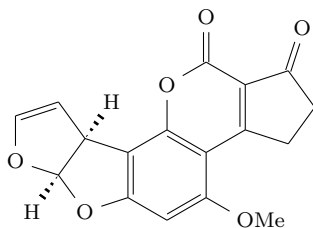


4 Determining Stereochemistry

3/18: Aflatoxin B1 is a toxin produced by a fungus which grows on a number of plant species, but is best known for causing liver carcinogenicity from contaminated peanuts.



The **unknown-C_5.46_2025** dataset contains a series of spectra which you should be able to identify (if this is untrue, let me know and I'll send out a list). For this exercise, I'd like you to identify the ROESY crosspeaks in experiment #9 and the NOESY crosspeaks in #37 as follows.

1. Assign all the protons in the molecule using the standard ^{13}C -directed approach.
2. Show the ROE/NOE crosspeaks on the structure of Aflatoxin B1 and explain whether any are missing that you would expect.
3. Confirm the stereochemistry of the bridged ring.
4. Experiment #13 shows a ^1H - ^{13}C HSQC in which the decoupling is turned off during acquisition; indicate on the structure which proton-carbon couplings are larger than usual and explain why you think this is.