New Data from Columbia University Illuminate Research in Chemistry [The First Step and the Cob(II)alamin Cofactor Inactive Particles Reactivation in the Updated Mechanism of the Methionine Synthase Process].

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Full Text:
2023 JUL 11 (NewsRx) -- By a News Reporter-Staff News Editor at Life Science Weekly -- Investigators discuss new findings in chemistry. According to news originating from New York City, New York, by NewsRx correspondents, research stated, "The Methionine Synthase process, in principle, can take an unlimited number of turnovers in the presence of the AdoMet substrate. In the absence of this substrate, the Methionine Synthase process lasts only about 2000 turnovers."

Funders for this research include National Science Foundation Grants; City University of New York High-performance Computing Center; Teragrid Science Gateways Program.

The news journalists obtained a quote from the research from Columbia University: "During 2000 turnovers, the entire amount of methylcob(II)alamin cofactor is converted into inactive cob(II)alamin particles. Nevertheless, the mechanism of the Methionine Synthase process determined previously lacks the presence of the AdoMet substrate. On the other hand, the first step of this mechanism was only mentioned earlier without its analysis. The CASSCF geometry optimization of the inactive cob(II)alamin cofactor particle plus the AdoMet ion substrate and of the methylcob(II)alamin cofactor particle plus homocysteine ion and histidine molecule joint models have been performed. CASSCF calculations show that the AdoMet particle transfers the methyl radical to the biologically inactive cob(II)alamin particle during their interaction, transforming it into the biologically active particle of methylcob(II)alamin. CASSCF geometry optimization of the second model leads to the Co-N bond's full cleavage."

According to the news reporters, the research concluded: "The two processes take place in the absence of the total energy barrier. The fully updated mechanism of the Methionine Synthase process has been drawn."

For more information on this research see: The First Step and the Cob(II)alamin Cofactor Inactive Particles Reactivation in the Updated Mechanism of the Methionine Synthase Process. Reactions, 2023,4(16):274-285. The publisher for Reactions is MDPI AG.

A free version of this journal article is available at https://doi-org.ezproxy.cul.columbia.edu/10.3390/reactions4020016.

Our news editors report that additional information may be obtained by contacting Tudor Spataru, Department of Chemistry, Columbia University, New York, NY 10027, United States.

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