Multidimensional mass spectrometry of multicomponent nonionic surfactant blends

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Ultra-performance liquid chromatography (UPLC) and ion mobility (IM) separation were coupled with mass spectrometry (MS) and tandem mass spectrometry (MS/MS) in order to characterize a commercially available complex nonionic surfactant mixture. The surfactant molecules are comprised of a glycerol core functionalized with units of poly(ethylene oxide) (PEO_n) and esterified by caprylic or capric fatty acids. Reverse-phase UPLC separated the mixture according to polarity into four fractions corresponding to no, mono-, di- and, tri- fatty acid containing compounds. Additional separation within each fraction was achieved according to the length of the fatty acid chains. Coeluting molecules of similar polarity were further separated by collisional cross section area using IM. Performed together, UPLC and IM allow for the detection of several ions that would otherwise be superimposed by isobaric species and enable confident structural elucidation through MS² fragmentation.



Liquid Chromatography Ion Mobility Mass Spectrometry Separation of a Multicomponent Nonionic Surfactant Blend