Molecular Mechanisms of Imidazole and Benzene Ring Binding in Proteins

A. V. Zhuravlev[1], B. F. Shchegolev[1]*, E. V. Savvateeva-Popova[1], and A. V. Popov[2]

[1]Pavlov Institute of Physiology, Russian Academy of Sciences, Naberezhnaya Makarova 6, 199034 St. Petersburg, Russia; fax: (812) 328-0501; E-mail: shcheg@mail.ru
[2]Sechenov Institute of Evolutionary Physiology and Biochemistry, Russian Academy of Sciences, pr. M. Toreza 44, 194223 St. Petersburg, Russia; fax: (812) 552-3012

Received April 28, 2008
Revision received September 15, 2008

Abstract—Aromatic bonds of amino acid radicals play an important role in arrangement of protein primary structure. Previously, the existence of a number of preferable conformations of aromatic dimers was shown theoretically and experimentally, the best known of which are parallel-displaced and perpendicular T conformations. To reveal principles that define preference of various conformations for His-His and Phe-His dimers, non-empirical quantum-chemical calculations of diimidazole and benzene-imidazole were carried out. Calculations were performed using the 6-31G** basis with account for electronic correlations in frames of MP2 and MP4 methods of perturbation theory. Comparative analysis of energetic and geometric parameters of the systems points to the preference of stacking contact or classical hydrogen bond in diimidazole. On the contrary, T conformation is maximally advantageous for benzene-imidazole.

DOI: 10.1134/S000629790908015X

Key words: stacking interaction, hydrogen bond, diimidazole, benzene-imidazole