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Pharmacophore of neonicotinoid insecticides

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Abstract:
Our recent study related to neonicotinoid pharmacophore was presented. The first topic described on the QSAR study with 17 variants of 2-nitroiminoimizolidine. The insect neuroblocking potency is proportionally related both to the Mulliken charge on the nitro oxygen atom and log P. The second raised the functional possibility of the 3-fluoropropyl group as an H-bond acceptor for the neonicotinoid skeleton. Its 2-nitroiminoimidazolidine derivative actually showed the insecticidal tendency common to the neonicotinoids bearing a 6-chloro-3-pyridylmethyl group, although the activating strength was not as high as expected. The third introduced a new type of neonicotinoid compounds of alkylene-tethered twin-structure. The insecticidal activity against American cockroaches was dependent on the tether length and maximized at the hexamethylene with the minimum lethal dose of 2.2 nmol/insects, comparable to that of imidacloprid.

Keywords:
pharmacophore, neonicotinoid, hydrogen bonding, divalent ligand, QSAR

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