot New Condensation Reaction of Unsymmetrical 1-Methylbarbituric Acid with BrCN and Various Aldehydes in the presence of Et₃N and/or Pyridine

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Many of heterocyclic furo[2,3-d]pyrimidines [1], spirobarbituric acids [2] and fused uracils [3,4] are well known as wide varieties of pharmaceutical and biological effects. Reaction of 1-methylbarbituric acid (1-MBA, 1) as an unsymmetrical barbituric acid with cyanogen bromide and various aldehydes (2) in the presence of triethylamine and/or pyridine afforded the salts of pyridinium- and/or triethylammonium-5-bromo-2,4,6-trioxohexahydro-1-methylpyrimidin-5-ide (3 and/or 4) and diastereomeric mixtures of new class of heterocyclic stable 5-aryl-1,1'-dimethyl- and 5-aryl-3,1'-dimethyl-1H,1'H-spiro[furo[2,3-d]pyrimidine-6,5'-pyrimidine]2,2',4,4',6'(3H,3'H,5'H)-pentaones (5-8) which are dimeric forms of 1-methyl barbiturate at the range of 0°C to room temperature. In the reaction of some aldehydes with 1 and BrCN were afforded at least three diastereomers. Another two aldehydes such as 4-cyano- and 2-hydroxybenzaldehydes gave exclusively two diastereomers in which binded to the salt of triethylammonium hydrobromide by intermolecular H-bond in ratio of 1:1. 4-Hydroxybenzaldehyde gave exclusively one diastereomer under the same condition. Aldehydes possessing strong electron-donor were produced exclusively two geometric isomers of Knoevenagel adduct (E- and Z-isomers). The mixture of diastereomers was deduced by ¹H NMR, ¹³C NMR and FT-IR spectroscopy.

REFERENCES