

## **Spectroscopic Characterizations of Dimers Formed during Thermo-oxidation of $\beta$ -Sitosterol**

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Thermo-oxidation of sterols, at temperatures typical for frying, leads to formation of oxidized derivatives, fragmented sterols, as well as oligomers. Recent research on sterol oxidation focuses mainly on the identification of oxysterol derivatives excluding compounds with high molecular mass. The aim of this work was to decipher the structure of dimers formed during  $\beta$ -sitosterol oxidation at 180°C in the presence of oxygen. Dimer fraction was separated by size-exclusion chromatography (SEC) after chromatographic precleaning using silica gel. Three methods were used to characterize dimers configuration: 1D and 2D NMR in solution state, IR and Raman spectroscopy. NMR and IR spectra revealed loss of hydroxyl group at C-3 on the A ring with double bond at C-5 preserved. NMR data indicated that dimers are formed through ether linkage ( $\delta\text{H}=3.3$  ppm,  $\delta\text{C}=76.3$  ppm), confirmed by IR ( $1093\text{ cm}^{-1}$ ). Furthermore HSQC and 2D COSY NMR experiments showed that ether bond is formed between C-3 and C-3' carbons of two sterol molecules. In conclusion, the predominant dimer formed during  $\beta$ -sitosterol oxidative degradation has configuration of 3,3'-sitosterol ether. In order to further verify chemical structure of dimers formed, analysis including application of solid state NMR and LC/MS/MS are underway.