Molecular Modeling Study of the Genotoxicity of the Sudan I and Sudan II Azo Dyes and Their Metabolites

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Supplementary Materials

Figure S1: The change in the overall number of hydrogen bonds over the 1 µs trajectory. Panel A: unadducted DNA; Panel B: DNA with Sudan dye adduct; Panel C: DNA with Sudan II dye adduct; Panel D: DNA with azobiphenyl adduct; Panel E: DNA with 4-aminobiphenyl adduct.
|       | No adduct | azo| 4-azobenzene | Sodan I | Sodan II |
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**Figure S2.** Heat Maps of 3DNA parameters changing over the course of the 1 µs MD trajectories of Sudan I and II, azobiphenyl, and 4-aminobiphenyl adducted DNA.