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A B3LYP study indicates the relationship between populations of the stable conformers and EAG activity in the insect pheromone Eldanolide

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Conformational analysis with B3LYP calculations has been carried out for the insect pheromone, Eldanolide, and its fluorinated analogues in order to clarify the origin of differences in the pheromone activity among these compounds. The calculations suggested that some conformers had distinctively higher energy for the fluorinated analogues and significant differences were found in the contribution of stable conformers to population between EAG-active compounds and EAG-inactive compounds. This fact indicates a possible mechanism to explain why the pheromone activity is critically influenced by the position of fluorination on Eldanolide.