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

**Synthesis and Biological Activities of N-Alkyl Derivatives of o-, m-, and p-Nitro (E)-4-Azachalcones and Stereoselective Photochemistry in Solution, with Theoretical Calculations**

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**Abstract:** The N-alkyl derivatisation and photochemical dimerisation of 3 o-, m-, and p-nitro substituted 4-azachalcones (1-3) yielded 3 new o-, m-, and p-nitro substituted (E)-N-decyl-4-azachalconium bromides, (2E)-1-(2-nitrophenyl)-3-(N-decyl-4-pyridinium bromide)-2-propen-1-one (4), (2E)-1-(3-nitrophenyl)-3-(N-decyl-4-pyridinium bromide)-2-propen-1-one (5), and (2E)-1-(4-nitrophenyl)-3-(N-decyl-4-pyridinium bromide)-2-propen-1-one (6), and 3 new dimers in solution, (1 $\beta$ , 2 $\alpha$ )-di-(3-nitrobenzoyl)-(3 $\beta$ , 4 $\alpha$ )-di-(4-pyridinyl) cyclobutane (7), (1 $\beta$ , 2 $\alpha$ )-di-(4-nitrobenzoyl)-(3 $\beta$ , 4 $\alpha$ )-di-(4-pyridinyl) cyclobutane (8a), and (1 $\beta$ , 2 $\beta$ )-di-(4-nitrobenzoyl)-(3 $\beta$ , 4 $\alpha$ )-di-(4-pyridinyl)cyclobutane (8b), stereoselectively. The monomeric compounds showed good antimicrobial activity against test micro-organisms. The most sensitive micro-organisms were Gram-positive bacteria. The monomers also showed high antioxidant activity, while the dimerisation products 7-8a,b were less active. Compound 6 was found to have similar or even higher activity when compared to the standard antioxidants Trolox<sup>R</sup> and vitamin C, respectively. The possible dimerisation products of compounds 1-3 were calculated theoretically. Experimental and theoretical calculations showed that  $\delta$ -truxinic type dimer is the most stable isomer.

**Key Words:** Nitro-(E)-4-azachalcones, nitro-(E)-N-decyl-4-azachalconium bromide, photodimerisation, antimicrobial and antioxidant activities

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