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ABSTRACTS

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ELECTRON IMPACT IONIZATION MASS SPECTRA OF SOME SUBSTITUTED DIPYRIDO[1,2-_a_:4,3-_d_]PYRIMIDINONES

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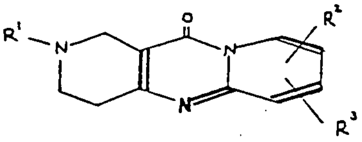
The aim of this study is to report the electron impact ionization mass spectra of 20 dipyrido[1,2-_a_:4,3-_d_]-pyrimidin-11-ones, the structures of which are represented in Table 1. The degree of aromaticity of the tricycle varies from compound to compound.

The substituents R^1, R^2 and R^3 of the dipyrido-[1,2-_a_:4,3-_d_]pyrimidin-11-ones did not have any decisive effect on their fragmentation. Instead the conjugation of the double bonds and the degree of aromatization directed the molecular cleavages very strongly. So these compounds can be divided into four groups (1 - 13, 14 - 15, 16 and 17 - 20), inside which there were many similarities in fragmentations.

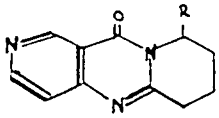
The molecular ions of all the compounds studied were quite stable. The ions $[M\text{-}PhCH_2]^+$ from compounds 1 - 6 and $[M\text{-}H]^+$ from 7 - 10 fragmented similarly. Characteristically they lost 28 m.u. By accurate mass measurements it was proved that the resulting peak was a doublet where the main component resulted from the loss of $H_2CN^{\cdot}$ and the minor component from the loss of CO. The former component lost further another 28 m.u. This time the main route corres-ponded to a loss of CO.

The fragmentation of compounds 14 and 15 was fairly scarce and it was dominated by loss of simple hydrocarbon fragments. In the spectrum of compound 16 the only significant peaks in addition to that of $M^{+\cdot}$ corresponded to the ions $[M\text{-}HCN]^{+\cdot}$ and $[M\text{-}HCN\text{-}CO]^{+\cdot}$. Splitting of hydrocarbon and CO fragments could be observed also in compounds 17 - 20.

Table 1. The structures of the studied compounds.

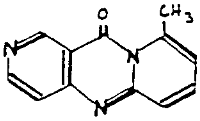


Compound	R^1	R^2	R^3
1	$PhCH_2$	H	H
2	PhCH2	6-Me	H
3	$PhCH_2$	7-Me	H
4	$PhCH_2$	8-Me	H
5	$PhCH_2$	9-Me	H
6	$PhCH_2$	7-Me	9-Me
7	H	H	H
8	H	H	6-Me
9	H	H	8-Me
10	H	H	9-Me
11	$PhCH_2$	6-OH	H
12	PhCO	9-Me	H
13	$HOCH_2CH_2CH_2$	9-Me	H

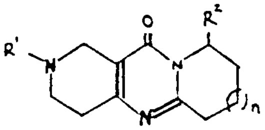


14 R = H

15 R = Me



16



17 $R^1 = R^2 = H$, $n = 1$

18 $R^1 = H$, $R^2 = Me$, $n = 1$

19 $R^1 = PhCH_2$, $R^2 = H$, $n = 1$

20 $R^1 = R^2 = H$, $n = 2$