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**Non-covalent interactions of the carcinogen (+)-anti-BPDE with exon 1 of the human K-ras proto-oncogene** JORGE H. RODRIGUEZ, CHRISTOS DELIGKARIS[1], Department of Physics, Purdue University — Investigating the complementary, but different, effects of physical (non-covalent) and chemical (covalent) mutagen-DNA and carcinogen-DNA interactions is important for understanding possible mechanisms of development and prevention of mutagenesis and carcinogenesis. A highly mutagenic and carcinogenic metabolite of the polycyclic aromatic hydrocarbon benzo[$\alpha$]pyrene, namely (+)-anti-BPDE, is known to undergo both physical and chemical complexation with DNA. The major covalent adduct, a promutagenic, is known to be an external (+)-trans-anti-BPDE-$N^2$-dGuanosine configuration whose origins are not fully understood. Thus, it is desirable to study the mechanisms of external non-covalent BPDE-DNA binding and their possible relationships to external covalent trans adduct formation. We present a detailed codon-by-codon computational study of the non-covalent interactions of (+)-anti-BPDE with DNA which explains and correctly predicts preferential (+)-anti-BPDE binding at minor groove guanosines. Due to its relevance to carcinogenesis, the interaction of (+)-anti-BPDE with exon 1 of the human K-ras gene has been studied in detail.

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