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Synthesis, Crystal Structure, and Biological Activity of 4-phenoxyacetyl-substituted methyl-3,4-dihydro-2*H*-1,4-benzoxazine

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ABSTRACT Two novel substituted benzoxazine derivatives have been synthesized through reduction, cyclization, and acylation reactions. The target compounds were characterized by IR, ^{1}H-NMR, ^{13}C-NMR, and HRMS. The single-crystal structures of the title compounds have been further determined by X-ray diffraction. 4-Phenoxyacetyl-3-methyl-3,4-dihydro-2*H*-1,4-benzoxazine (**4a**) crystallizes in orthorhombic system, space group $P2_12_12_1$ with a=8.0411(16) Å, b=8.1386(16) Å, c=21.799(4) Å, V=1426.6(5) Å^3, Z=4, D_c=1.319 g/cm^3, μ=0.091 mm^{-1}, F(000)=600, and the final R_1=0.0335 and $wR_2(I>2\sigma(I))$=0.0841. 4-Phenoxyacetyl-3,6-dimethyl-3,4-dihydro-2*H*-1,4-benzoxazine (**4b**) crystallizes in orthorhombic system, space group $Pca2_1$ with a=23.811(5) Å, b=8.3061(17) Å, c=7.9338(16) Å, V=1569.1(6) Å^3, Z=4, D_c=1.259 g/cm^3, μ=0.086 mm^{-1}, F(000)=632, and the final R_1=0.0342 and $wR_2(I>2\sigma(I))$=0.0827. The title compounds are assembled into a 3*D* supramolecular structure by hydrogen bonds. Compounds **4a** and **4b** showed safener activity on maize against the injury of 2,4-Dbutyl ester.

KEYWORDS Substituted benzoxazine derivatives, synthesis, single-crystal structure, safener activity.

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