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Synthesis and Structure-Activity Relationships of Dinotefuran Derivatives: Modification in the Tetrahydro-3-furylmethyl Part

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Abstract:
The (±)-tetrahydro-3-furylmethyl moiety, which is a characteristic part of the novel neonicotinoid dinotefuran, was found by research in which acetylcholine was selected as the lead compound. SAR (structure-activity relationships) for the tetrahydrofuran part indicated that the non-substituted moiety showed the highest level of activity, 4- and 5-substituted moieties showed intermediate levels, and 2- and 3-substituted moieties lost the activity. Conformational analysis of these compounds indicated that the substituents changed little the hypothetical active conformation of dinotefuran. Computational analysis proved that dinotefuran, a methoxypropyl compound and other neonicotinoids well overlapped, and dinotefuran adopts the active conformation more easily than the methoxypropyl compound.

Keywords:
neonicotinoids, (±)-tetrahydro-3-furylmethyl, dinotefuran, acetylcholine, structure-activity relationships (SAR), 3D-QSAR

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