Molecular modeling of the ?9?10 nicotinic acetylcholine receptor subtype

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This study reports the comparative molecular modeling, docking and dynamic simulations of human ?9?10 nicotinic acetylcholine receptors complexed with acetylcholine, nicotine and ?-conotoxin RgIA, using as templates the crystal structures of Aplysia californica and Lymnaea stagnalis acetylcholine binding proteins. The molecular dynamics simulations showed that Arg112 in the complementary ?10(-) subunit, is a determinant for recognition in the site that binds small ligands. However, Glu195 in the principal ?9(+), and Asp114 in the complementary ?10(-) subunit, might confer the potency and selectivity to ?-conotoxin RgIA when interacting with Arg7 and Arg9 of this ligand.