Shota Rustaveli National Science Foundation of Georgia
(SRNSFG)
Basic Research Grant Project
Summary

(Up to 250 words)

Project Title	Quantum-chemical description of amino acids propensity for peptide bond formation
Host Institution	Ivane Javakhishvili Tbilisi State University

Abstract

Peptide bond formation is ribosomal catalytic reaction. In addition, the peptide bond formation is influenced by inductive and steric effects of R-groups. Therefore, some R-groups may promote of the peptide bond formation but other may prevent it. For the quantitaive description of these influences modern quantum-chemical method - Density Functional Theory (DFT) has been used. Using the method the bond orders of carbonyl and amino groups (PCO, PNH) and lengths of corresponding bond (RCO, RNH), difference values of charge between C and N atoms (?q), as well as the activation energy (?E#) and the reaction energy (?E) have been calculated. Using these electronic, structural and energetic characteristics the formula of propensity of amino acids for the peptide bond formation was constructed.