

SYNTHESIS OF SOME 5,6-DIAMINO-AS-TRIAZIN-3(2H)-ONES AND THEIR REACTIVITY
FOR THE CYCLISATION TO THE DERIVATIVES IN THE NOVEL RINGS, 6-AZAPURINE,
6,8-DIAZAPURINE, AND 4,7-DIAZAPTERIDINE

Keiji Kaji, Hironu Nagashima, Hirohisa Oda, and Masami Kawase
Gifu College of Pharmacy
East 5-6-1, Mitahora, Gifu

Synthesis of some derivatives in the novel ring systems, imidazo[4,5-e]-as-triazine(6-azapurine), y-triazolo[4,5-e]-as-triazine(6,8-diazapurine), and as-triazino[6,5-e]-as-triazine(4,7-diazapteridine), has been described.

2-Benzyl-6-bromo-as-triazine-3,5(2H,4H)-dione reacted smoothly with ammonia and benzylamine to give 6-amino- and 6-benzylamino-2-benzyl-as-triazine-3,5(2H,4H)-dione respectively. Selective thionation of these amino derivatives, by heating with phosphorus pentasulphide in pyridine, to lead to 6-amino- and 6-benzylamino-2-benzyl-as-triazin-3(2H)-one-5(4H)-thione, effectively proceeded and subsequent aminodethiolation of the latter also readily went on to afford 5,6-diamino-, 5-amino-6-benzylamino-, 5-benzylamino-6-amino-, and 5,6-dibenzylamino-2-benzyl-as-triazin-3(2H)-one.

An oxidative mode of cyclisation by heating the appropriate 5,6-diamino compounds with triethyl orthoformate or benzaldehyde in nitrobenzene for a few hours furnished a successful procedure for the preparation of 2-benzyl-5H- and 2,5-dibenzyl-imidazo[4,5-e]-as-triazin-3(2H)-one, or 2-benzyl-5H-, 2,5-dibenzyl-, and 2,7-dibenzyl-6-phenyl-imidazo[4,5-e]-as-triazin-3(2H)-one.

5,6-Diamino- and 5-amino-6-benzylamino-2-benzyl-as-triazin-3(2H)-one reacted readily with nitrous acid to afford 2-benzyl-5H- and 2,5-dibenzyl-y-triazolo[4,5-e]-as-triazin-3(2H)-one respectively, while the 5-benzylamino-6-amino derivative was unable to undergo the cyclisation in the reaction condition.

6-Amino- and 6-benzylamino-5-(1'-methylhydrazino)-2-benzyl-as-triazin-3(2H)-one, derived easily from 6-amino- and 6-benzyl-as-triazin-3(2H)-one-5(4H)-thione by the action of methylhydrazine at the room temperature respectively, were heated in formic acid to furnish the cyclisation to 2-benzyl-6H- and 2,8-dibenzyl-5-methyl-as-triazino[6,5-e]-as-triazin-3(2H)-one respectively, although 5-hydrazino-6-amino-2-benzyl-as-triazin-3(2H)-one was likely to undergo another mode of cyclisation in the reaction with triethyl orthoformate.