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## Nucleosides, Nucleotides and Nucleic Acids

Publication details, including instructions for authors and subscription information:

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## Mass Spectrometric Study of Modified Uridines and Their N<sup>3</sup>—Isomers

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**To cite this Article** Sochacki, Marek(1990) 'Mass Spectrometric Study of Modified Uridines and Their N<sup>3</sup>—Isomers', *Nucleosides, Nucleotides and Nucleic Acids*, 9: 3, 461 — 462

**To link to this Article:** DOI: 10.1080/07328319008045175

**URL:** <http://dx.doi.org/10.1080/07328319008045175>

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# MASS SPECTROMETRIC STUDY OF MODIFIED URIDINES AND THEIR N<sup>3</sup>-ISOMERS

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**Abstract:** The mass spectral fragmentations of modified uridines and their N<sup>3</sup>-isomers are discussed in context of the b+41 ion formation.

In the present work the electron impact mass spectra of modified uridines (1) and their N<sup>3</sup>-isomers (2) (Figure 1) have been analyzed.

The main fragmentation pathways of all investigated compounds correspond to known EI fragmentation of underivatized nucleosides. However, in the mass spectra of N<sup>3</sup>-isomers (2) an interesting peak b+41 (at m/z 41 units higher than the peak corresponding to the pyrimidine base) has been observed. The intensity of the b+41 ion may be used to

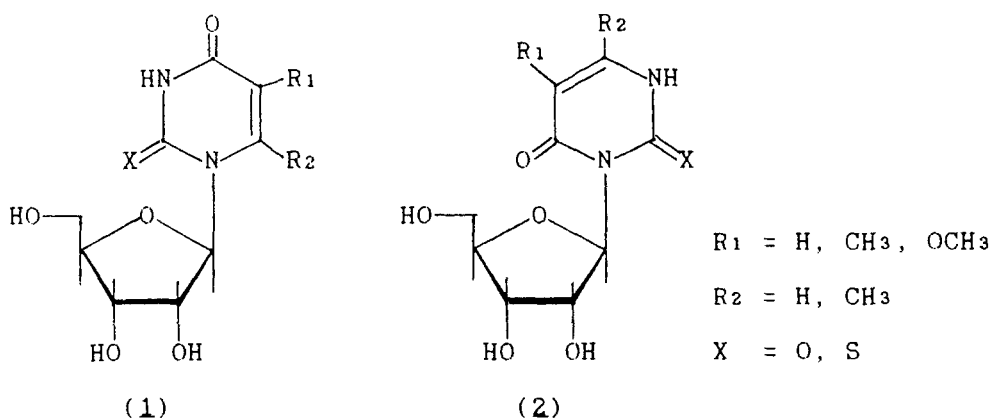


FIGURE 1. Structures of modified uridines.

TABLE 1. Relative intensity of the b+41 ion in the mass spectra of modified uridines and their N<sup>3</sup>-isomers

Compound			70 eV		15 eV	
R <sub>1</sub>	R <sub>2</sub>	X	N <sup>1</sup> -isomer	N <sup>3</sup> -isomer	N <sup>1</sup> -isomer	N <sup>3</sup> -isomer
H	H	O	1.8	6.4	1.6	11.1
CH <sub>3</sub>	H	O	1.0	8.3	0.4	14.0
OCH <sub>3</sub>	H	O	0.2	1.4	0.1	1.6
H	CH <sub>3</sub>	O	3.5	8.0	4.1	9.0
H	H	S	26.9	11.5	27.2	16.3
OCH <sub>3</sub>	H	S	4.6	1.5	4.8	1.8

differentiate N<sup>1</sup>- from N<sup>3</sup>-isomers of modified uridines (Table 1).

The detection of the b+41 ion in the mass spectra of N<sup>3</sup>-isomers of modified uridines and in model compounds: N- $\beta$ -D-ribofuranosylpyrimidone-2, N- $\beta$ -D-ribofuranosylpyridone-2 as well as in 2-thiouridines<sup>1</sup> provides some additional information concerning the mechanism which has been proposed for the production of this ion in the fragmentation of cytidines<sup>2</sup> and 3-deazauridine<sup>3</sup>. The carbonyl or thiocarbonyl group adjacent to the N-glycosidic bond and the conjugated double bond seem to be necessary for the b+41 ion formation. The sulphur atom at the 2-position significantly facilitates production of this ion, while chemical nature of substituents at 4-, 5- or 6-position has relatively less influence.

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