The Efficacy of Lycopene: A Cancer Therapy Evaluated Through Its Binding Energy to Oncoproteins

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While it is a relatively well-researched cancer therapy study, the difference in efficacy between lycopene isomers has not been explored. This carotenoid is mainly utilized for its antioxidant abilities, which allows it to capture free-roaming reactive oxygen compounds called reactive oxygen species (ROS). The ROS molecules are highly reactive, and this can cause instances where they activate harmful cellular signaling pathways, leading to irregular or uncontrolled outcomes that cause cancer proliferation. Using the software MD GROMACS, the energy interactions of a system with a lycopene isomer (the cis-15-lycopene and the all-trans-lycopene), an oncoprotein, and ROS particles can be derived. The controlled trials will contain only the oncoprotein and the ROS molecules. The three oncoproteins utilized are the KRAS G12A (6l4H), the NDRG3-C30S (5vp7), and the Her2 Mutant (8vqe), they are also referred to by the PDB ID its derived from. The given data shows the experimental groups exhibited a comparatively much higher repulsive force, as seen in the LJ (Lennard-Jones) energy data and the highly positive Coulombs, unlike the negative Coulombs recorded in the control trial. This indicates that the lycopene isomers significantly reduced the attractive interactions between the ROS and oncoproteins, thus restricting the activation of the pathways. Furthermore, when comparing the isomers' data, the trans isomer exhibited slightly better results with only two oncoproteins. This indicates that the most optimal isomer may vary per system, but the difference is negligible overall. Lycopene could be utilized in immunotherapy to increase its effectiveness and viability as an option for patients with pre-existing conditions who may not be able to undergo high-intensity treatments.

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