Comparison of fully optimized α-and 3_{10}-helices with extended β-strands. An ONIOM density functional theory study.

Autorzy

Robert Wieczorek

J. J. Dannenberg

Rok wydania

2004

Czasopismo

Journal of the American Chemical Society

Numer woluminu

126

Strony

14198-14205

DOI

10.1021/ja048831i

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

We compare the structures and energies of β-strands, α-helices, and 3_{10}-helices for capped polyalanines, acetyl(ala)$_N$NH$_2$, for values of N from 2 to 18, using completely optimized mixed DFT/AM1 calculations. Non-pairwise additive cooperativity is manifest from the variation of the relative energies, helical strain, dipole moments, and H-bond lengths of both types of helices, but especially for the α-helices. While the gas-phase 3_{10}-helices are more stable for small polyalanines, largely due to the additional H-bond, the α-helices become relatively more stable as the polyalanines increase in size.

Słowa kluczowe

Chemical structure, Cooperativity, Energy, Molecular structure, Peptides and proteins

Adres publiczny

https://doi.org/10.1021/ja048831i

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html