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Study on the Chelation Treatment in the Beta thalassemias Using Bio-chemical and Computational Analysis SEMIN AHN, Foxcroft School , RICHARD KYUNG, CRG-NJ — Thalassemia is an inherited blood disorder caused by reduced or absent synthesis of the beta chains of hemoglobin that result in anemia. Iron is very toxic to tissue. Under normal circumstances in humans iron is transported bound to a carrier protein called transferrin. Transferrin transports iron into certain tissues. Because the iron is bound to this protein, other tissues are protected from the toxic effects of free iron. The result shows variable outcomes ranging from highly active to less active depending on the use of the iron-chelating agent. In this project, we assessed the thermodynamical and stereochemical safety of several types of chelating agent and its derivatives that could be used as biological agents in thalassemia treatment. Also other factors were checked to assess the efficiencies of the iron-chelating agent. A molecular editing program was used to model, optimize, and compare the resulting molecular optimization energies and other characteristics of the chelating agent. By figuring out the most efficient type of chelating agent, people who suffer from thalassemia can get help for the treatment.

Richard Kyung
CRG-NJ

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