Cooperativity of hydrogen bonding network in microsolvated biotin, the ligand of avidin class proteins.

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Rok wydania

2019

Czasopismo

Journal of Molecular Modeling

Numer woluminu

25

Strony

361/1-361/7

DOI

10.1007/s00894-019-4253-7

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Biotin is well known to be bound with exceptional strength by the avidin class of proteins. This ability comes from a match between the biotin-binding pocket of the protein and the structural elements of biotin, including its ureido and thiolane rings. Here we investigate the solvation shell of biotin in water as revealed by classical force field molecular dynamics with GAFF force field. Snapshots from the classical molecular dynamics were then used to generate microsolvated structures. Details of hydrogen bonding patterns present in these microsolvated structures were studied by symmetry-adapted perturbation theory (SAPT). Interaction energy values for small models of biotin hydrated by 5 or 6 water molecules show that the cooperativity constitutes 15–22% of the total interaction energy and corresponds roughly to formation of one additional hydrogen bond to biotin. The SAPT analysis shows the differences underlying hydrogen bonds of similar strength (with oxygen or sulfur atoms as the hydrogen bond acceptors, and with nitrogen atom playing a dual role of the donor and acceptor).

Słowa kluczowe

Biotin, Avidin ligand, Microsolvation, Hydrogen bonding cooperativity, Interaction energy, Symmetry-adapted perturbation theory

Adres publiczny

http://dx.doi.org/10.1007/s00894-019-4253-7

Strona internetowa wydawcy

http://link.springer.com