

Partial structural studies of fucosylated chondroitin sulfate (FuCS) using attenuated total reflection fourier transform infrared spectroscopy (ATR-FTIR) and chemometrics

ABSTRACT

The compound fucosylated chondroitin sulfate from three sea cucumber species *Holothuria atra*, *Stichopus horrens*, and *Holothuria arenicola* was extracted and purified using strong ion exchange chromatography. The structure and sulfation patterns on their fucose branches were partially characterized and compared using liquid, gas chromatography-mass spectrometry, infrared spectroscopy, and chemometrics. The monosaccharide composition was consistently a 1:1 molar ratio of glucuronic acid to N-acetylgalactosamine while the fucose molar ratio was statistically different among the three species. Normal IR spectra exhibited a broad band at the region of 850–830 cm^{-1} assigned to the sulfate $\text{C}-\text{O}-\text{S}$ group. This band was resolved in the second derivative spectra into two or three bands corresponding to the difference of sulfation patterns among sea cucumber species. Principal component analysis (PCA) confirmed the difference in the sulfate substitution region with additional discrimination of the combination amide $\text{N}-\text{H}$ and $\text{C}=\text{O}$ group, sulfate $\text{S}=\text{O}$ region, and skeletal region 1050–980 cm^{-1} . The hierarchical clustering analysis (HCA) successfully grouped each sea cucumber FuCS in the same cluster. Nevertheless, the comparison of the FuCS structure was simplified using chemometrics analysis.