Video S1.

Results of 100 ns of CG-MD of the interaction between SFN (gray colored spheres), NF-κB chain A (cyan surface), NF-κB chain B (mauve surface) and DNA (green backbone; yellow stick bases). The initial position of SFN was derived from docking simulations (see Results section for detailed description) considering only NF-κB chain A. The presence of the nucleic acid induces SFN to change its position within the first 30 nanosec (6 sec in the video), exploring a different binding site at the interface between DNA and NF-kB. The final pose was retained for the remaining simulation time. CG-MD, coarse-grained molecular dynamics; SFN, sulforaphane.