Molecular Structure of
5-Chloro-2-[p-t-butylphenyl]benzoxazole.
Relation Between Structure and Antimicrobial
Activity of 2,5-Disubstituted Benzoxazoles

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As part of our investigation on antimicrobial agents, the structure of 5-chloro-2-[p-t-butylphenyl]benzoxazole is reported: C₁₇H₁₆ClNO, mol. mass 285.77, monoclinic, space group: C2/c; a = 32.164(6), b = 6.756(1), c = 13.710(3); = 92.73(3)° V = 2975.8(10) ³; dₓ = 1.276 g cm⁻³; Z = 8; F(000) = 1200; μ(CuKα) = 2.219 mm⁻¹. Final R = 0.0658 for 2621 reflections with F > 4 (F). Final atomic coordinates for this 2,5-disubstituted benzoxazole were used as a starting point in molecular modelling of remaining 32 derivatives searched as antimicrobial agents. Electronic parameters calculated with quantum chemistry methods and classical Hansch’s constants were applied in searching for structure-activity correlation. It was established that geometrical parameters (area and volume) and LUMO energy values seem to be most important for the activity.