New insights on the molecular features and electrophysiological properties of dinotefuran, imidacloprid and acetamiprid neonicotinoid insecticides

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Résumé en anglais	Structural features and hydrogen-bond interactions of dinotefuran (DIN), imidacloprid (IMI) and acetamiprid (ACE) have been investigated experimentally through analyses of new crystal structures and observations in structural databases, as well as by Density Functional Theory quantum chemical calculations. Several conformations are observed experimentally in the solid state, highlighting the large flexibility of these compounds. This feature is confirmed by the theoretical calculations in the gas phase, the numerous and different energetic minima of the three neonicotinoids being located within a 10kJ/mol range. Comparisons of the observed and simulated data sheds light on the hydrogen-bond (HB) strength of the functional group at the tip of the electronegative fragment of each pharmacophore (NO(2) for DIN and IMI and CN for ACE). This effect originates in the 'push-pull' nature of these fragments and the related extensive electron delocalization. Molecular electrostatic potential calculations provide a ranking of the two fragments of the three neonicotinoid in terms of HB strength. Thus, the NO(2) group of DIN is the strongest HB acceptor of the electronegative fragment, closely followed by the cyano group of ACE. These two groups are significantly more potent than the NO(2) group of IMI. With respect to the other fragments of the three neonicotinoids, the nitrogen atom of the pyridine of IMI and ACE are stronger HB acceptors than the oxygen atom of the furanyl moiety of DIN. Finally, compared to electrophysiological studies obtained from cockroach synaptic and extrasynaptic receptors, DIN appears more effective than IMI and ACE because it strongly increases dose-dependently the ganglionic depolarisation and the currents amplitudes. These data suggest that DIN, IMI and ACE belong to two subgroups which act differently as agonists of insect nicotinic receptors.
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