



New insights on the molecular recognition of imidacloprid with *Aplysia californica* AChBP: a computational study

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Auteur	Ceron-Carrasco, José Pedro [1], Jacquemin, Denis [2], Graton, Jérôme [3], Thany, Steeve Hervé [4], Le Questel, Jean-Yves [5]
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Résumé en anglais	<p>The binding of imidacloprid (IMI), the forerunner of neonicotinoid insecticides, with the acetylcholine binding protein (AChBP) from <i>Aplysia californica</i>, the established model for the extracellular domain of insects nicotinic acetylcholine receptors, has been studied with a two-layer ONIOM partition approach (M06-2X/6-311G(d):PM6). Our calculations allow delineating the contributions of the key residues of AChBP for IMI binding. In particular, the importance of Trp147 and Cys190-191, through weak CH...pi interactions and both van der Waals and hydrogen-bond (H-bond) interactions, respectively, are highlighted. Furthermore, H-bonds between hydroxyl groups of both Ser189 and Tyr55 and the IMI nitro group are pointed out. The participation of Ile118, whose main chain NH and carbonyl group are hydrogen-bonded with the IMI pyridinic nitrogen through a water molecule, is characterized. Our simulations also indicate the presence of a significant contribution of this residue through van der Waals interactions. The various trends obtained by the calculations of the pairwise interaction energies are confirmed through a complementary noncovalent interaction (NCI) analysis of selected IMI-AChBP amino acid pairs. Indeed, the contribution of a halogen-bond interaction between IMI and AChBP, recently proposed in the literature, is corroborated by our NCI analysis.</p>
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