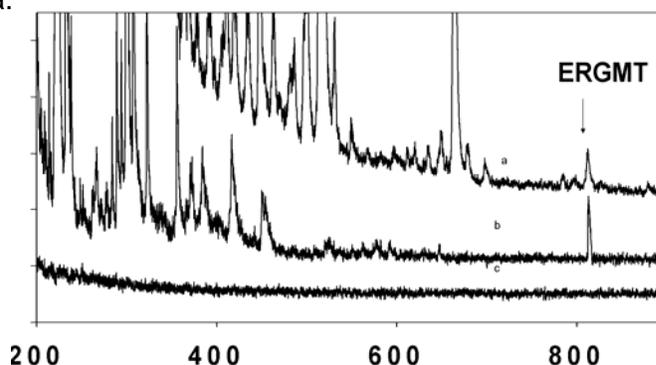


In-Situ Derivatization and Identification of Peptides by Vacuum Ultraviolet Postionization Mass Spectrometry for Bacterial Biofilms

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Inter cell signaling using molecules like lactones and peptides is a fundamental activity carried out by most cell types. Detection of these molecular species by matrix assisted laser desorption ionization (MALDI) or secondary ion mass spectrometry (SIMS) can be complicated by low ionization yields and/or high fragmentation. Single photon vacuum ultraviolet (VUV) postionization is one method that shows great promise for enhancing ionization yields with a minimum of fragmentation. The fluorine laser is an intense laboratory source of vacuum ultraviolet radiation, but the 7.87 eV photons it generates are lower in energy than the ionization potential of many target species. A method is described here whereby derivatization of peptides with a 7.87 eV photoionizable chromophore allows efficient fluorine laser postionization of the entire labeled peptide and reduces the complexity of the mass spectrum. F2 laser desorption postionization (LDPI) mass spectrum of underivatized biofilms of *Bacillus subtilis* do not show significant peaks above 150 Da due to the lack of species which can be ionized by 7.87 eV photons. In-situ polycyclic aromatic hydrocarbon derivatized biofilms, which selectively form primary and secondary amine and carboxylic acid groups in the biofilms, show significant mass peaks above 150 Da.

Separate studies were carried out for identification of these peaks by solid phase extraction of these species followed by electrospray mass spectrometry. These methods allow quorum sensing species in complex biofilms to be analyzed and can produce a two dimensional mass spectrometric image of a biofilm.



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Laser desorbed post ionized mass spectra show that an anthracene tag and SPI allow the quorum sensing peptide, ERGMT, to be detected within a biofilm. The upper two curves (a & b) are of *B. subtilis* with and without a biofilm, respectively. Both show a pronounced signal at the anthracene-tagged ERGMT peptide mass. The lower curve (c) which is the same *B. subtilis* biofilm without derivatization shows no discernable mass signals.

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