

Supplementary Materials: Molecular Modeling Studies on the Interactions of Aflatoxin B1 and Its Metabolites with Human Acetylcholinesterase. Part II: Interactions with the Catalytic Anionic Site (CAS)

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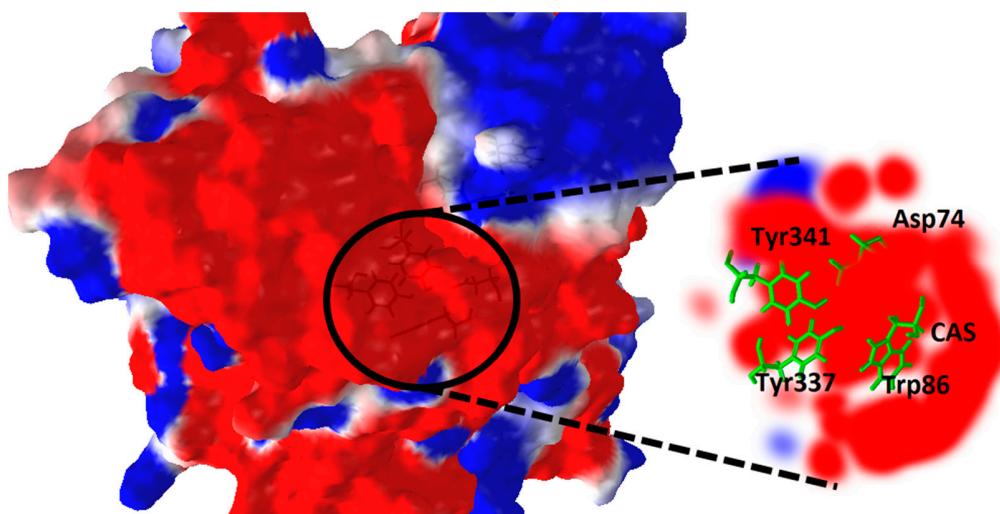


Figure S1. Map of electrostatic potential for the CAS. Regions of higher electrostatic potentials are represented in blue while lower electrostatic potentials are in red.

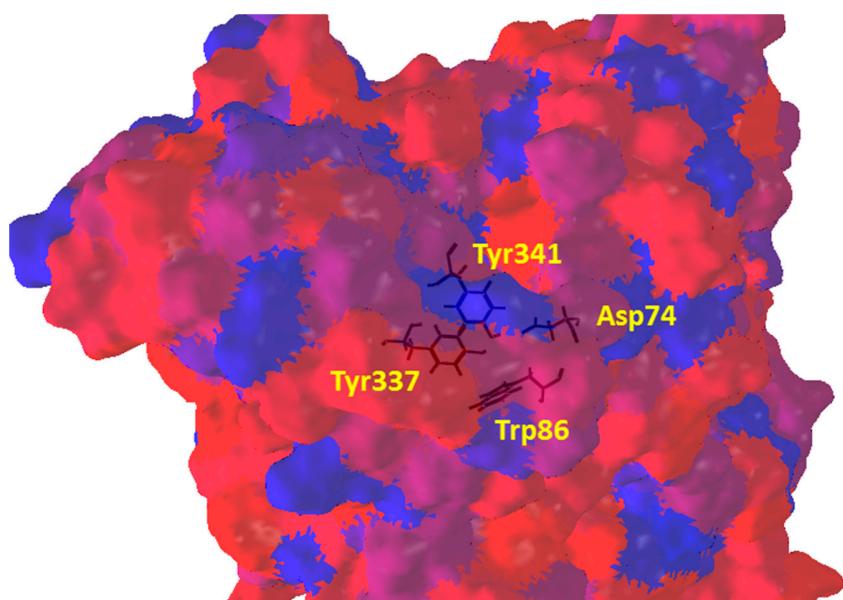


Figure S2. Solvent accessible surface for the protein. Hydrophilic areas are represented in red and hydrophobic areas are represented in blue.

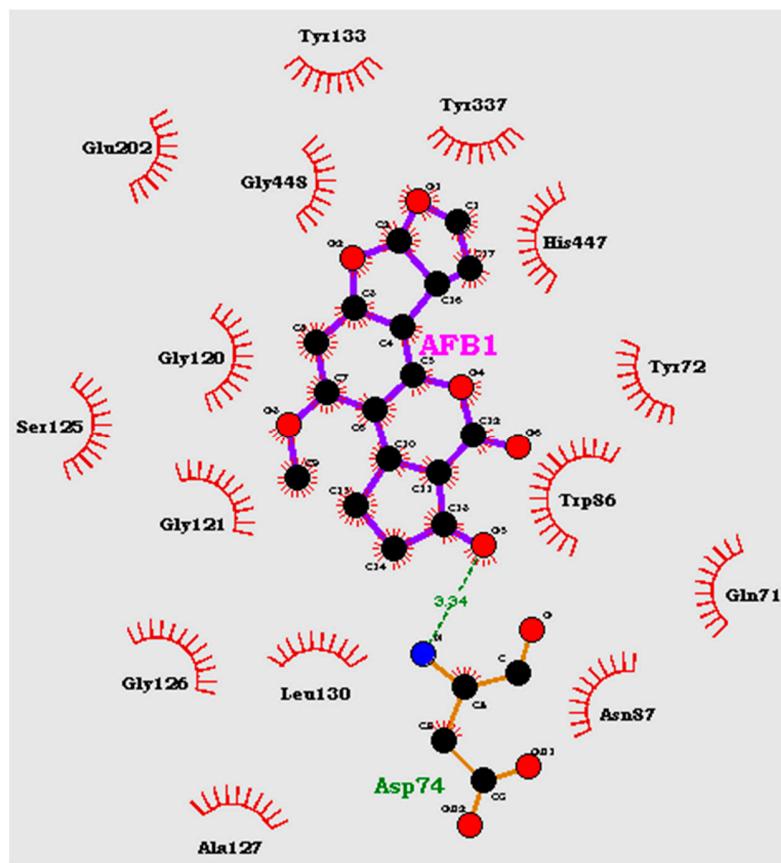


Figure S3. 2D representation of the best pose of AFB1 on CAS.

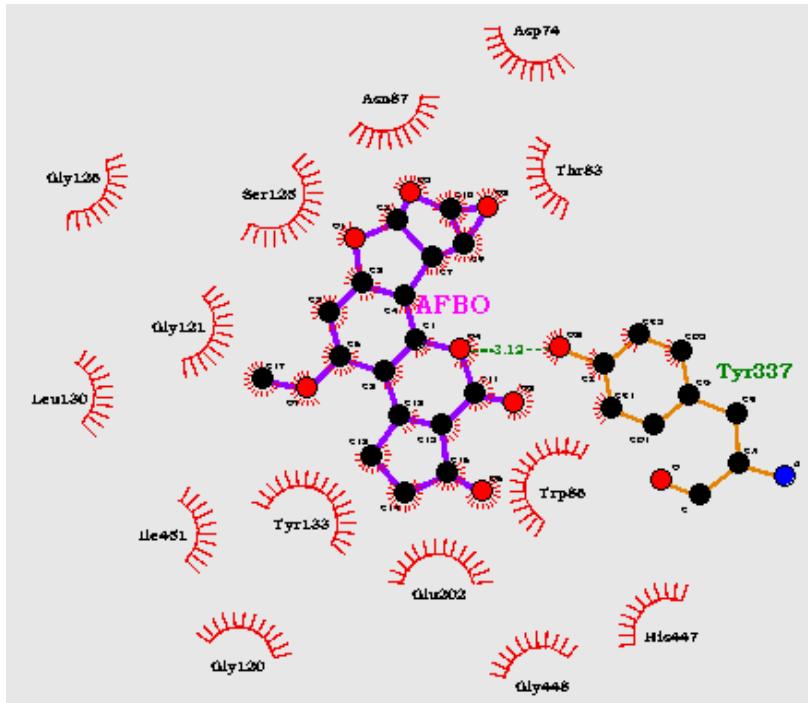


Figure S4. 2D representation of the best pose of AFBO on CAS.

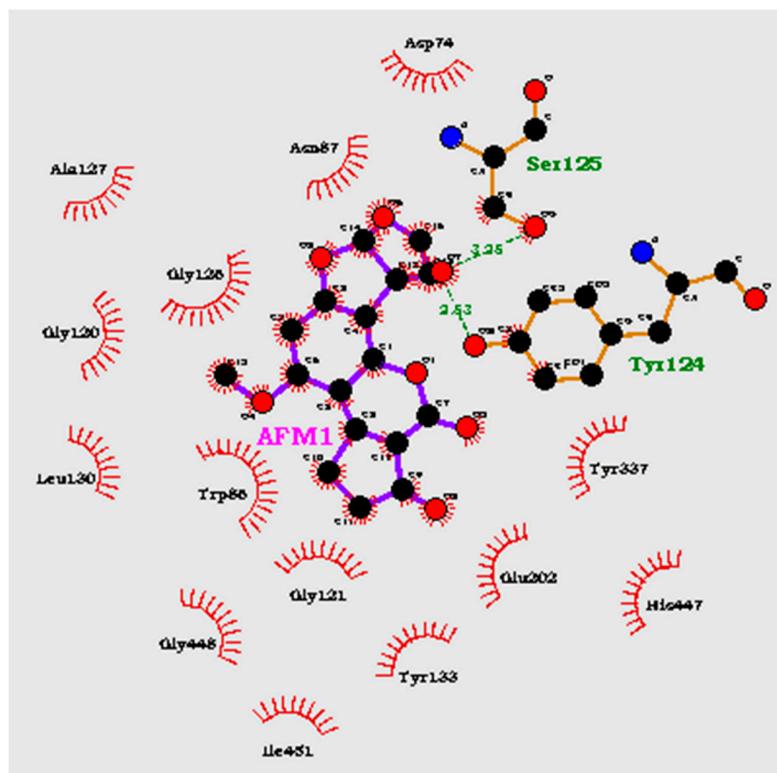


Figure S5. 2D representation of the best pose of AFM1 on CAS.

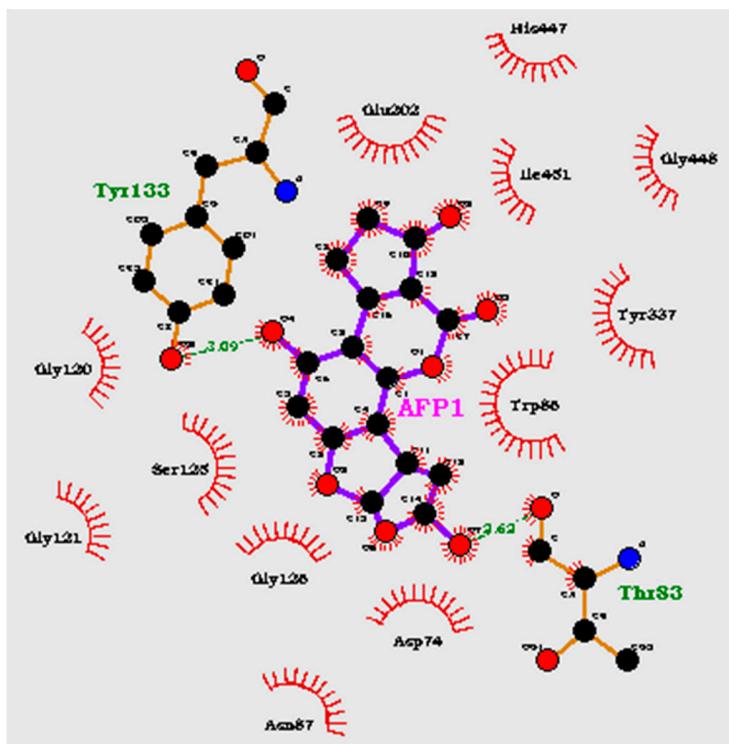


Figure S6. 2D representation of the best pose of AFP1 on CAS.

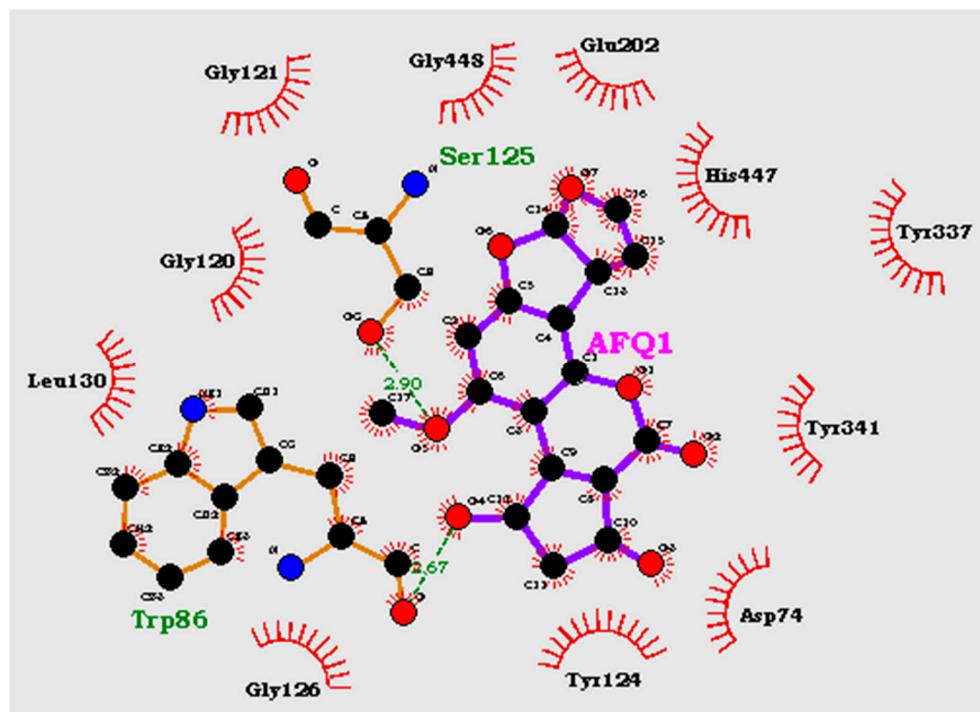


Figure S7. 2D representation of the best pose of AFQ1 on CAS.

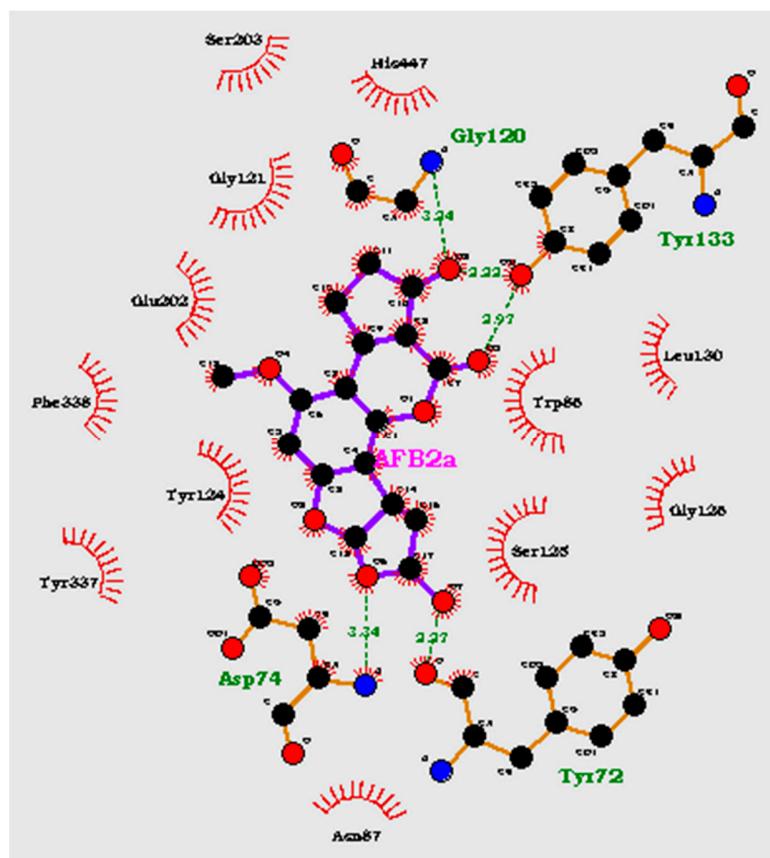
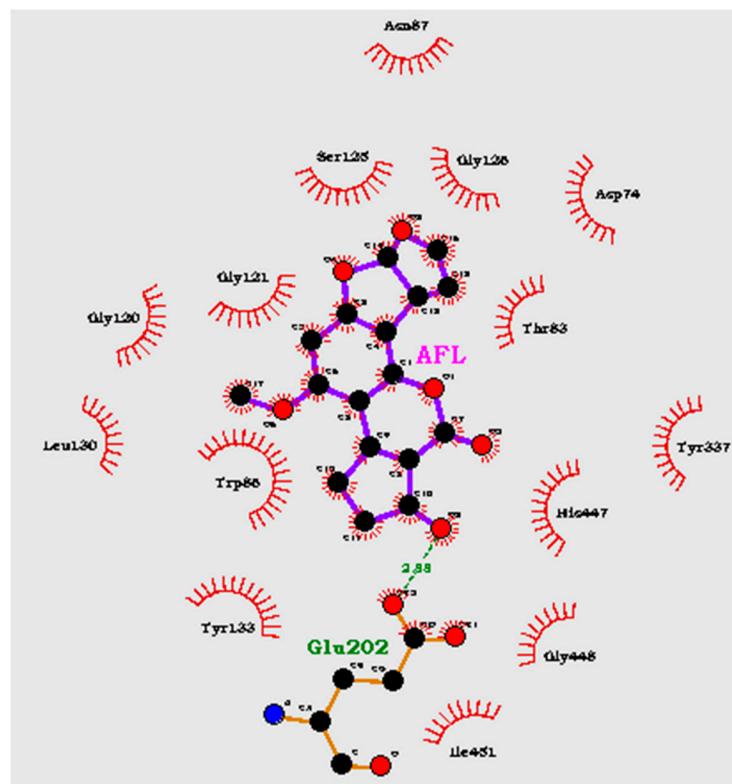
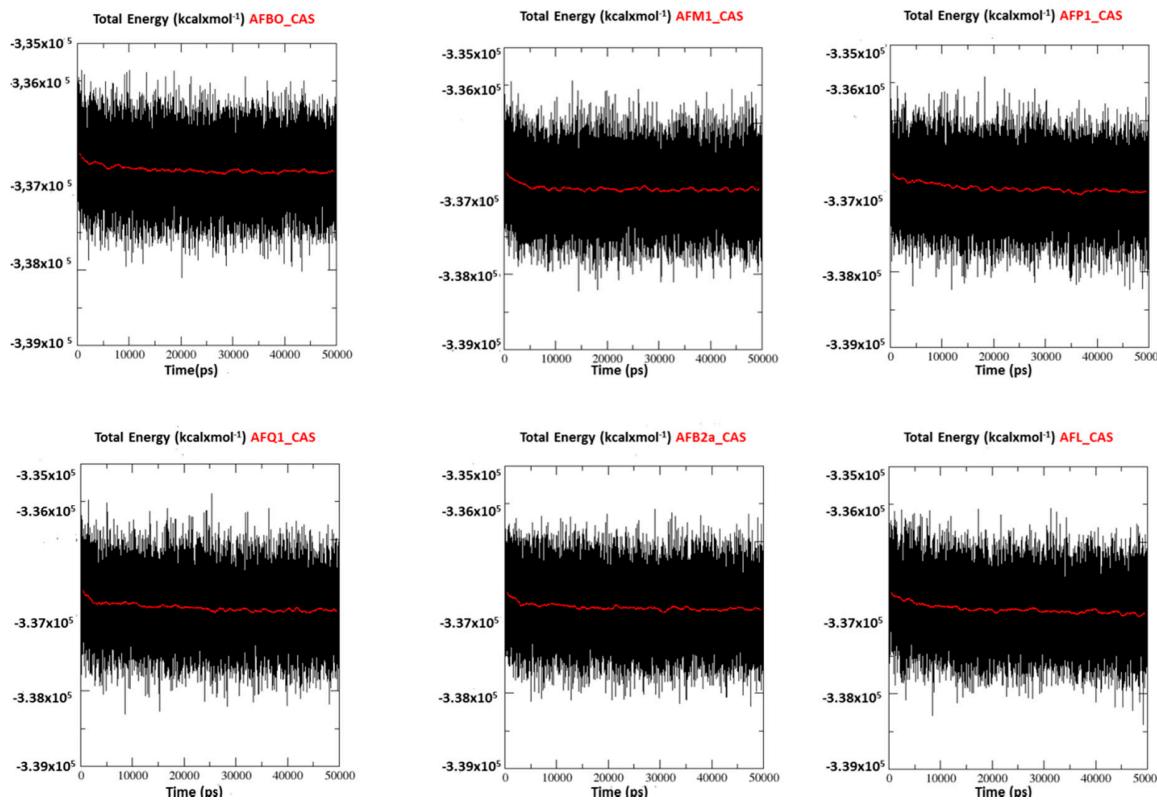


Figure S8. 2D representation of the best pose of AFB2a on CAS.

**Figure S9.** 2D representation of the best pose of AFL on CAS.**Figure S10.** Variation of total energy for the complexes HssAChE/AFB1-metabolites on the CAS of HssAChE.

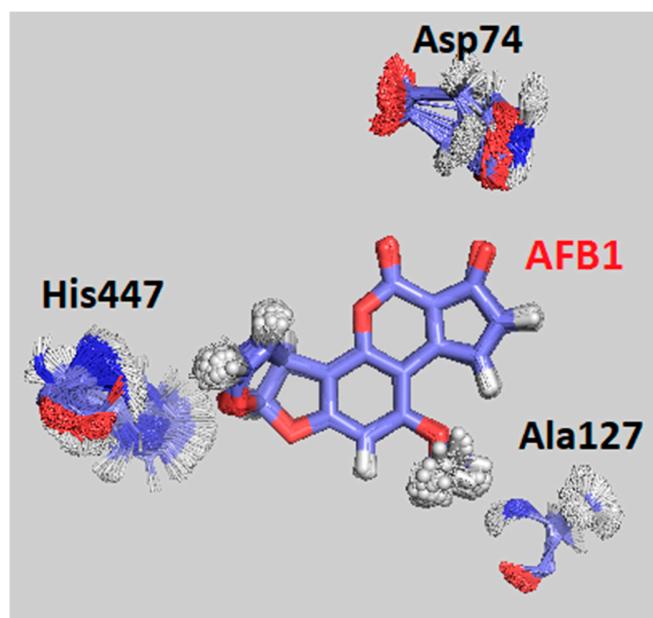


Figure S11. Superposition of frames for the complex *HssAChE/AFB1* on the CAS during 50 ns of MD simulations.

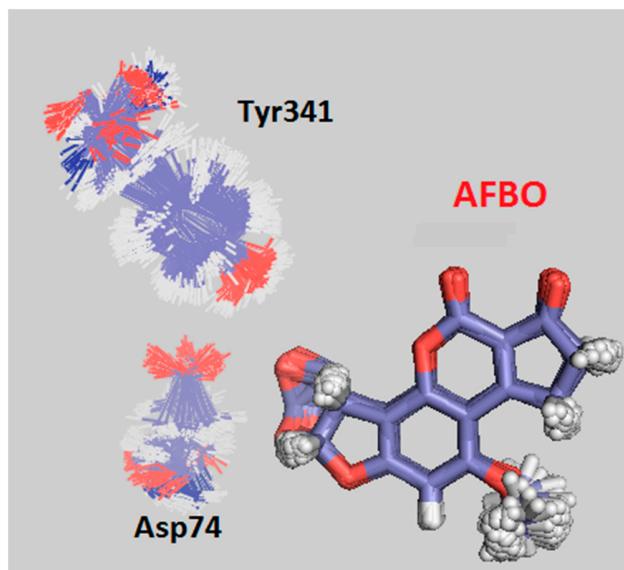


Figure S12. Superposition of frames for the complex *HssAChE/AFBO* on the CAS during 50 ns of MD simulations.

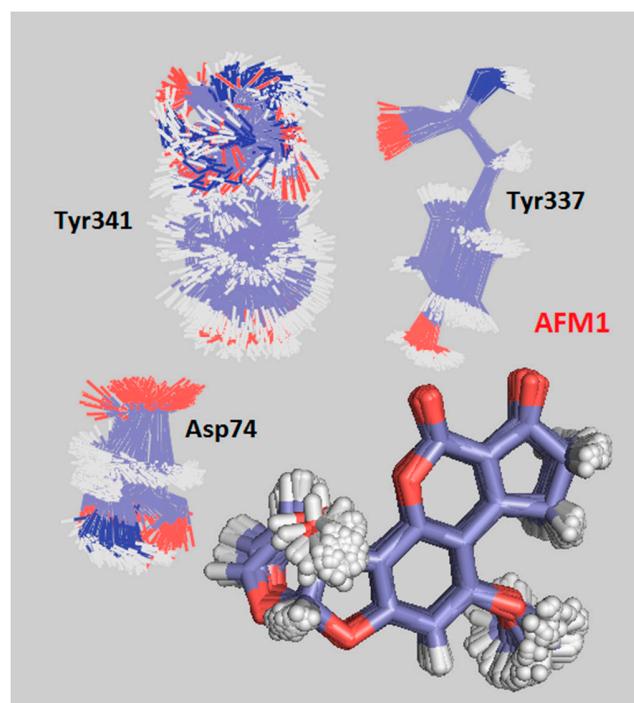


Figure S13. Superposition of frames for the complex *HssAChE/AFM1* on the CAS during 50 ns of MD simulations.

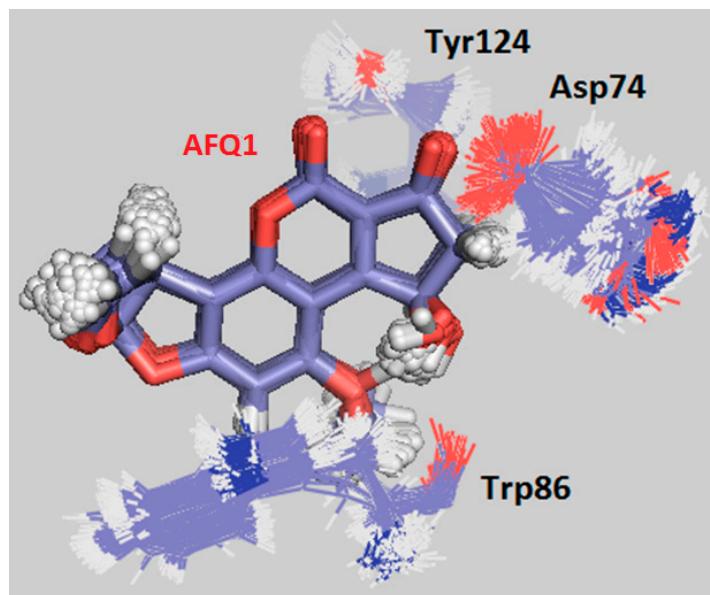


Figure S14. Superposition of frames for the complex *HssAChE/AFQ1* on the CAS during 50 ns of MD simulations.

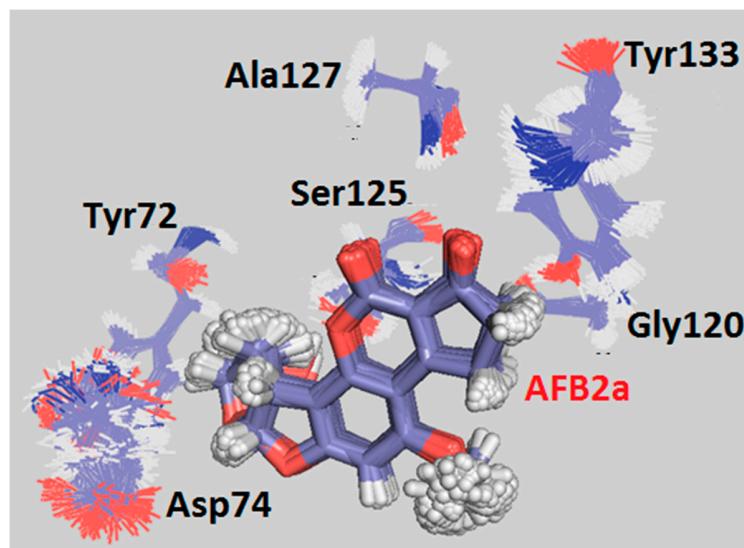


Figure S15. Superposition of frames for the complex *HssAChE*/AFB2a on the CAS during 50 ns of MD simulations.

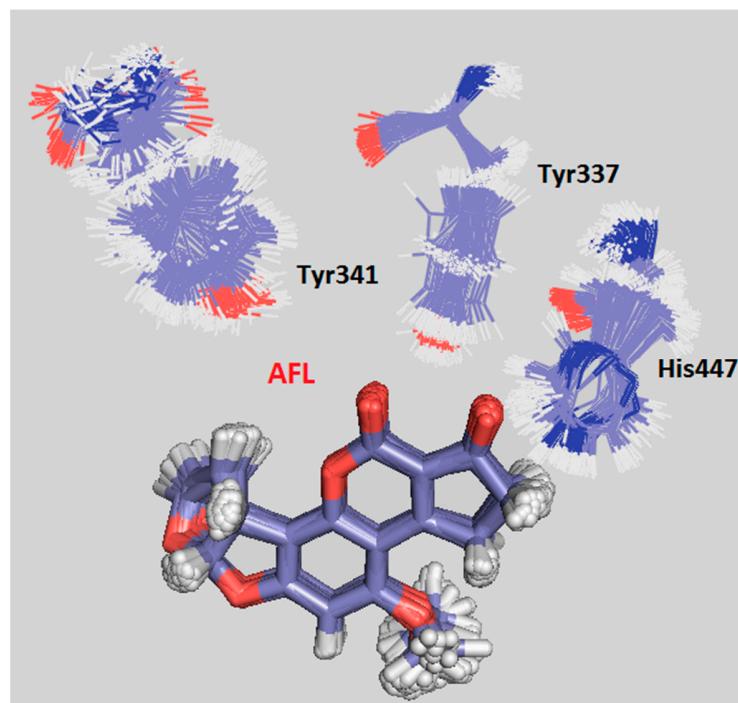


Figure S16. Superposition of frames for the complex *HssAChE*/AFL on the CAS during 50 ns of MD simulations.