Anti-Cancer Structure Investigations in Computational Chemistry

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This poster synthesizes two projects, one focusing on the characterization of orthobenzyne, the other focusing on the cycloaddition reaction between a modified cyclopropane group and a nitrone. Both projects are related to cancer research, as both molecules containing diradicals related to orthobenzyne and molecules containing the product of the cycloaddition reaction have been proposed as having antitumor applications. Calculations for the orthobenzyne characterization have been performed using Columbus 7.0 with the MCSCF, MRCI-SD, and MR-AQCC methods using the basis sets cc-pVDZ and cc-pVTZ. In relation to the cycloaddition reaction, one particular interest is the bonding of a calcium ion catalyst with the cyclopropane's electron-withdrawing groups. Calculations are being performed to investigate this bonding mechanism in Gaussian 03 using the B3LYP method with the 6-31+G** basis set.