

Creating Crosslinking Compounds to Cure Cancer

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Currently, there are some ways cancer is clinically treated but most methods have adverse effects. A way that cancer is commonly treated is by using chemotherapeutic drugs. Chemotherapy works by stopping and slowing the growth of cancerous cells. Chemotherapeutic drugs do not only attack cancerous cells but also healthy cells. Although targeted chemotherapy is not extremely prevalent in the clinical side of cancer treatment, research is being done on ways to make this possible. There is a method called DNA crosslinking that is being tested for targeted chemotherapy. Crosslinking is the action of one polymer chain bonding to another polymer chain. This works by the compound being activated with UV light to create a crosslink with DNA. Once the crosslink is formed between the cancerous cell DNA and the compound, there is a disruption in DNA replication triggering apoptosis. If the technology of DNA crosslinking could be adapted to clinical cancer treatment, then targeted chemotherapy would be achievable. In this project, several potential targeted chemotherapeutic compounds were modeled using Gaussian09 software. Energy absorption levels were analyzed and compared to determine the most favorable chemotherapeutic compound. Then the compound was adapted into UCSF CHIMERA software to analyze compound cross linking ability.