Calculation of Binding Free Energy for Nanodiamond Particles and Aflatoxin B_1

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Computer modeling simulations have been used in combination with experimental work to investigate detoxification of mycotoxins using functionalized nanodiamond particles. Aflatoxin B_1 is a known carcinogen that is among the top five most detrimental mycotoxins found in the world's food supply. Basic material modeling techniques will be used to explore possible trends in surface stability and availability of functional group binding sites. Preliminary modeling efforts include the use of mm-pbsa and mm-gbsa methods to calculate binding energetics between functional groups found on the surface of nanodiamonds and aflatoxin B_1. Calculations presented in the paper include binding energies for two solvated complexes containing aflatoxin B_1 and small diamondoid molecules, one with no functional group the other containing a hydroxyl group on the diamond surface.

Sponsored by the Materials World Network program of the National Science Foundation.