This thesis is about computing lifetimes of excited states of molecules by using semiempirical methods in simulations of molecular dynamics. Pyrimidine nucleobases and three aza-derivatives were chosen as reference molecules. Simulations of molecular dynamics by program MNDO99 were performed with these molecules and static spectra were computed by programs Gaussian and Orca. All the examined molecules have femtosecond lifetimes of second excited states, pyrimidine nucleobases have also short lifetimes of first excited states in hundreds of femtoseconds. The computed first excited states of aza-derivatives have lifetimes in tens or hundreds of picoseconds and suggest that the higher stability of the states is related to the smaller number of amino groups attached to the ring.