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Physical and Thermodynamic Analysis of Nano-scaled Aryl Azo Molecules Causing Dermal Disease JAE HYUNG LEE, RICHARD KYUNG, Choice Research Group — Recently, computational biomedical simulation technology is perceived as a means of new approach to an alternative method for future solution of research on chemical agents causing dermal disease. As the use of artificial colorant molecules increases, scientist have tried to study those complexes as they are believed to be able to affect human dermal cells. In this paper, we have tested selectivity and stereochemical aspects for several types of aryl azo compounds and their derivatives as a biological agent causing dermal disease. For this purpose, we used chemical computer programs to model, optimize, and compare the resulting molecular enthalpy of the aryl azo clusters. The theoretical structure of each feasible nano-scaled compounds has been studied in this project. Based on the predicted stability of each molecule, it can be predicted which compound can be used more efficiently to assess the thermodynamic stability. Optimization configuration energy was collected in order to compare each chemical compound's stability. Calculations show some compounds converge easily to lower in enthalpy, which makes them suitable to use as biochemical compound in the disease treatment.

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