

Supplementary Materials: Interaction of Ochratoxin A and its thermal degradation product 2'R-Ochratoxin A with Human Serum Albumin

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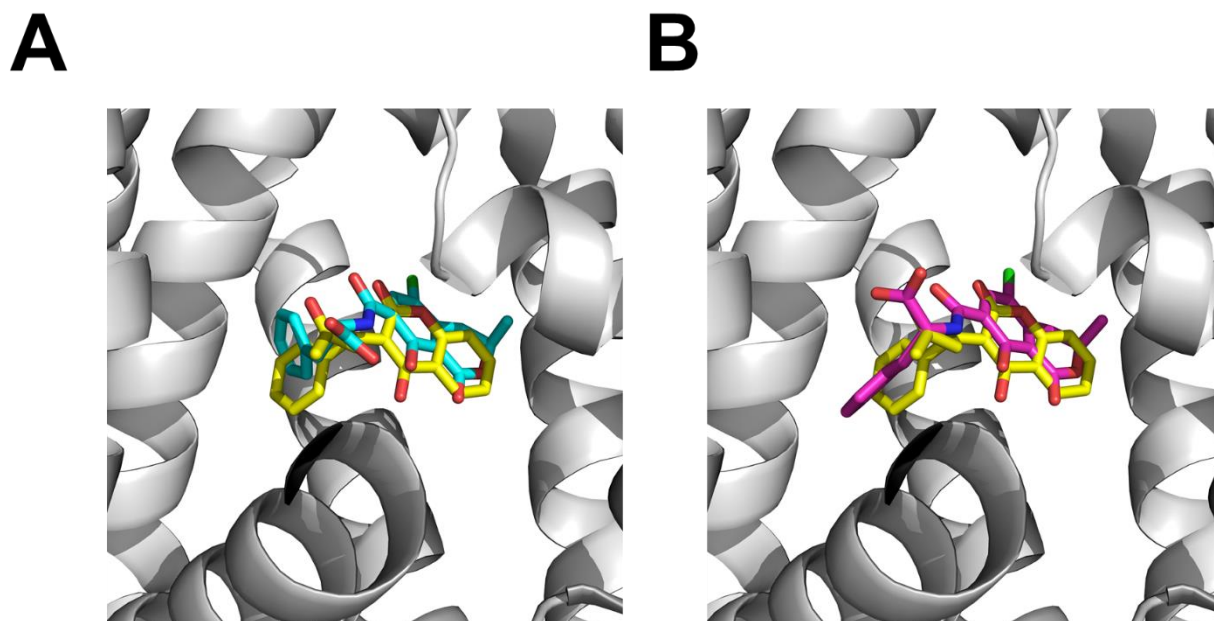


Figure S1. Structural alignment of the ligands. Comparison of OTA (**A**, blue) and 2'R-OTA (**B**, magenta) aligned onto Warfarin (yellow) in the crystal structure of the complex with HSA (grey, cartoon representation) (PDB ID: 1H9Z) after energetic relaxation of OTA and 2'R-OTA in the presence of HSA.

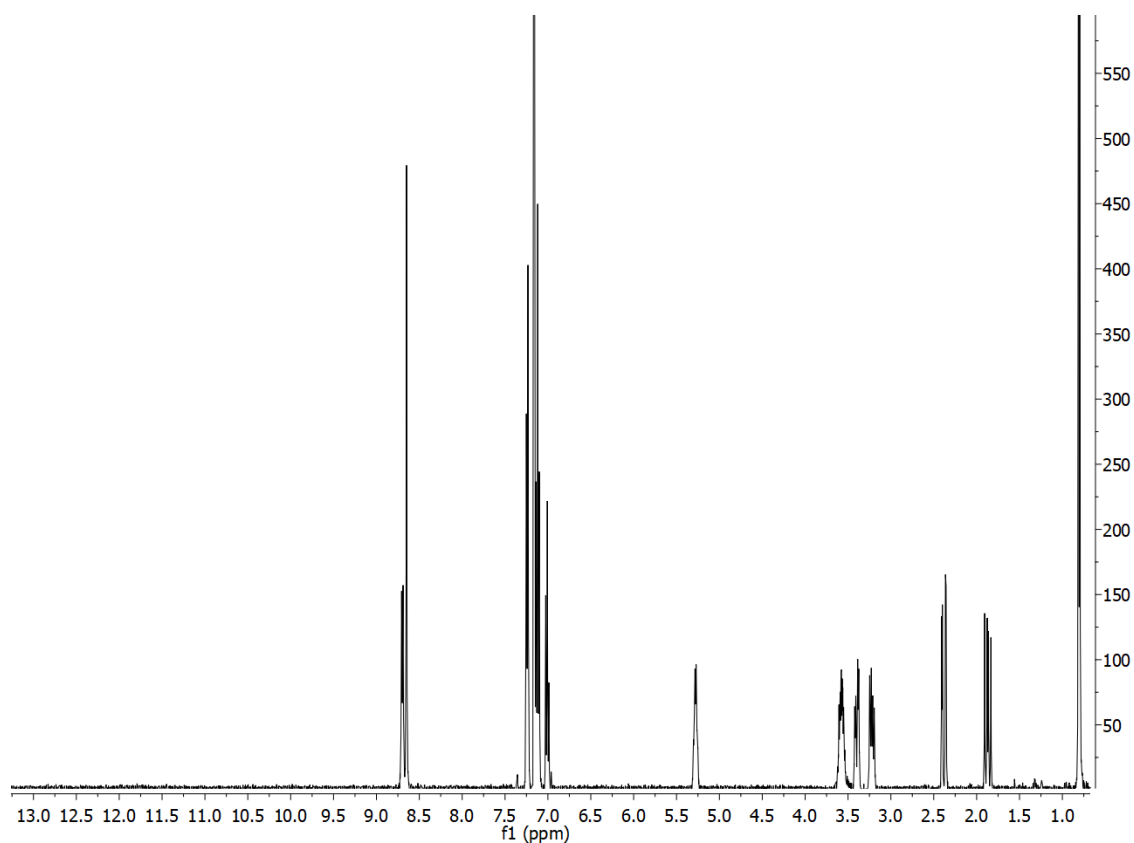


Figure S2. ^1H -NMR (400 MHz, Benzene- d_6) spectra of ochratoxin A. Ochratoxin A: ^1H NMR (400 MHz, Benzene- d_6) δ 8.70 (H-10, d, J = 6.8 Hz, 1H), 8.65 (H-6, s, 1H), 7.24 (H-5'+H-9', d, J = 7.5 Hz, 2H), 7.12 (H-6'+H-8', t, J = 7.5 Hz, 2H), 7.01 (H-7', t, J = 7.4 Hz, 1H), 5.28 (H-2', m, 1H), 3.58 (H-3, ddd, J = 11.9, 6.1, 3.4 Hz, 1H), 3.40 (H-3'b, dd, J = 14.1, 5.0 Hz, 1H), 3.22 (H-3'a, dd, J = 14.0, 7.3 Hz, 1H), 2.38 (H-4b, dd, J = 17.3, 3.4 Hz, 1H), 1.87 (H-4a, dd, J = 17.3, 11.9 Hz, 1H), 0.80 (H-11, d, J = 6.3 Hz, 3H).

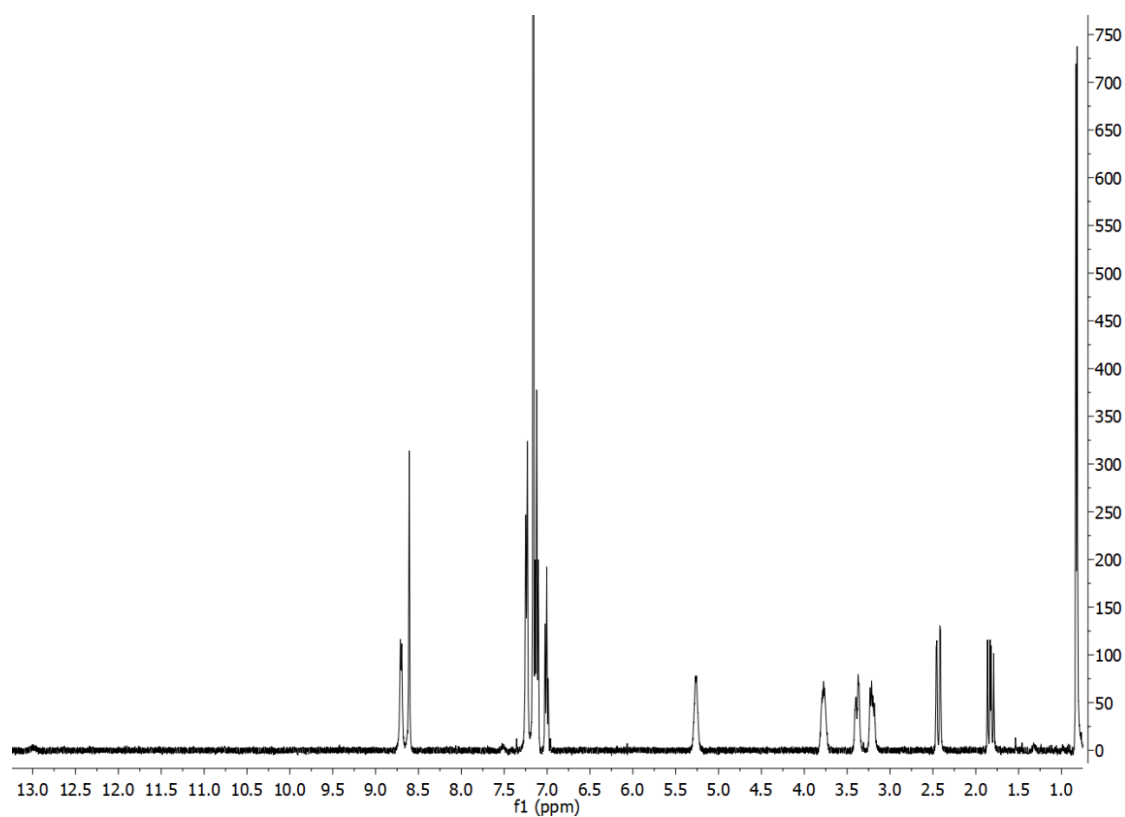


Figure S3. ^1H -NMR (400 MHz, Benzene- d_6) spectra of 2'*R*-ochratoxin A. 2'*R*-ochratoxin A: ^1H NMR (400 MHz, Benzene- d_6) δ 8.70 (H-10, d, J = 6.6 Hz, 1H), 8.61 (H-6, s, 1H), 7.24 (H-5'+H-9', d, J = 7.5 Hz, 2H), 7.12 (H-6'+H-8', t, J = 7.5 Hz, 2H), 7.01 (H-7', t, J = 7.3 Hz, 1H), 5.25 (H-2', m, 1H), 3.83 – 3.72 (H-3, m, 1H), 3.38 ((H-3'b, dd, J = 14.1, 4.6 Hz, 1H), 3.21 (H-3'a, dd, J = 14.1, 7.3 Hz, 1H), 2.44 (H-4b, dd, J = 17.3, 3.3 Hz, 1H), 1.83 (H-4a, dd, J = 17.3, 12.0 Hz, 1H), 0.82 (H-11, d, J = 6.3 Hz, 3H).

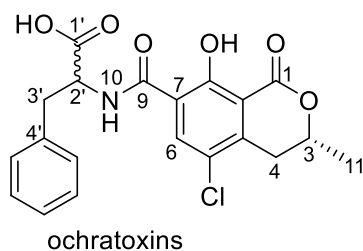


Figure S4. Molecular structure of the ochratoxins OTA and 2'*R*-OTA with labeled atoms.

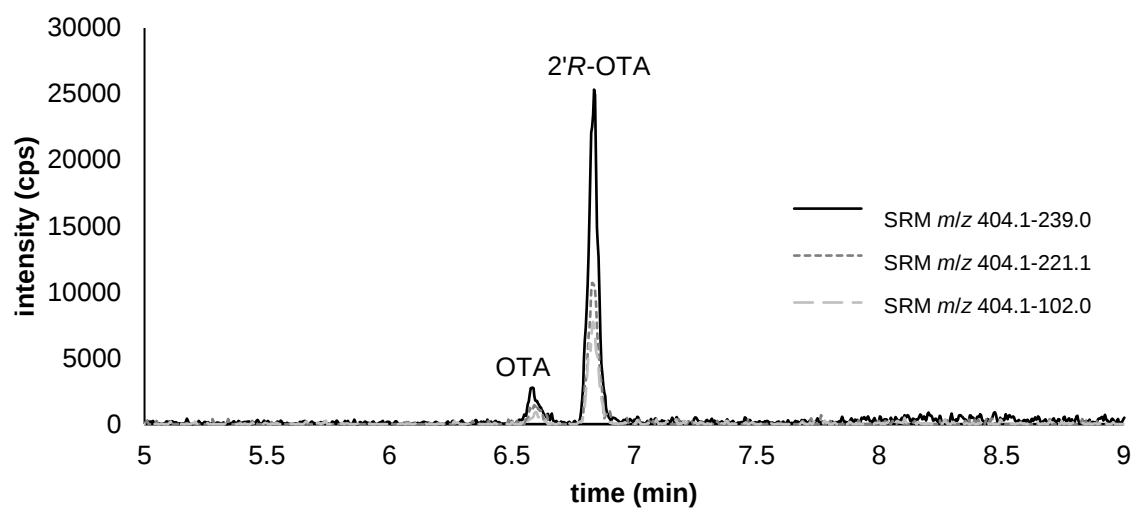


Figure S5. HPLC-MS/MS chromatogram of OTA and 2'R-OTA with the three transitions from the dialysis chamber without HSA after 5.5h. cps: counts per second.