Mitomycin antitumor compounds. Part 1. CD studies on their molecular structure.

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The UV-Vis and circular dichroism (CD) spectra of several mitomycin antitumor compounds and some of their derivatives were analyzed in order to attribute the proper assignment to their electronic transitions. The lowest energy $\pi \rightarrow \pi^*$ transition was found to depend on the effect of the auxochromic group in the aromatic ring, whereas the three $n \rightarrow \pi^*$ transitions, present at around 240, 400 and 560 nm, are related to the C(9)=O of the carbamoyl group and to the C(8)=O and the C(5)=O of the quinone, respectively. The chirality of the C(9) is responsible for the sign of the Cotton effect (CE) at around 240 nm, whereas the substituents of the chromophore for mitosane derivatives and the conformation of the carbamoyloxymethyl group at C(9) determine the CE sign of the $^1A \rightarrow {}^1L_b$ transition. When the aziridine ring was opened and mitosenes derivatives were obtained, CD spectra did not differ significantly among the compounds and the bands associated to the different transitions had similar Cotton effect. Our findings suggest that the differences in the CD spectra, observed between mitosanes and mitosenes, are probably related to the more rigid molecular structure of the mitosene derivatives and the different conformations in solution of the C(9) side chain.

Słowa kluczowe

Mitomycin, Mitosane, Mitosene, Circular dichroism, Transition assignment

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