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Coffee Protects From Cancer

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Abstract

From our INDO/SCF-CI quantum mechanical calculations between twelve possible structures of Paracetamol (PA) molecule, it has been concluded that PA molecule has the cis-conformer only without conformation with the trans-form. This has been verified by IR, UV spectroscopic studies. The ionization potentials and electron affinities of Purines and Pyrimidens in addition to caffeine have been calculated by the same method of quantum mechanical calculations, INDO. It has been found that caffeine molecule has the lowest ionization potential, 8.7185 eV and PA molecule has the highest electron affinity, 4.1497eV.

Paracetamol (Acetaminophen) is 4- hydroxylacetanilide and it has world wide use as analgesic and antipyretic medication that is readily absorbed after administration and has few side effects and little toxicity when used in the recommended dose. Several studies of the clinical side effects of Paracetamol, PA, were carried out and it has been concluded that PA has many side effects such as allergic and skin, hematol, renal, pregnancy and lactation, carcinogenesis.

The dipole moment, ionization potential and electron affinity of PA molecule have been calculated and have the following values 2.3761D, 9.9131 eV and 4.1497 eV, respectively. It is clear that PA molecule has a high ionization potential and this means that it is difficult if it is not impossible to give an electron to other molecules. The electron affinity of PA molecule is sufficient to withdraw an electron from the other molecules namely the nucleic acid bases of the cell as well as from caffeine to its LUMO leaving the cell with ionized nucleus i.e. PA molecule acts as an electron acceptor and the nucleic acid bases act as electron donors.

Therefore, the long use of high dose of PA causes the carcinogenesis and caffeine molecule gives an electron easier than the nucleic acid bases to PA molecule at 272 nm. Therefore, caffeine molecule protects the cell in general from the carcinogenic materials and it is advisable to drink one cup of coffee at the morning every day to avoid cancer from the free radicals along the day.