Spectroscopic properties of Ochratoxin A and B

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Ochratoxin A (OTA) is an ubiquitous mycotoxin and natural food contaminant which is produced by several storage fungis such as *Aspergillus ochraceus*, *Aspergillus niger* and *Penicillium verrucosum*. OTA can occur in a large variety of food, e.g. in cereals, beans, nuts, spices, fruits, coffee, beer and wine. Because of carry-over effects it can also be found in meat especially in kidneys of animals fed with contaminated feed. Moreover, in animal experiments this toxin was identified as immunotoxic, genotoxic, teratogenic, hepatotoxic, and potentially carcinogenic for humans.

OTA (s. Fig.) is composed of an isocoumarin unit connected to a phenylalanine unit. The photophysics of OTA is determined by intra- and intermolecular proton transfer reactions. These dynamic characteristics can be investigated using absorption, steady state and time resolved fluorescence spectroscopy.[1]

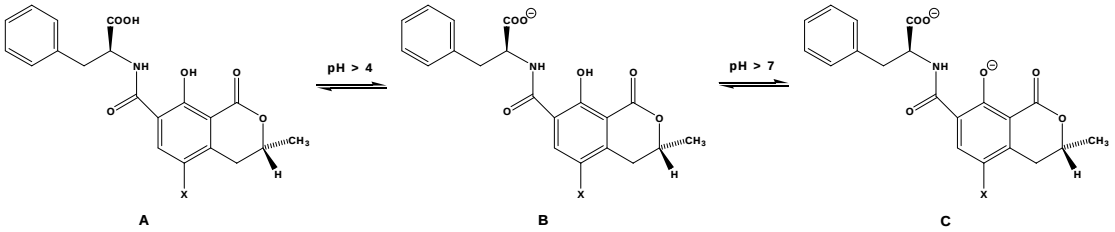

Figure: Deprotonation of Ochratoxin A (X=Cl) and B (X=H)

Structure A and B show an absorption maximum at λ_{abs} = 333 nm. In ethanolic solution (pH > 4) the phenolic group of the isocoumarin moity is stabilized by a keto-enol-tautomerism (B). After addition of base the dianion is builded (C) and the absorption maximum is red-shifted, while the fluorescence emission maximum shifts from 455 to 427 nm. Furthermore, in time-resolved fluorescence experiments non-monoexponential decay kinetics are observed. Due to the excited-state reactions the photophysical processes are complex and further analytical information is indispensable for a sensitive and selective in-situ detection of OTA and related compounds (e.g. OTB) in food and feed.
Therefore, diffuse reflectance spectra in the UV/Vis and NIR spectral range from 200 nm < λ < 2500 nm are collected in addition and analysed according to the Kubelka-Munk-Theory.[2]

References

[1] Chu, F.S., 1974. Studies on Ochratoxins. CRC Critical Reviews in Toxicology, 2, 499-523
[2] Kubelka, P., Munk, F., 1931. Ein Beitrag zur Optik der Farbanstriche. Zeitschrift für technische Chemie, 11a, 593-601