Biochemical Simulations using QM/MM Techniques

by

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Abstract:

QM/MM simulations are increasingly used to model chemical reactions in large systems. Most of the system is treated by a classical force field (MM), while the reaction itself is described by quantum mechanics (QM).

While this approach significantly speeds up single-point calculations, geometry optimizations and molecular dynamics sampling still cause significant difficulties.

I will describe methods to overcome these challenges. Then I will focus on the unraveling of the reaction mechanism of Monoaminoxidase as well as on force field simulations of protein-protein interactions. The binding of tumor necrosis factor to its receptor will be covered as well as the interaction of the epidermal growth factor with its receptor.

Both lead to signal induction in the cell.

Friday, December 13th, 2013, 13:00

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