**Dear Professor Branislav Ž. Nikolić**

Kindly finds attached the manuscript entitled " Mechanistic, energetic and structural studies of carbon nanotubes functionalized with penicillamine" by Hosein Shaki, Ali Morsali, Heidar Raissi, Mohammad Hakimiand S. Ali Beyramabadi for possible publication as a full length article in **Journal of the Serbian Chemical Society.**

The Authors warranty that the manuscript submitted to the Journal for review is original, has been written by the stated authors and has not been published elsewhere; is currently not being considered for publication by any other journal and will not be submitted for such a review while under review by the Journal; the manuscript contains no libellous or other unlawful statements and does not contain any materials that violate any personal or proprietary rights of any other person or entity.

As you are aware, nanosciences have developed at a tremendous speed in recent years, but most of the researches done in this discipline have been experimental and based on trial and error. Since the ultimate aim of molecular sciences is in their capacity to predict the processes based on theoretical foundations, especially quantum mechanics, understanding the mechanism of nanoprocesses is of paramount importance in reducing the trial and error in experiments.

Unfortunately, in spite of the speedy development of nanosciences, there has been few studies in the field of mechanism of these processes due to high computational costs and the complexity of the nanoprocesses and the majority of the theoretical papers lack the mechanistic investigation (finding intermediates and transition states).

Nowadays, in the field of drug delivery, carbon nanotubes have experimentally presented their capacity in passing through the cell shell. Accordingly, scientists believe that they can use them in releasing drug in the cell, particularly in the diseases such as cancer and AIDS. Concerning the increasing importance of carbon nanotubes in drug delivery, effort has been made in this manuscript to analyze the mechanism of covalent and nancovalent functionalization of drug penicillamine onto COCl and COOH functionalized carbon nanotubes. These results could be applied to other similar drugs and chemical species being absorbed on carbon nanotubes.

Yours Sincerely

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