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: $C_{17}H_{16}ClNO$, mol. mass 285.77, monoclinic, space group: *C*2/*c*; *a* = 32.164(6) , *b* = 6.756(1) , *c* = 13.710(3) ; = 92.73(3)° *V* = 2975.8(10) ^{3}; d_x = 1.276 g cm^{-3}; *Z* = 8; *F*(000) = 1200; μ(CuK) = 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.