

Evaluation of peripheral effects for gamma carboxylase effective in blood coagulation and relating proteins using QM/MM methods

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Abstract: Vitamin K-dependent carboxylation is an essential posttranslational modification that converts specific glutamate residues to gamma-carboxyglutamate (Gla) residues in vitamin K-dependent (VKD) proteins that catalyzes by Vitamin K-dependent gamma glutamyl carboxylase [1]. The Gla domains mediate the binding of blood coagulation proteins to membrane surfaces [2]. VKD proteins, included clotting factors (such as factor (F) II, FVII, FIX and FX) and natural anticoagulants (such as protein C, protein S and protein Z) [1]. These proteins play roles in blood coagulation [3]. Molecular dynamics is a simulation methodology often used for studying the conformational rearrangements of molecules and their interactions with other molecular species in a range of environments [4]. Molecular dynamics simulations can be used effectively to understand macromolecular structure-to-function relationships [5] and simulate structures and properties of materials [4]. The crystallographic structure of enzyme and vitamin k-dependent proteins (coagulation factors) is taken from bioinformatics servers. Based on QM/MM methods and using related soft wares, these enzyme and proteins are calculated under different condition. According to analysis of results in format of plot, activity rate in this enzyme are evaluated in diverse temperature and environment. Also interaction of coagulation proteins with enzyme are studied in different condition compared to other factors. These results can be used in pharmaceutical researches.

Keywords: gamma glutamyl carboxylase, coagulation protein, QM/MM

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