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Chemical Sciences

Title

Improved resolution of hydrocarbon structures and constitutional isomers in complex mixtures
using Gas Chromatography-Vacuum Ultraviolet-Mass Spectrometry (GC-VUV-MS)
(Supplementary Info)

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Improved resolution of hydrocarbon structures and constitutional isomers in complex mixtures using Gas Chromatography-Vacuum Ultraviolet- Mass Spectrometry (GC-VUV-MS)

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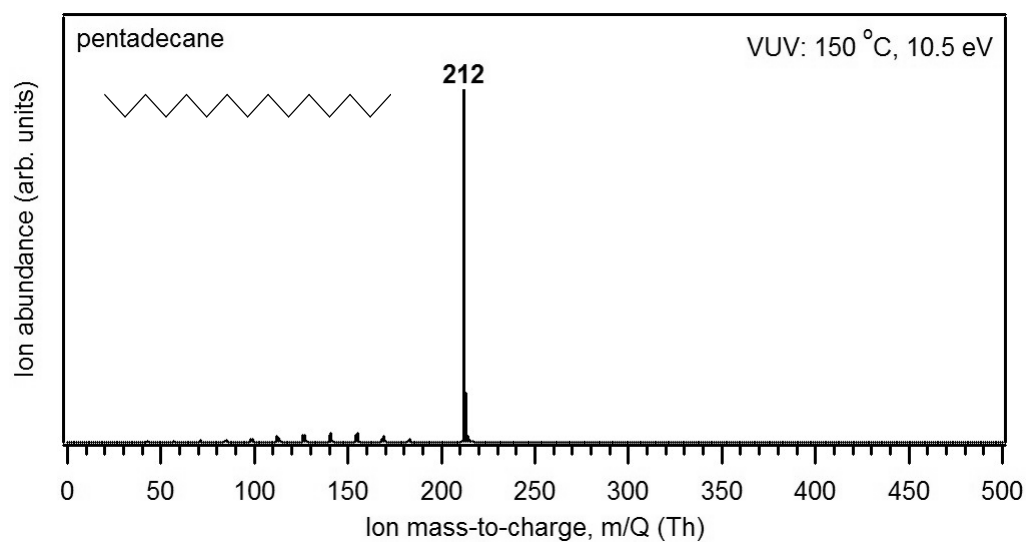
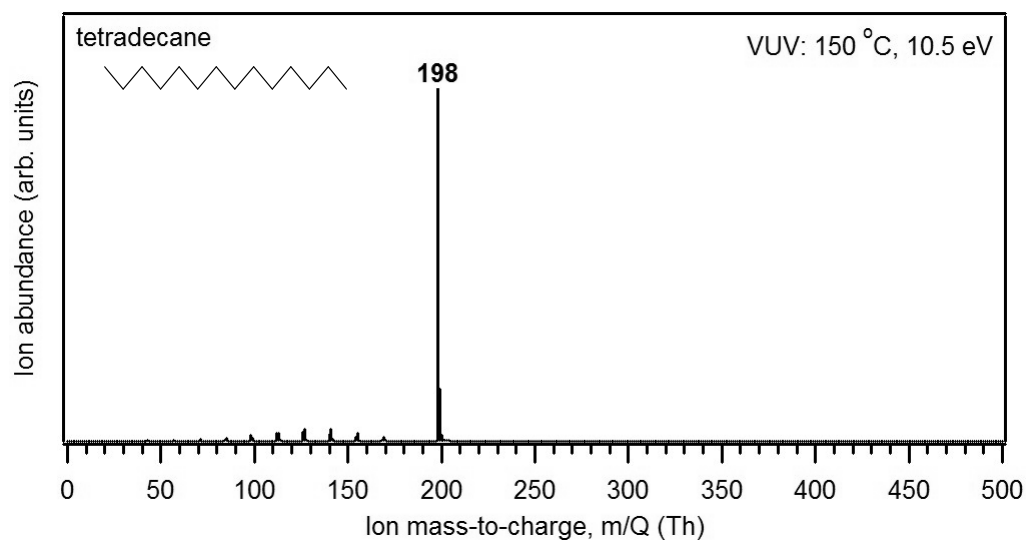
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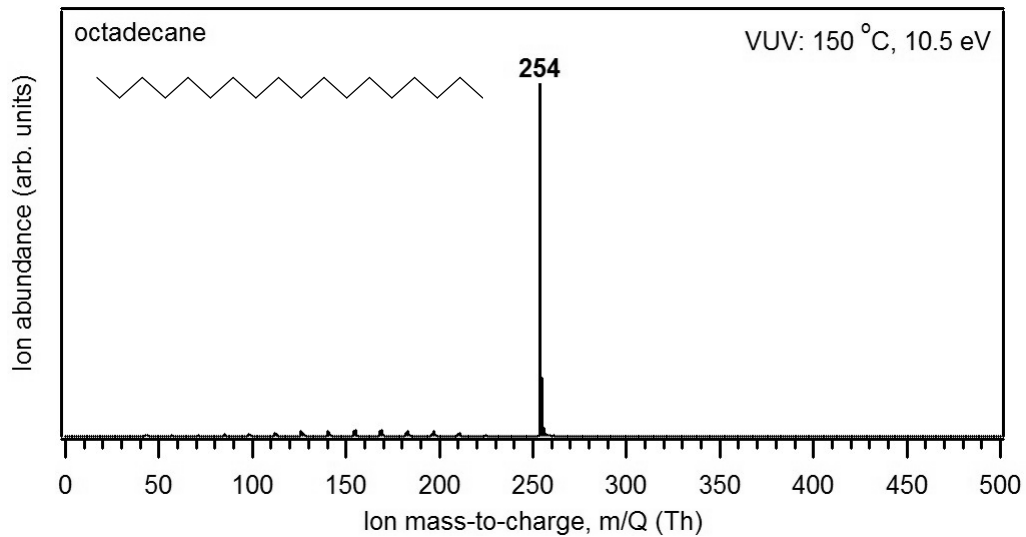
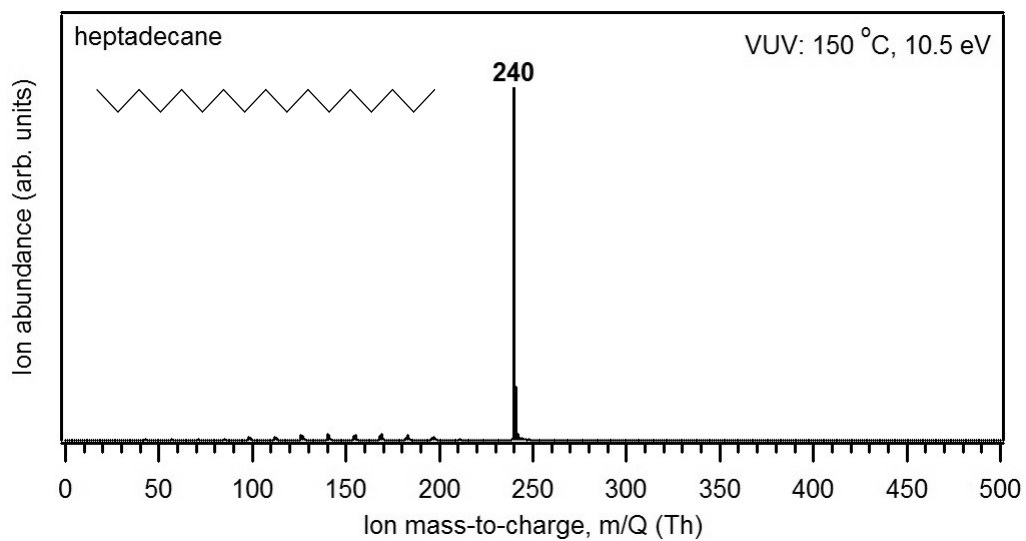
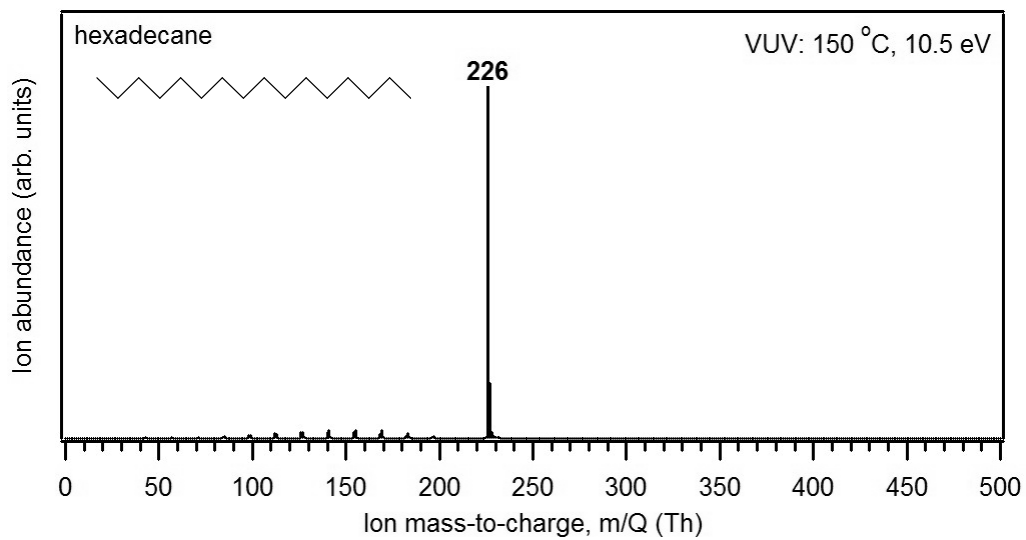
This supplementary information contains the mass spectra of known compounds using vacuum ultraviolet (VUV) ionization at transfer temperatures of 150 °C (38 compounds) and 275 °C (84 compounds). Parent ion is shown in bold (not shown for chlorinated compounds because the prevalence of both ³⁵Cl and ³⁷Cl leads to multiple "parent" ions). Mass spectra using electron impact (EI) ionization for all reported compounds are available online from the NIST WebBook (reference provided in manuscript).

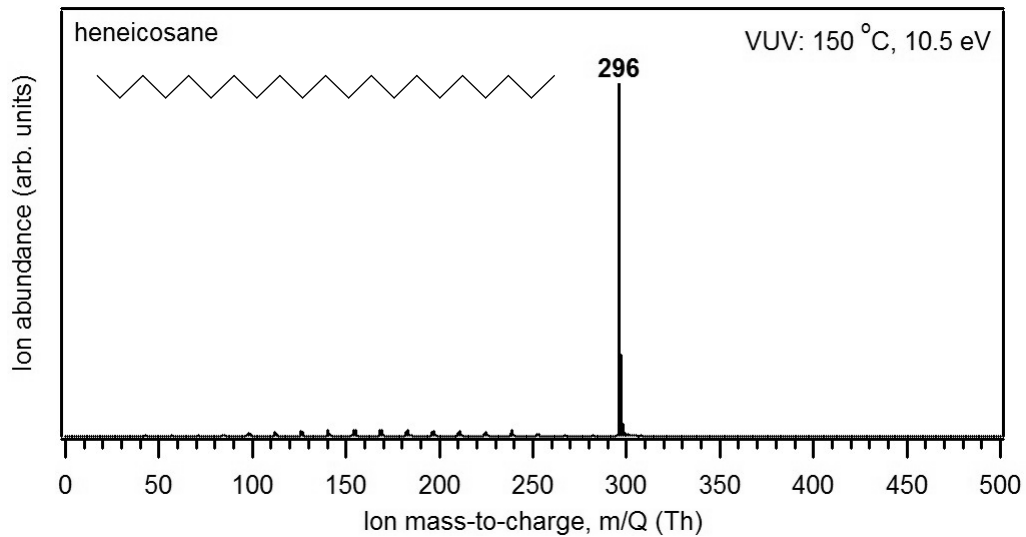
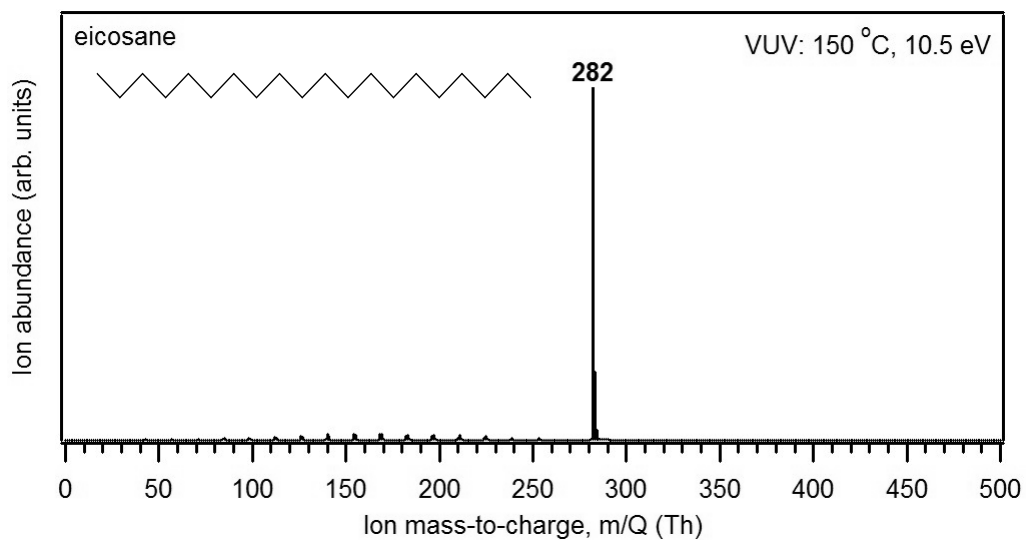
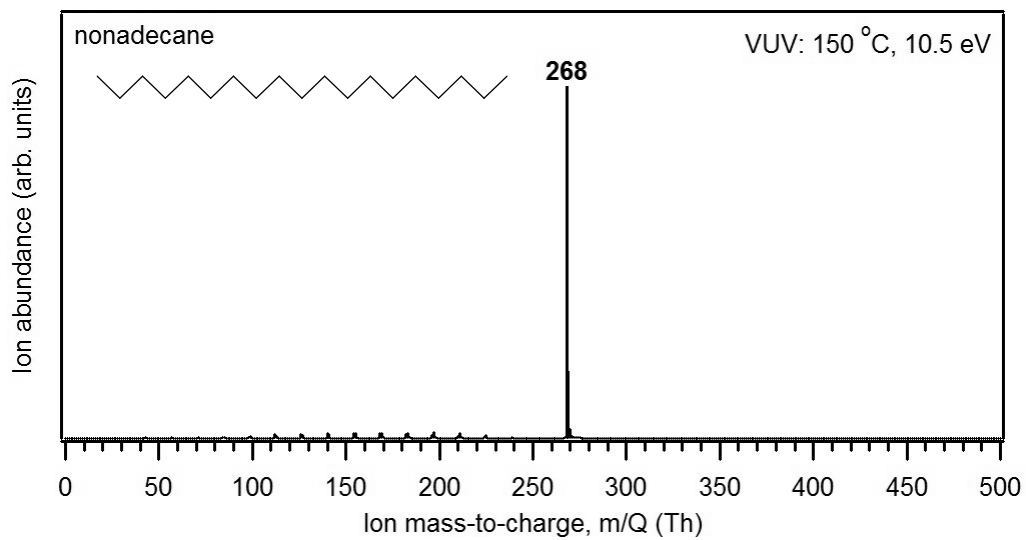
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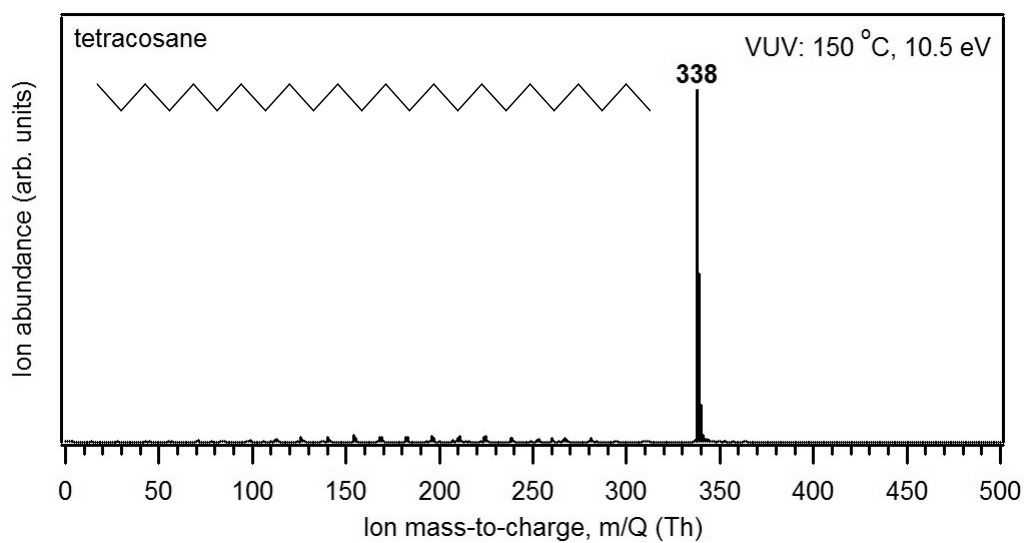
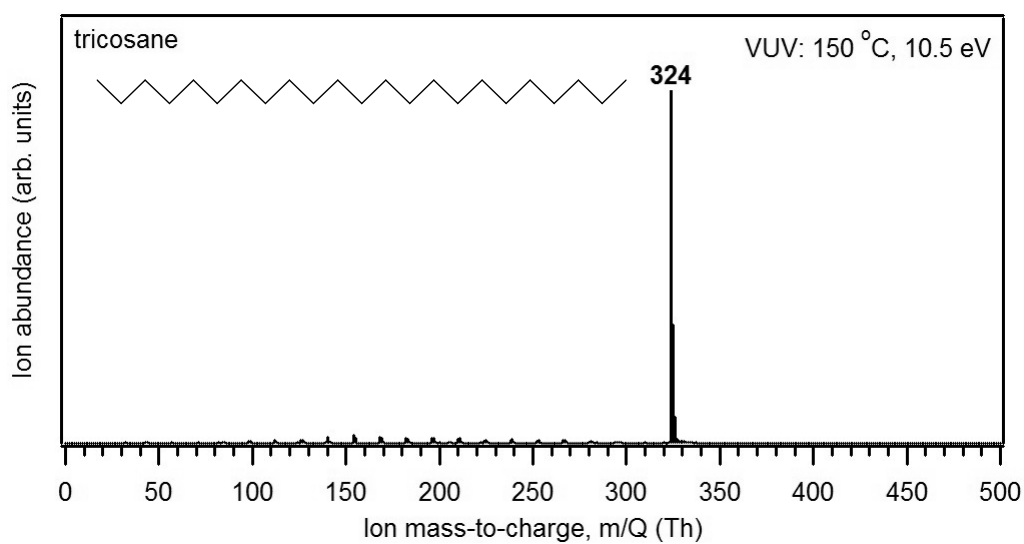
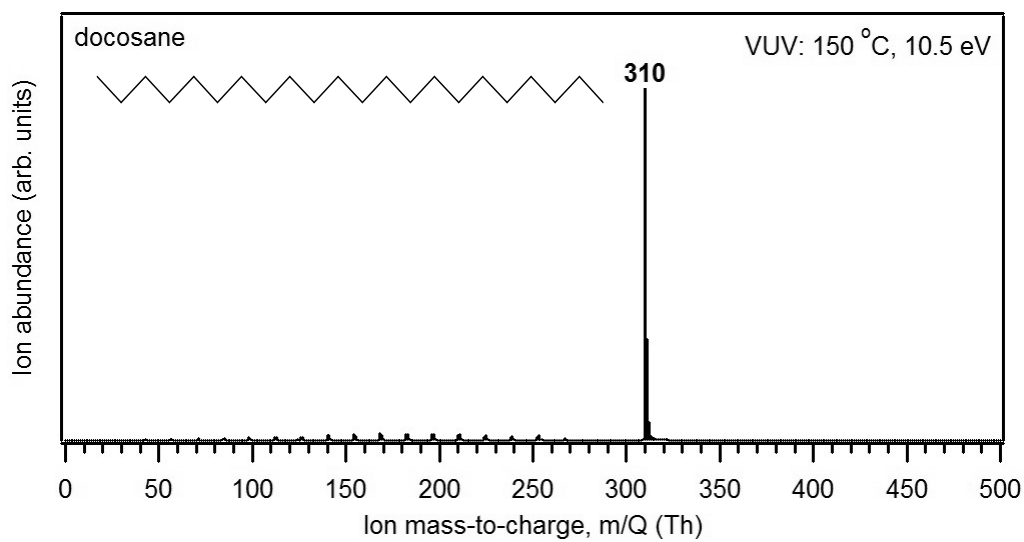
S.1. Spectra at a transfer temperature of 150 °C

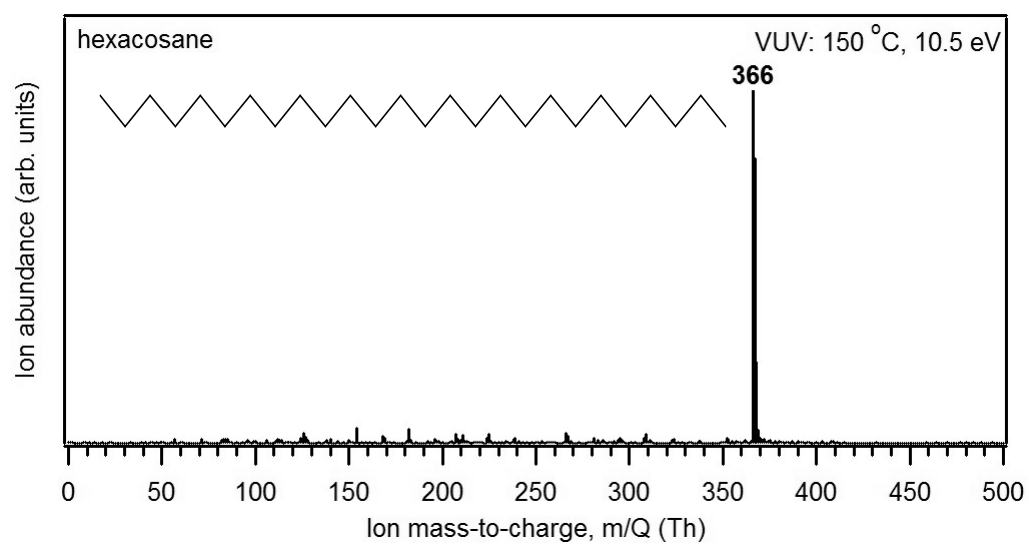
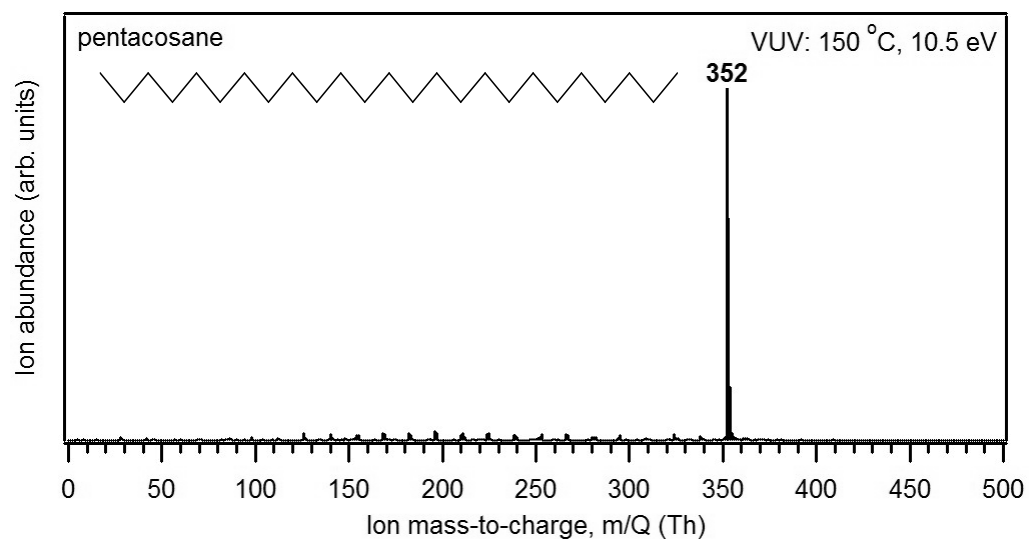
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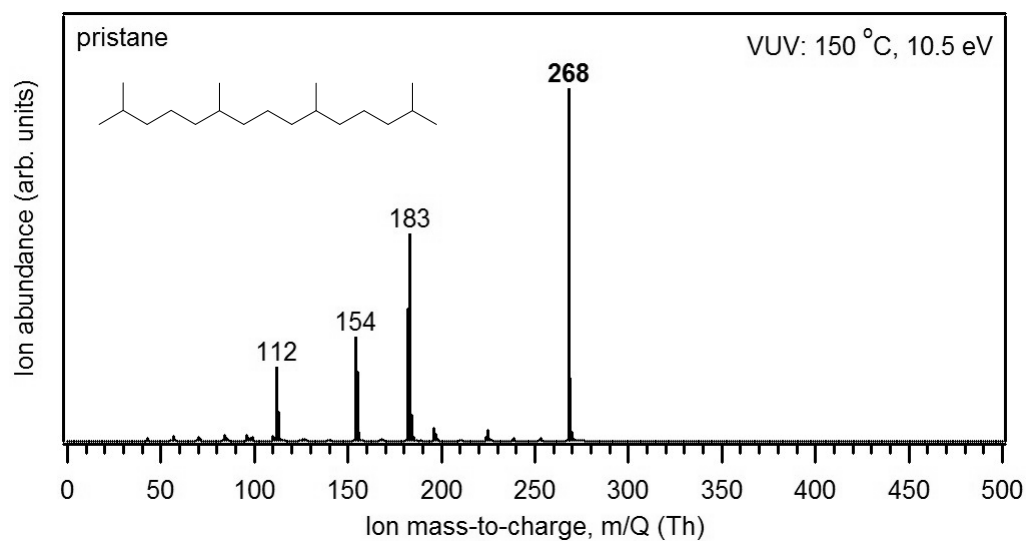
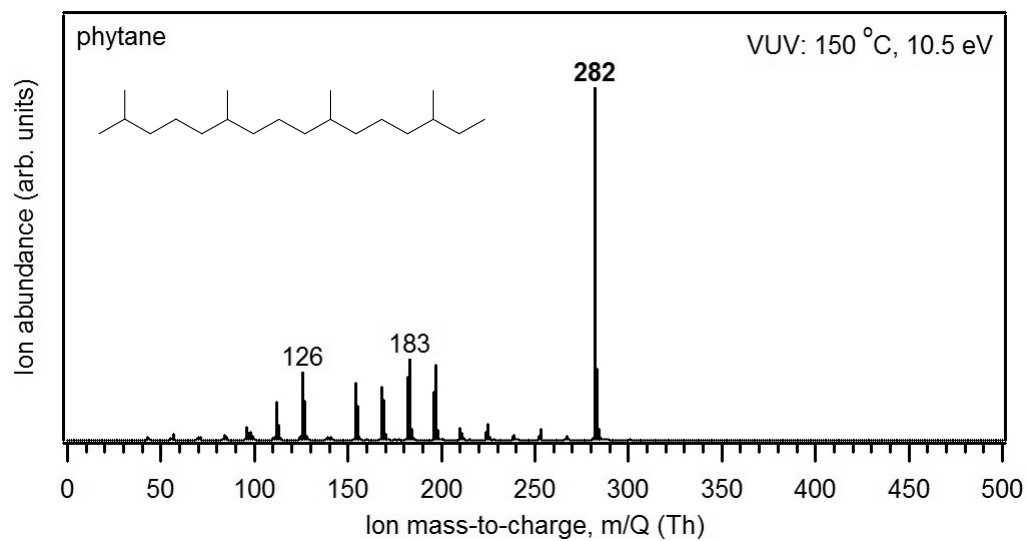


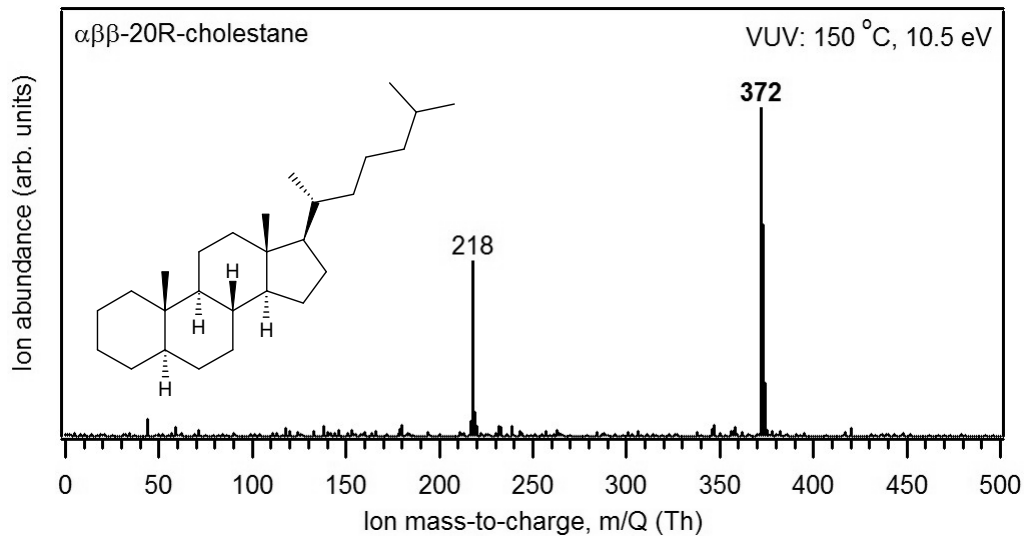
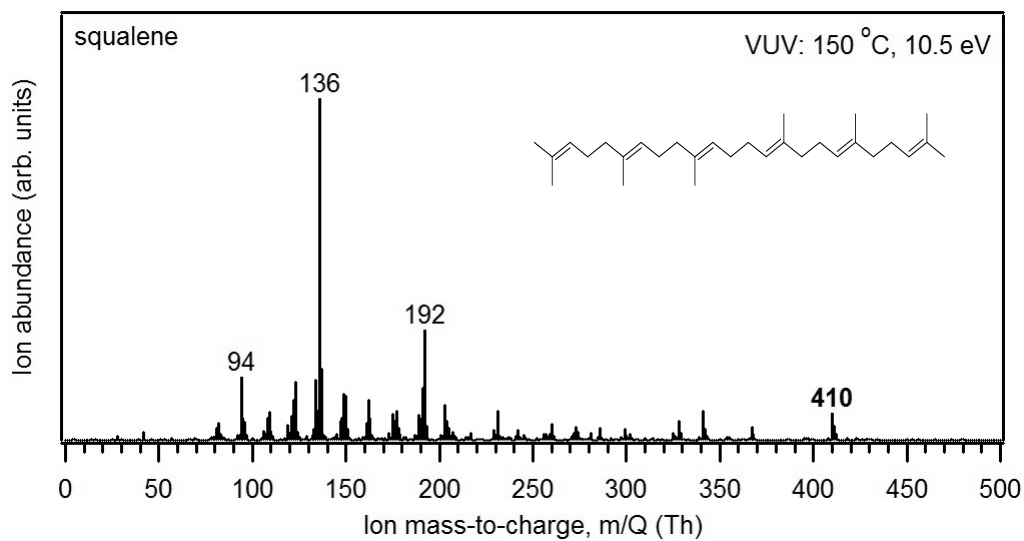
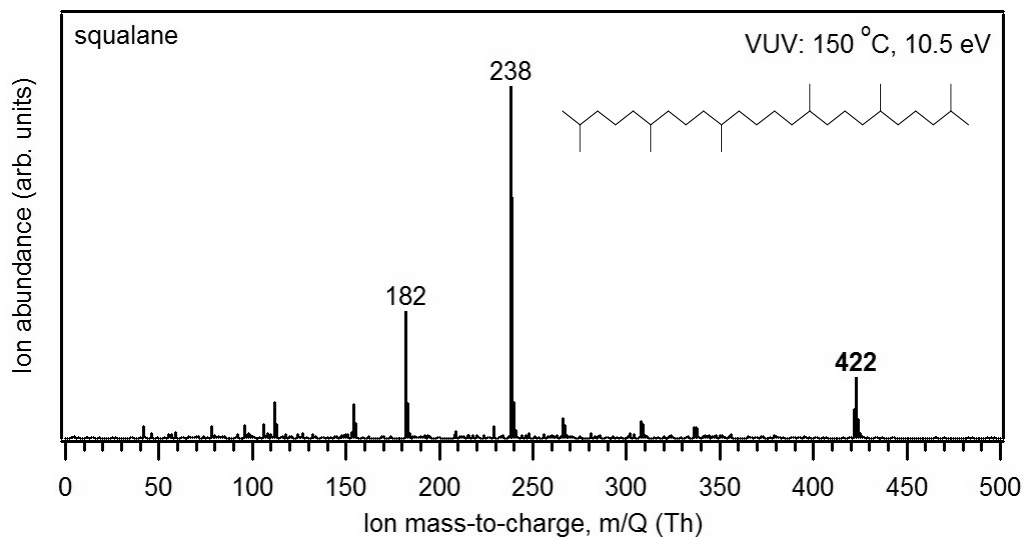




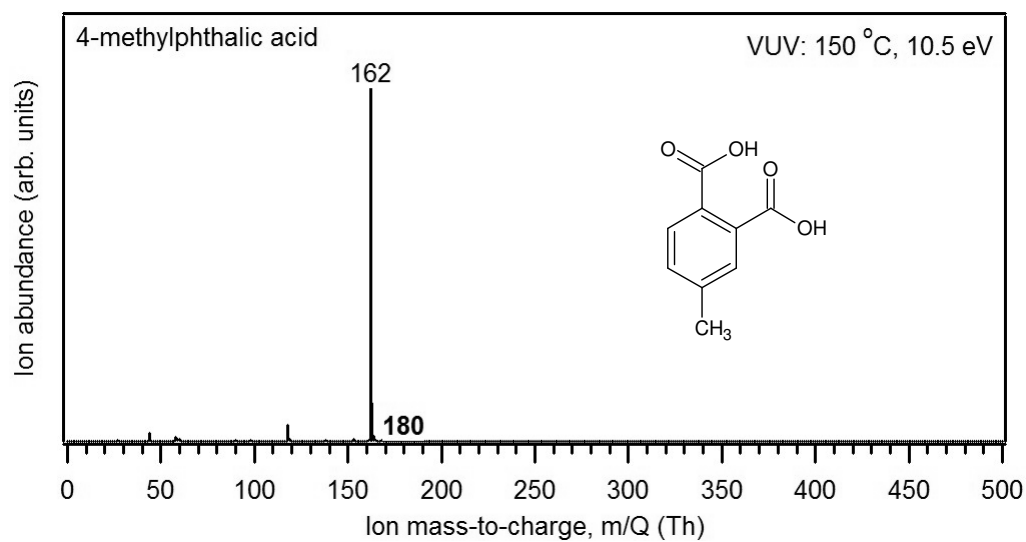
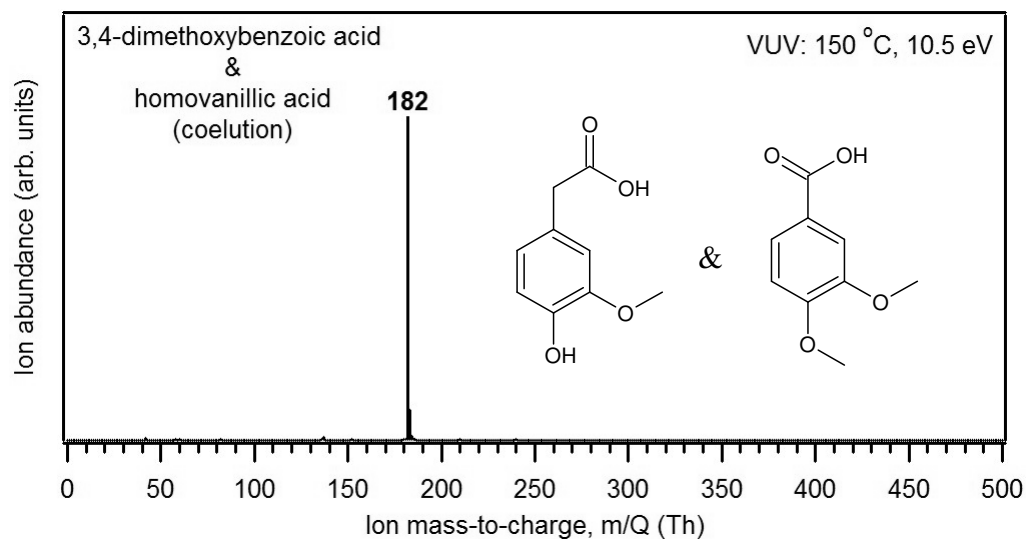


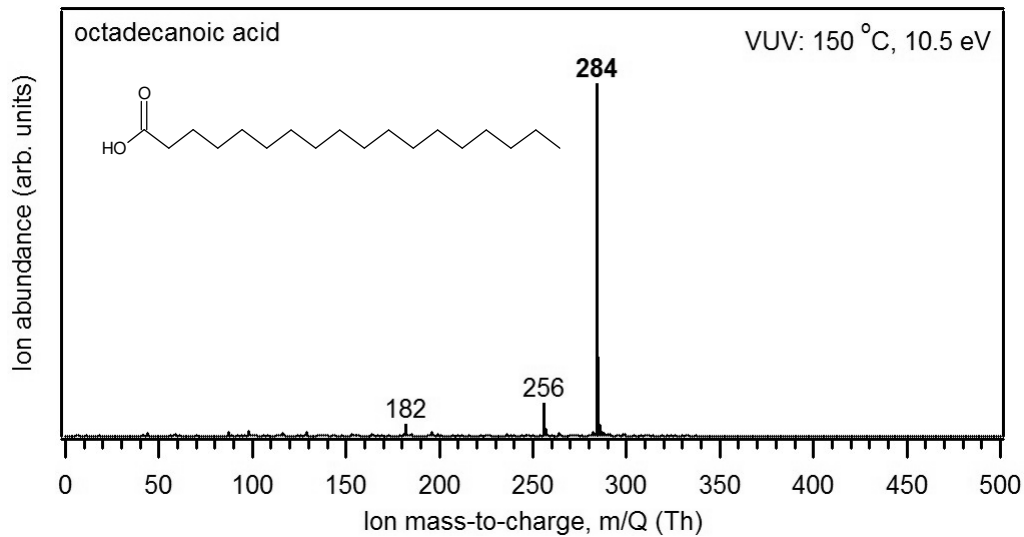
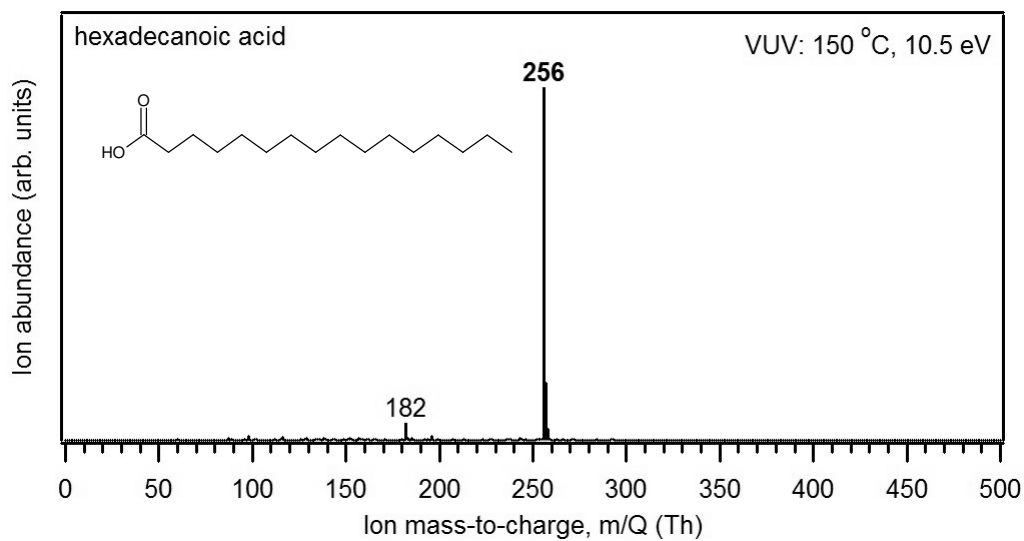
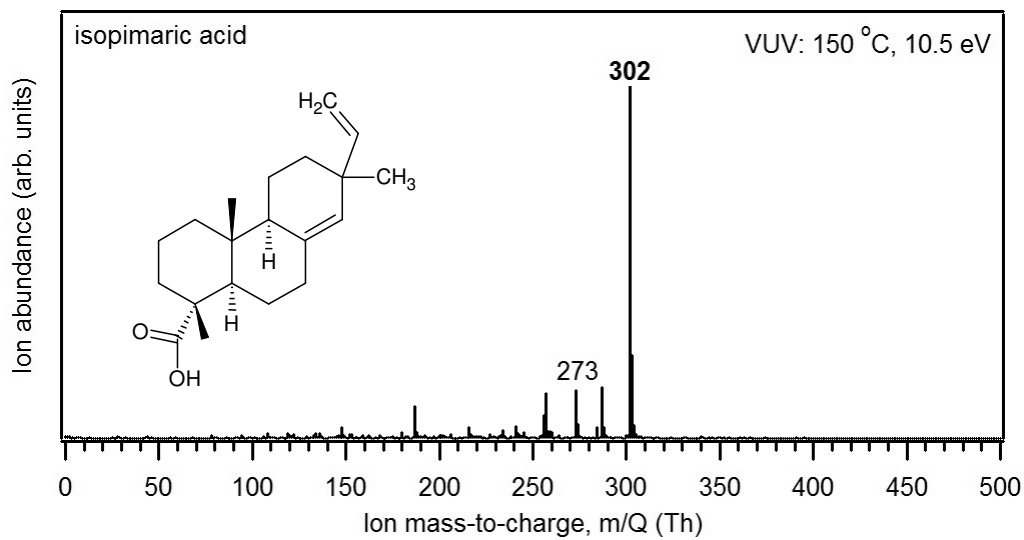
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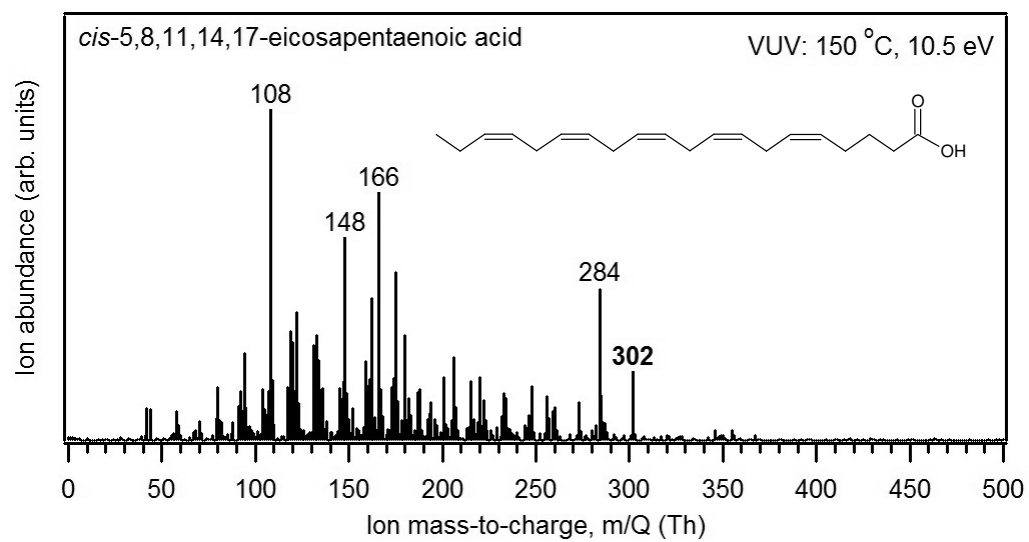




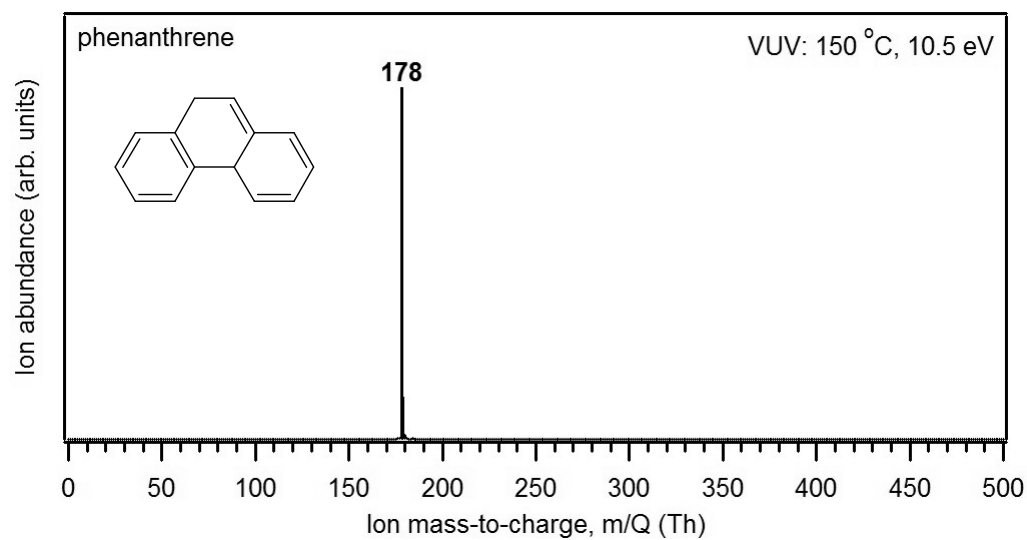
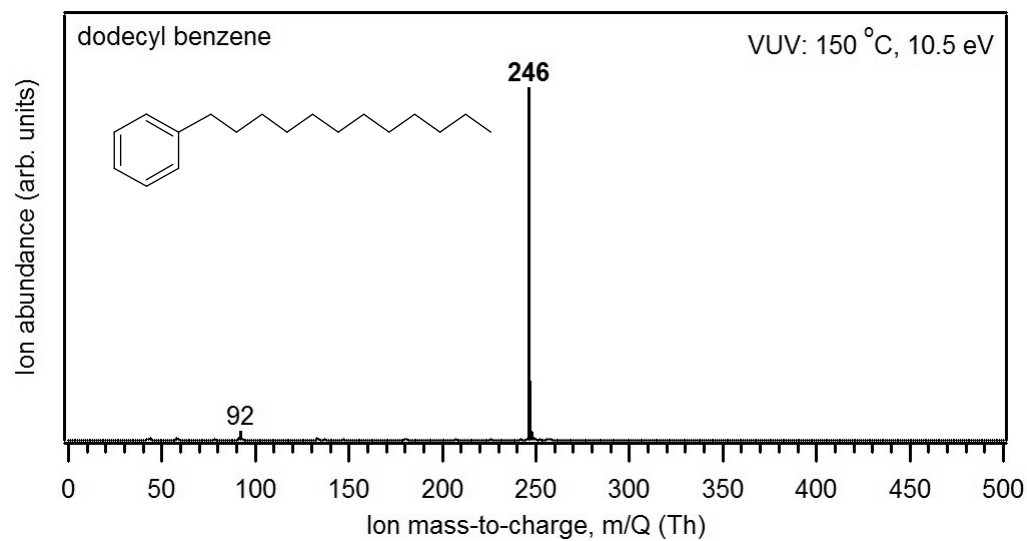
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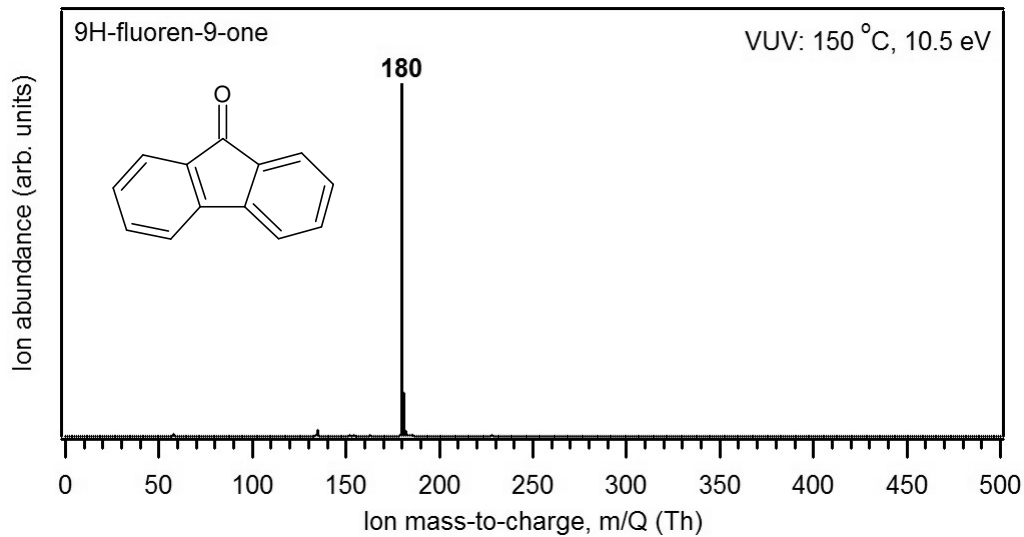
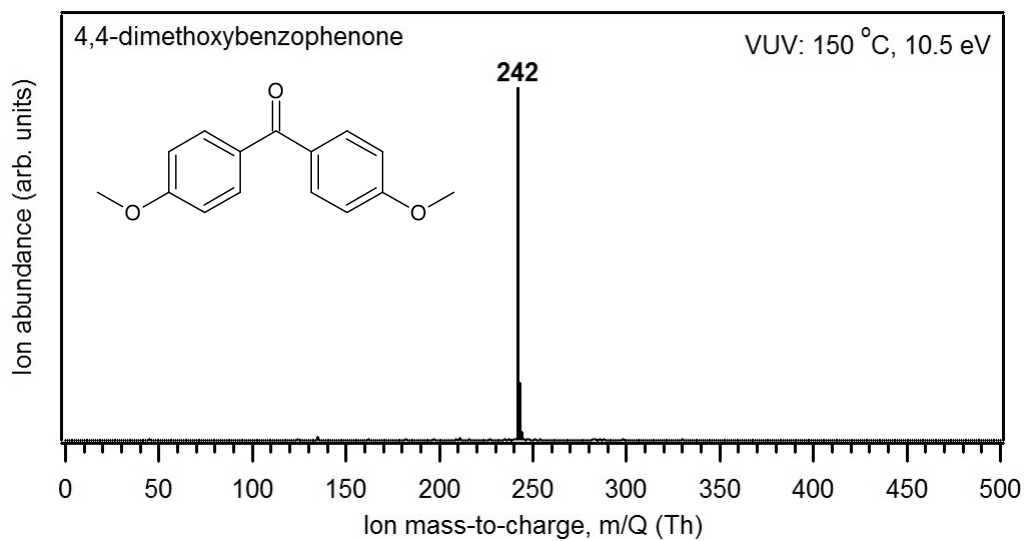
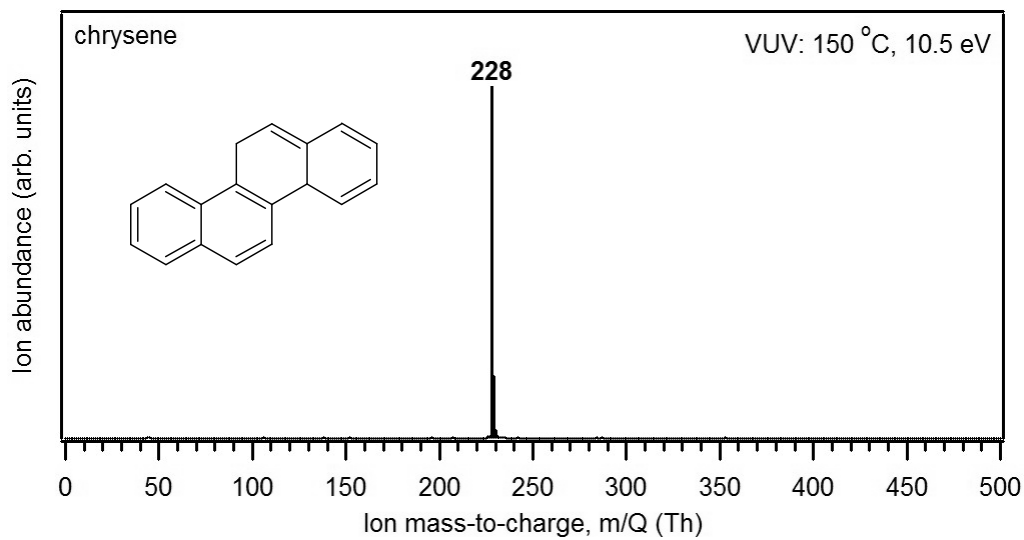


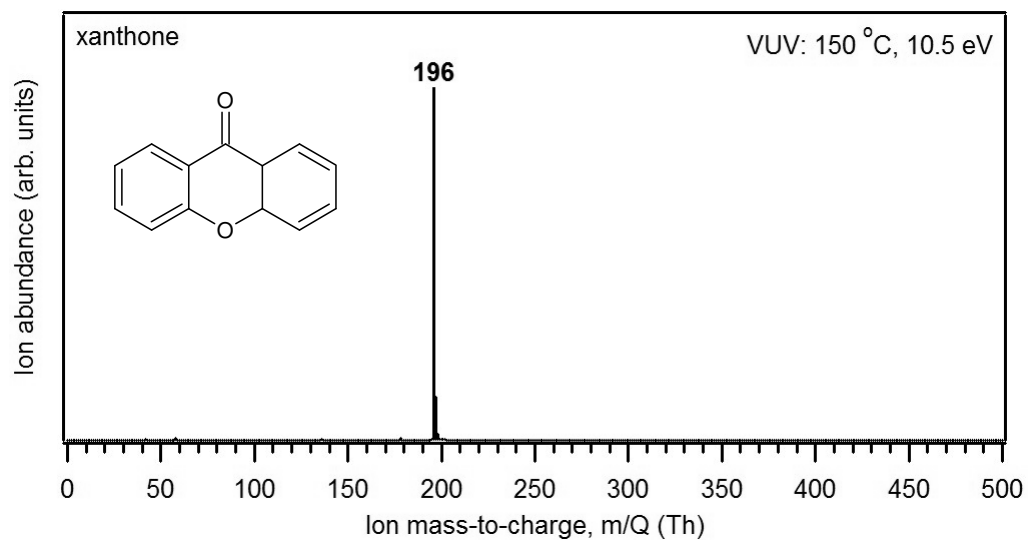
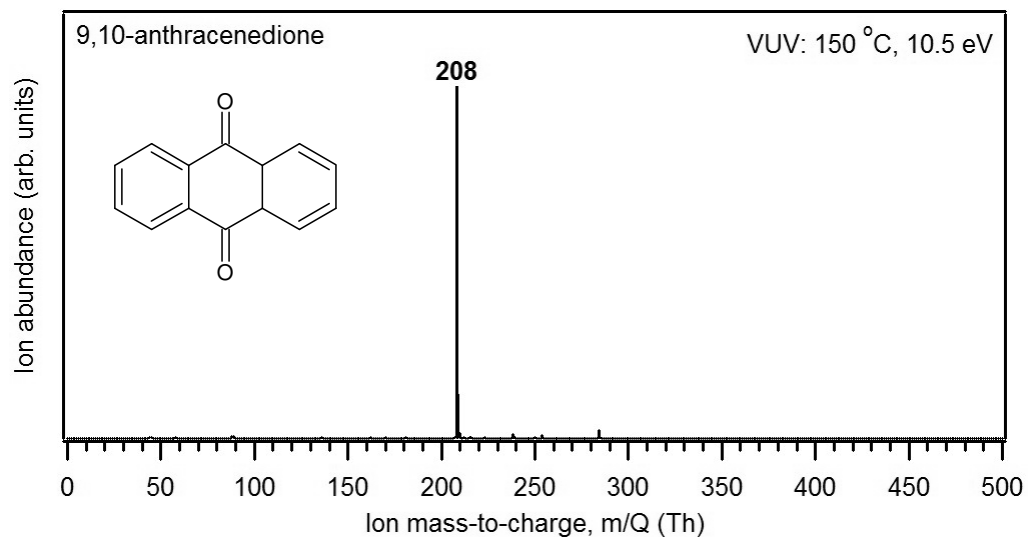




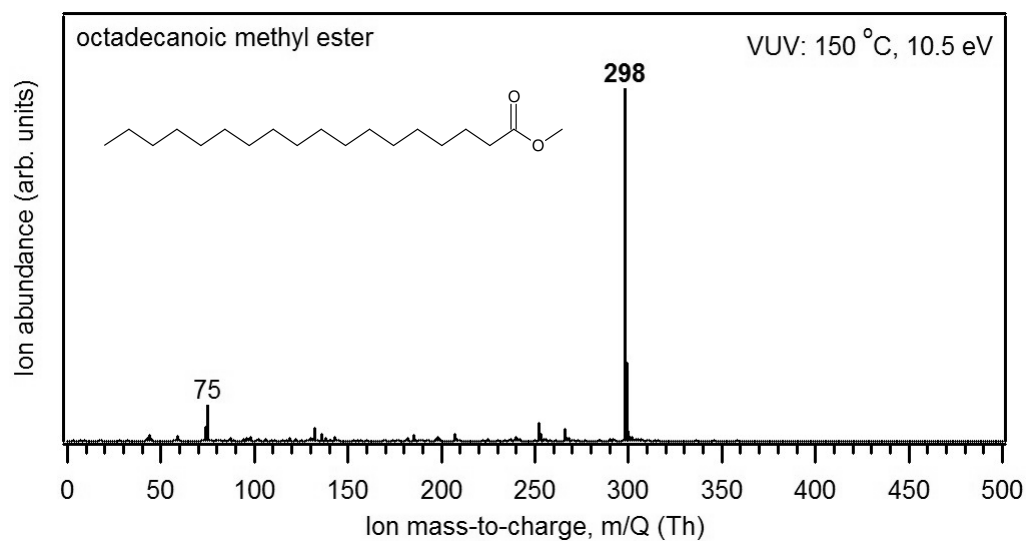
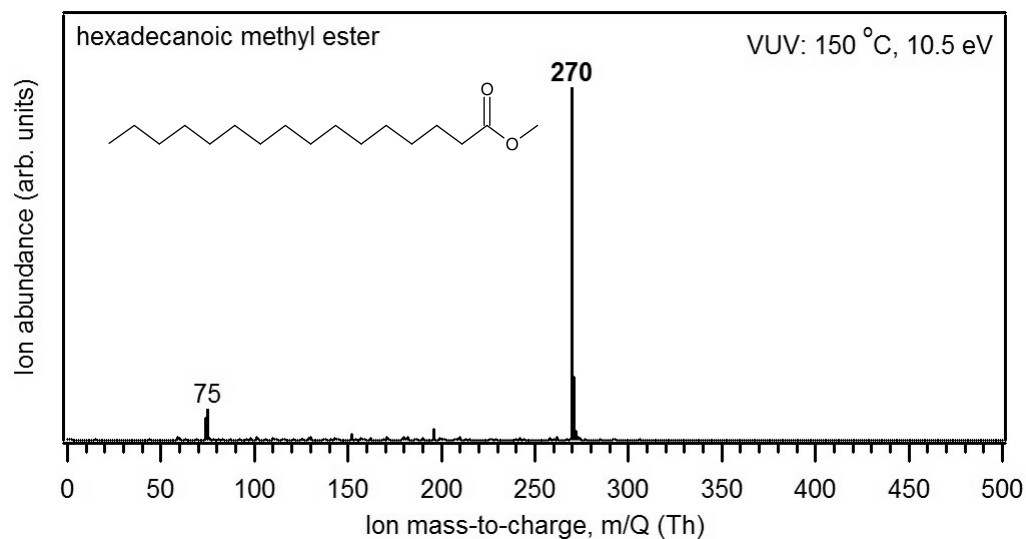
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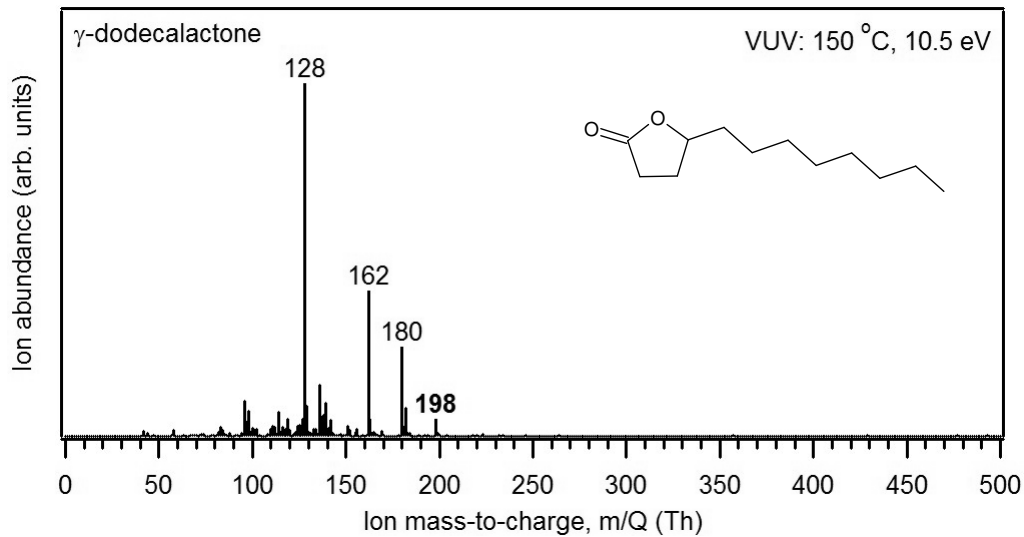
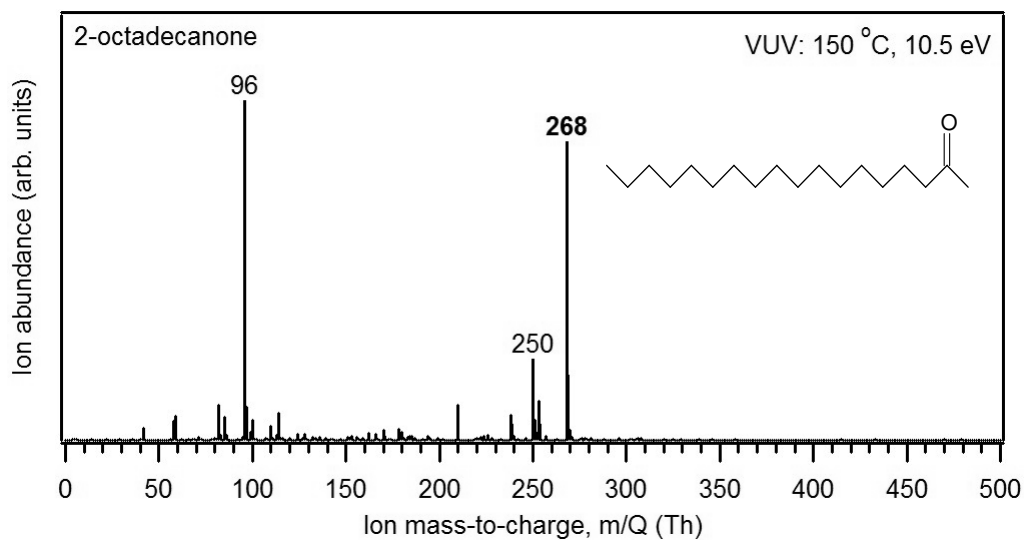
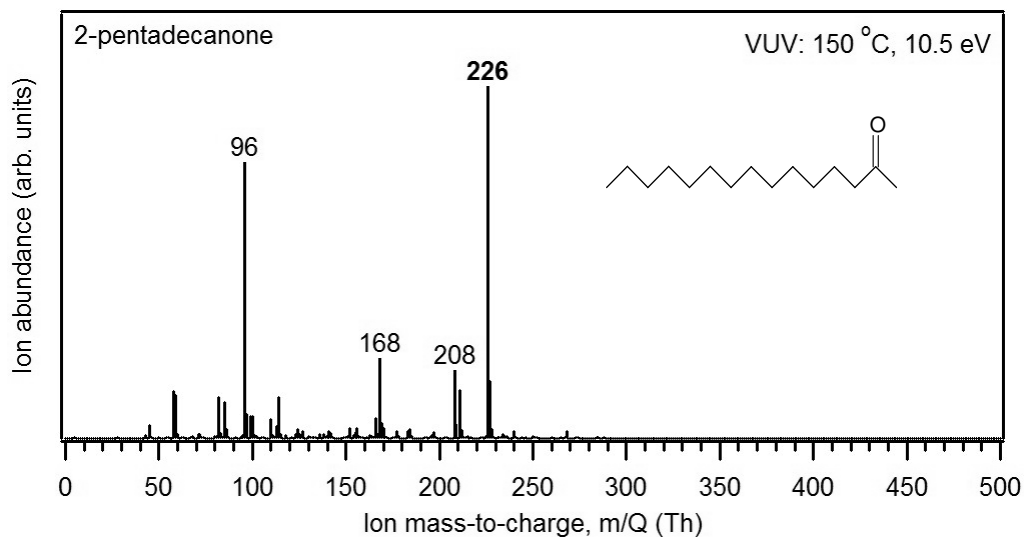


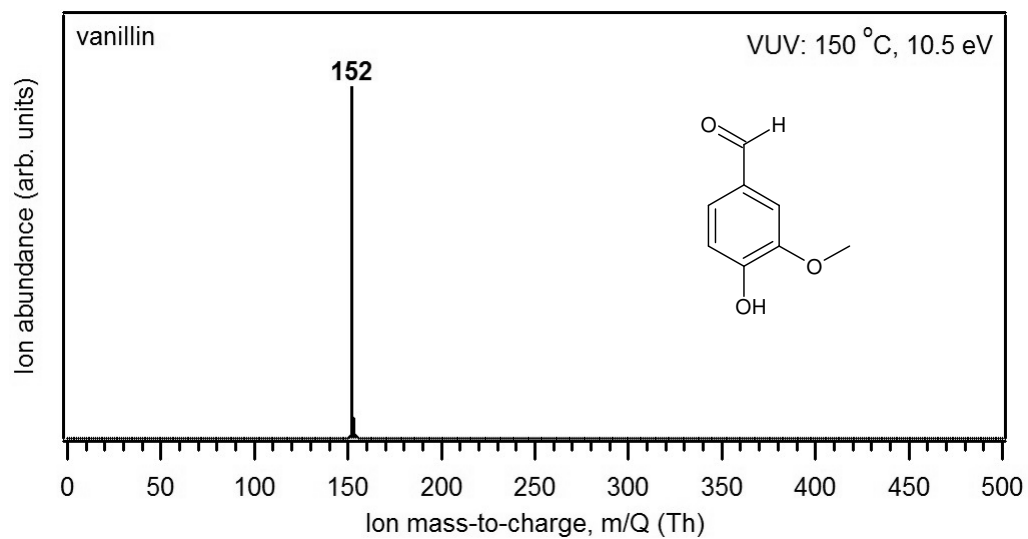
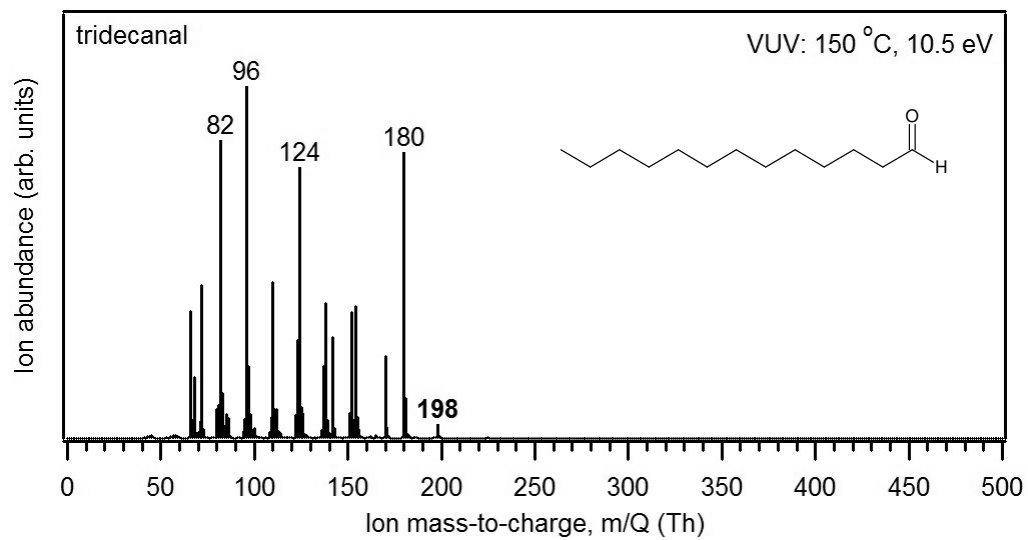




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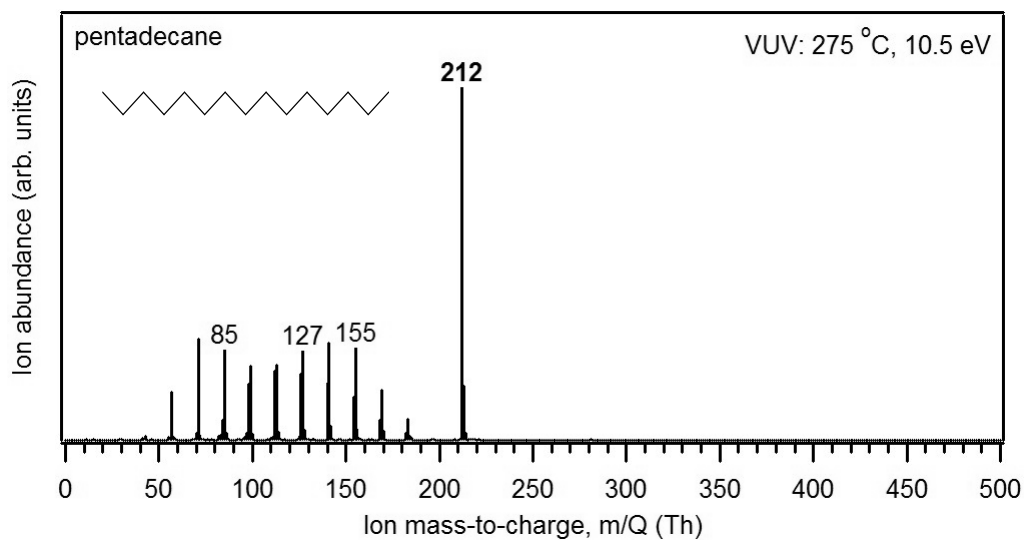
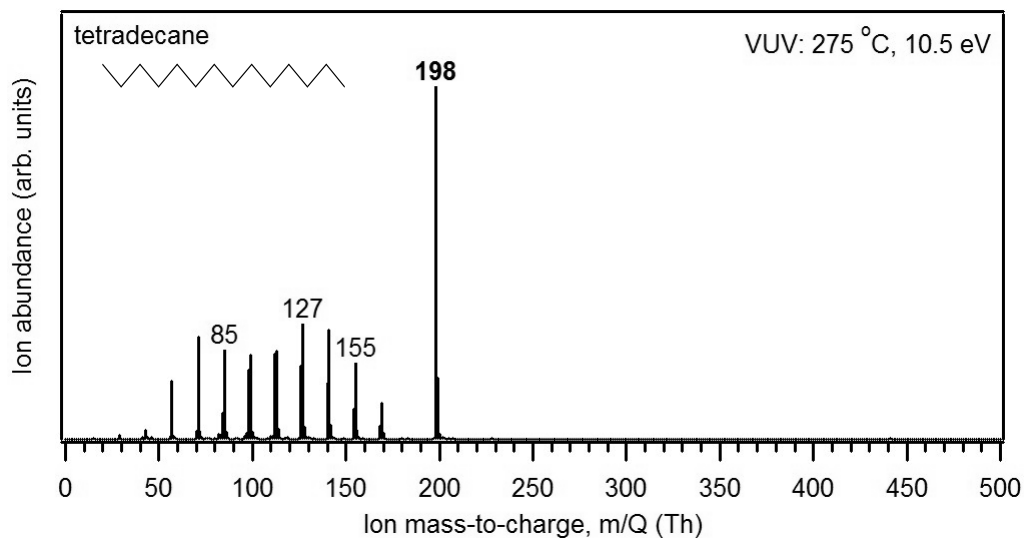


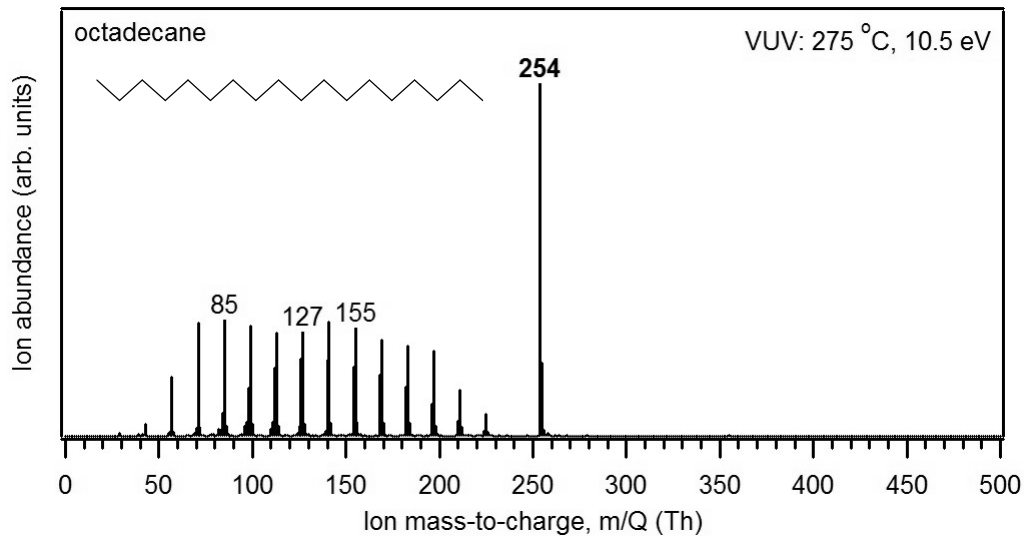
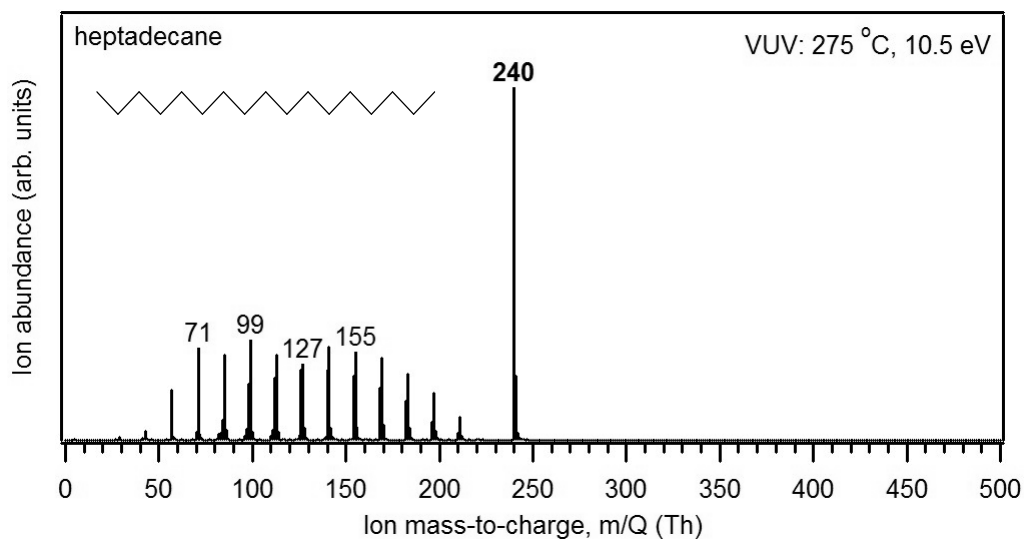
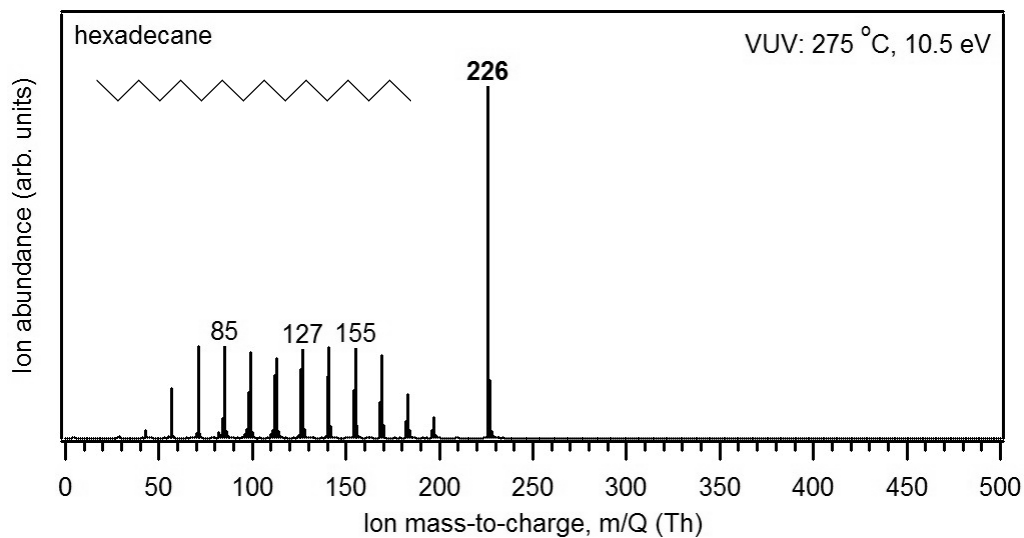


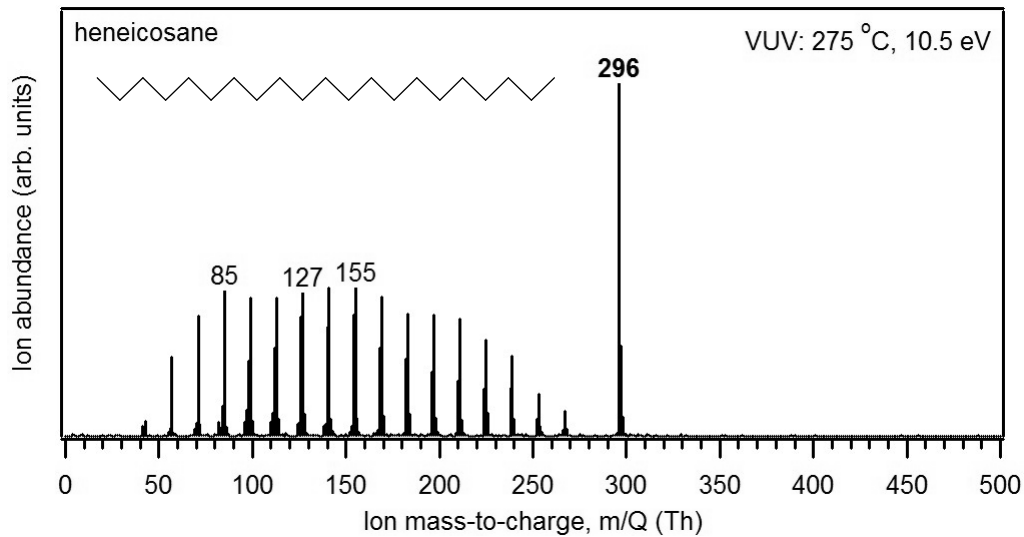
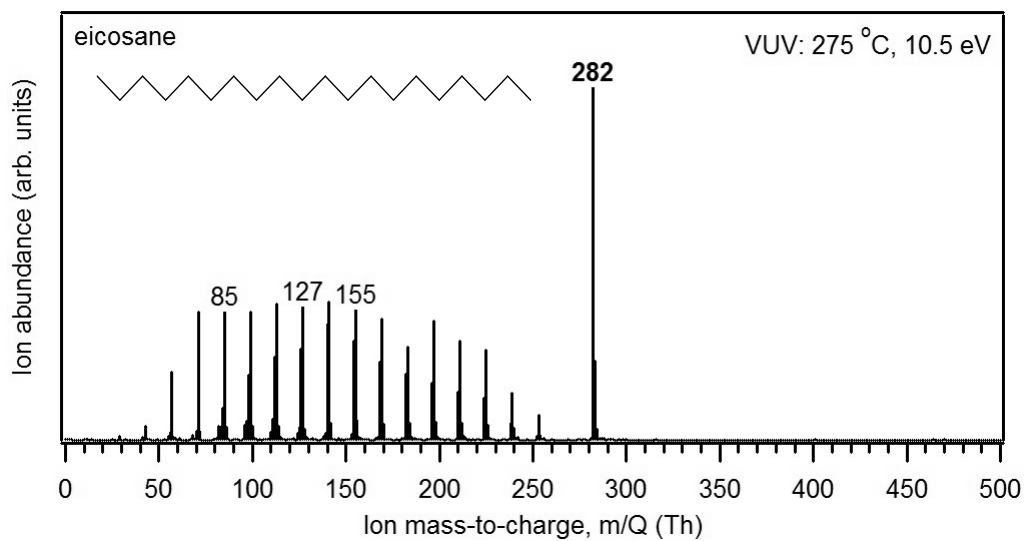
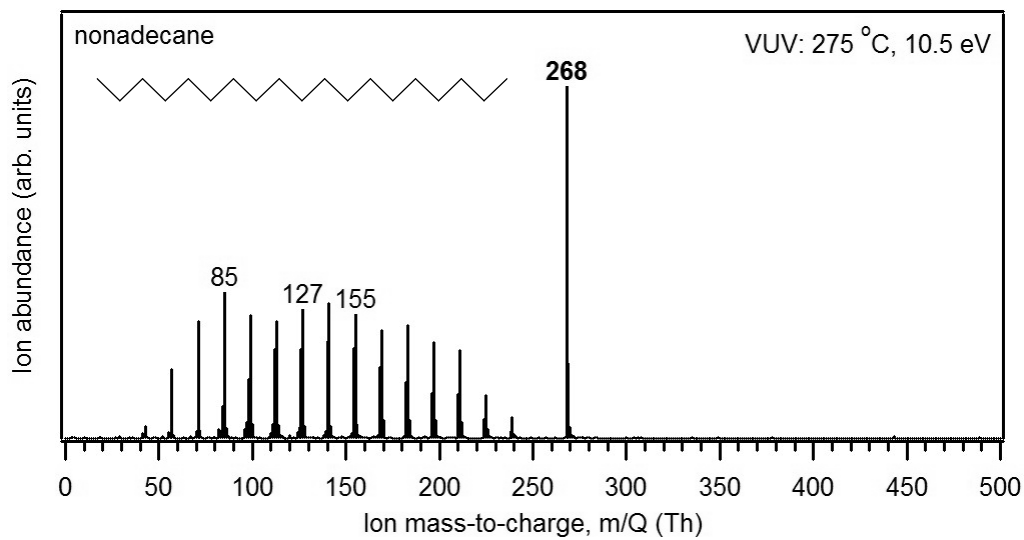


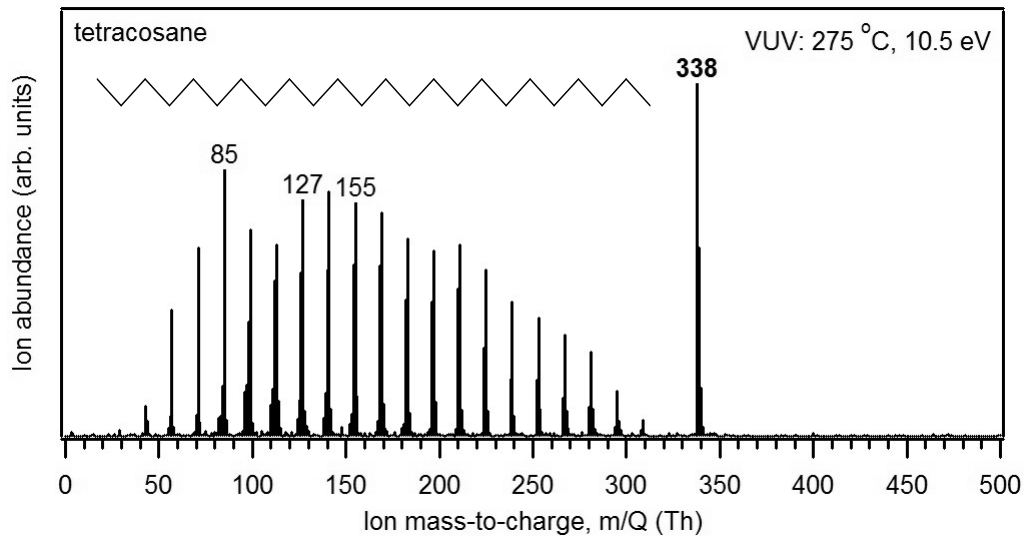
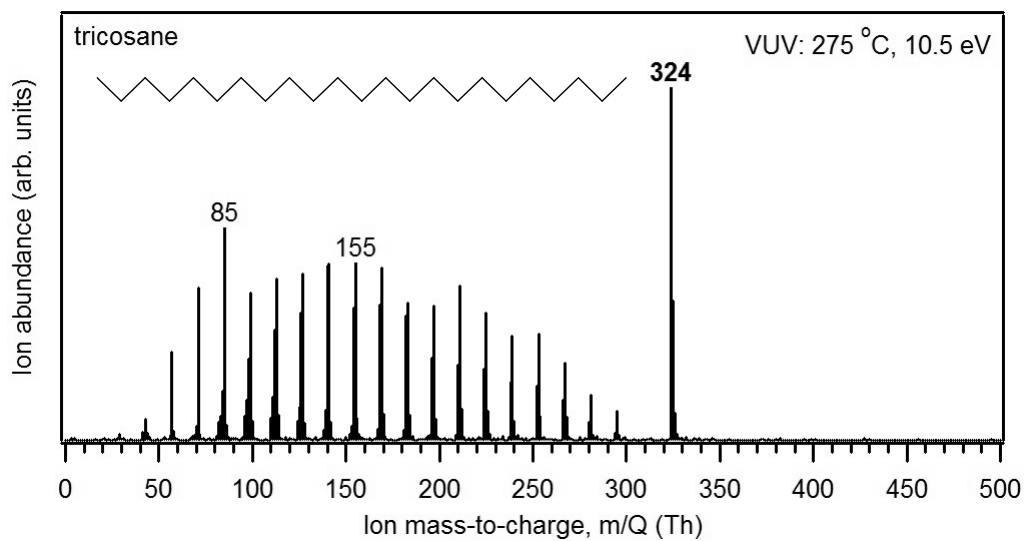
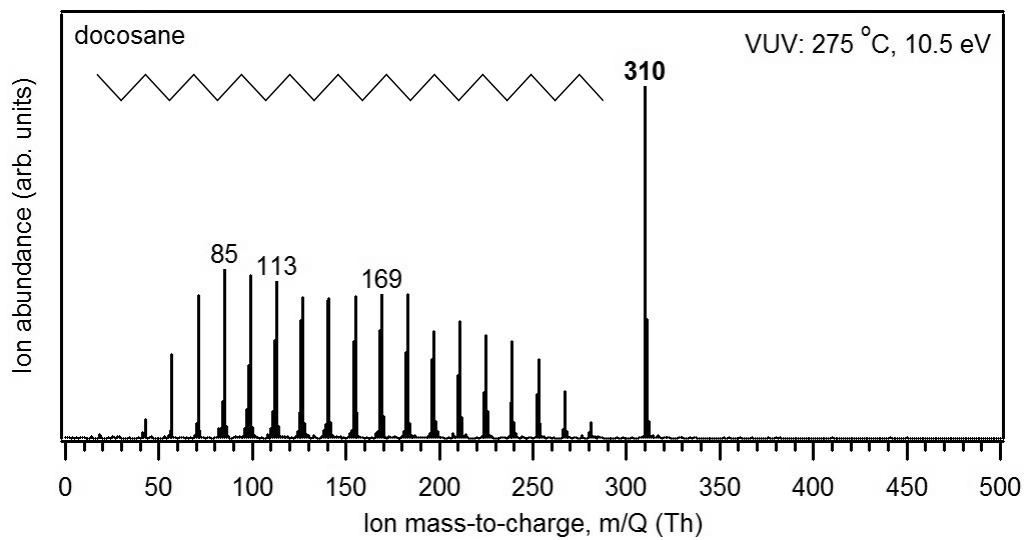
S.2. Spectra at a transfer temperature of 275 °C

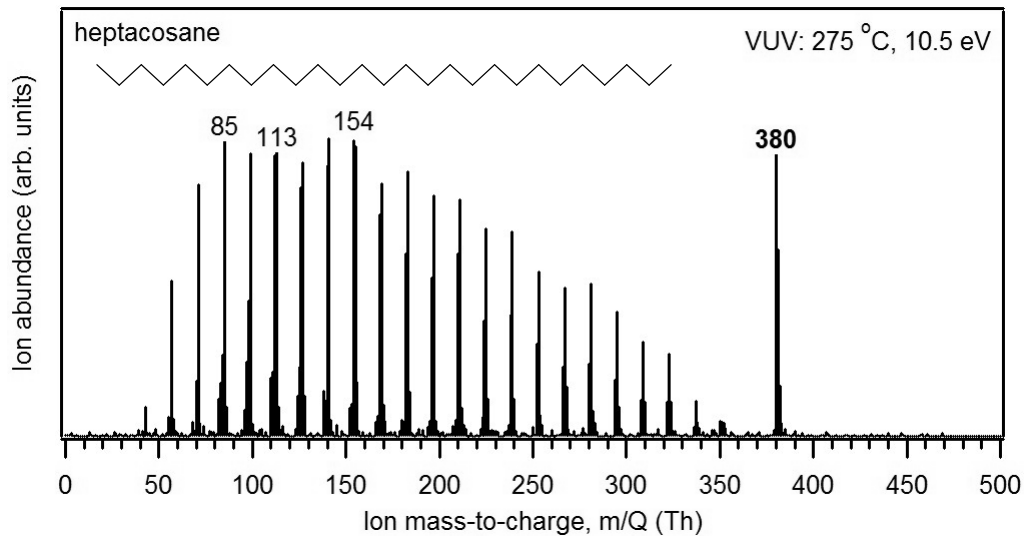
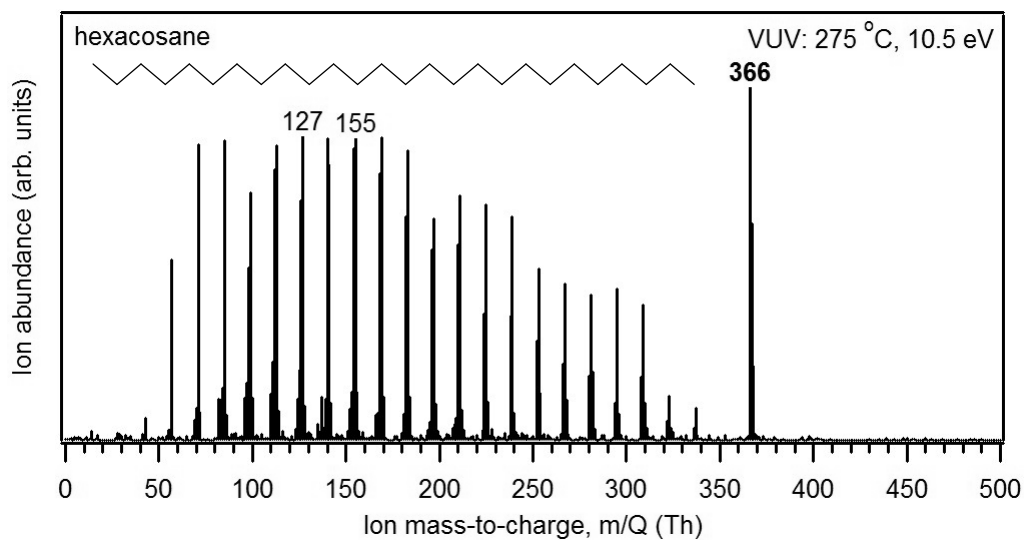
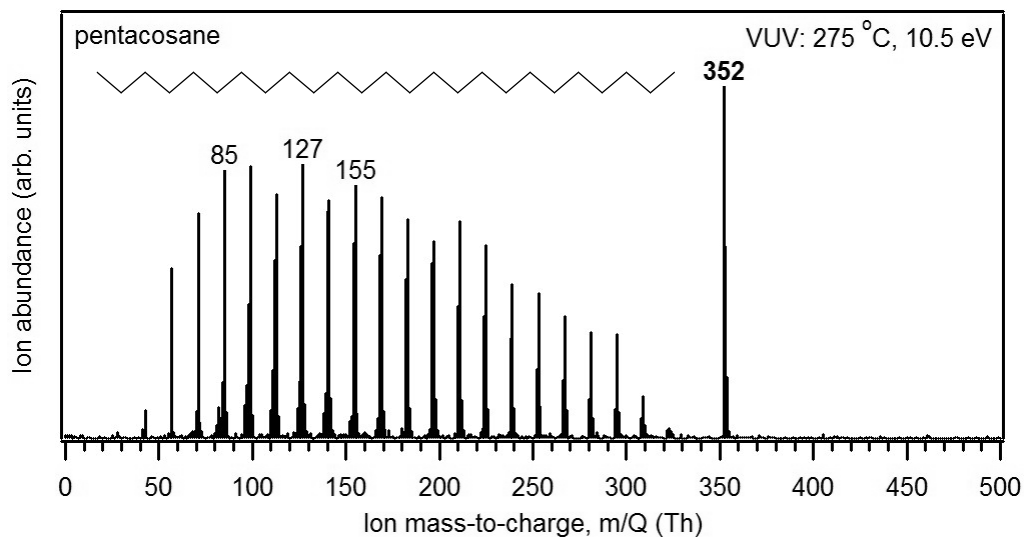
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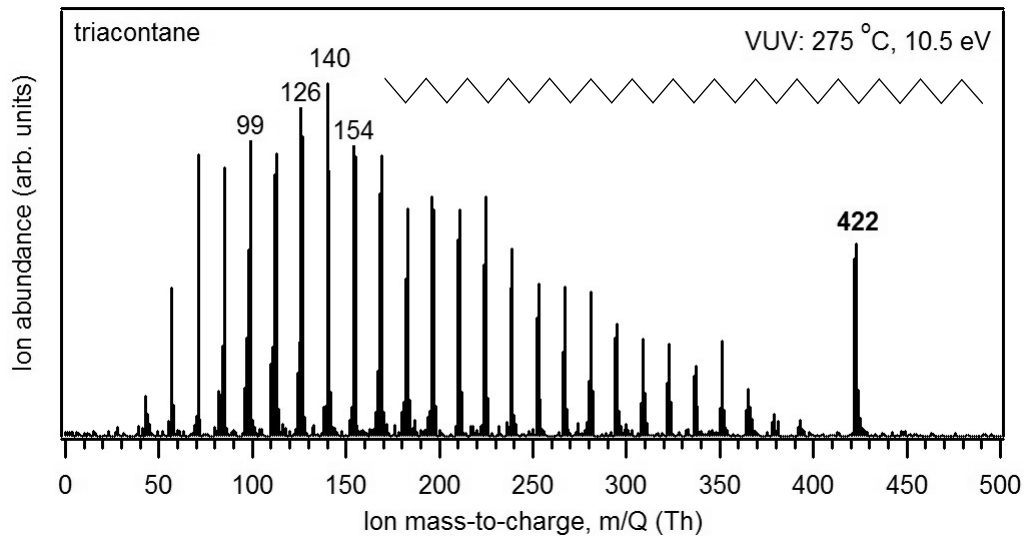
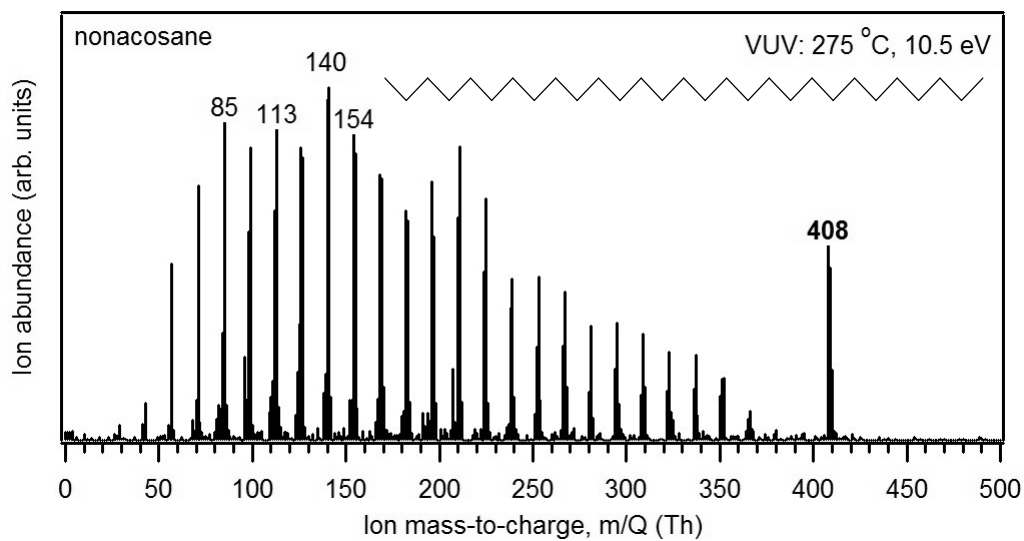
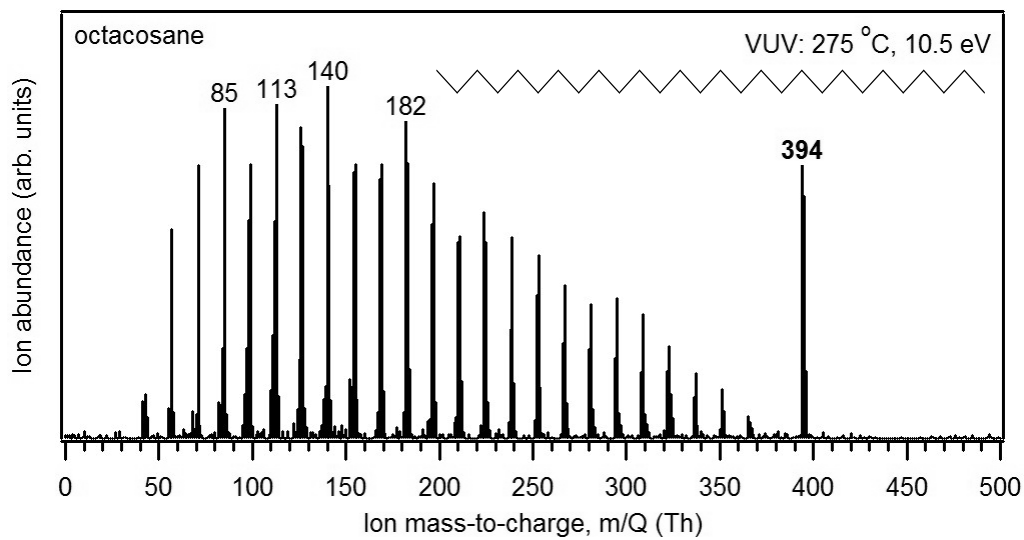


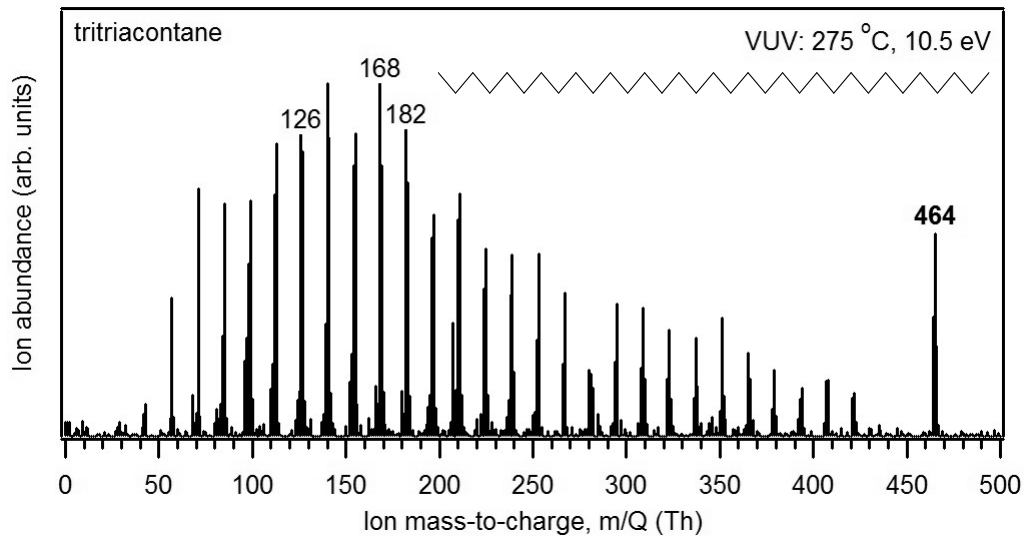
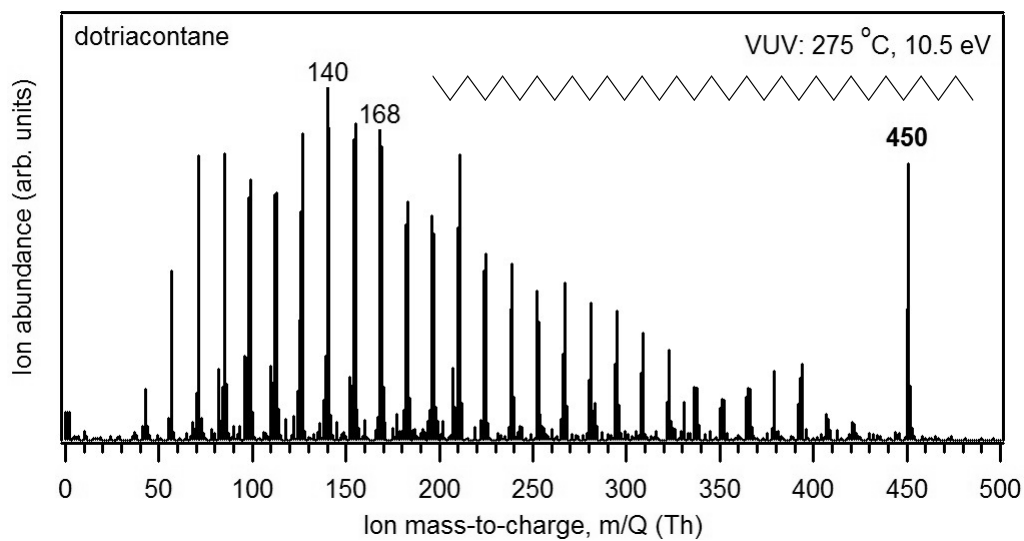
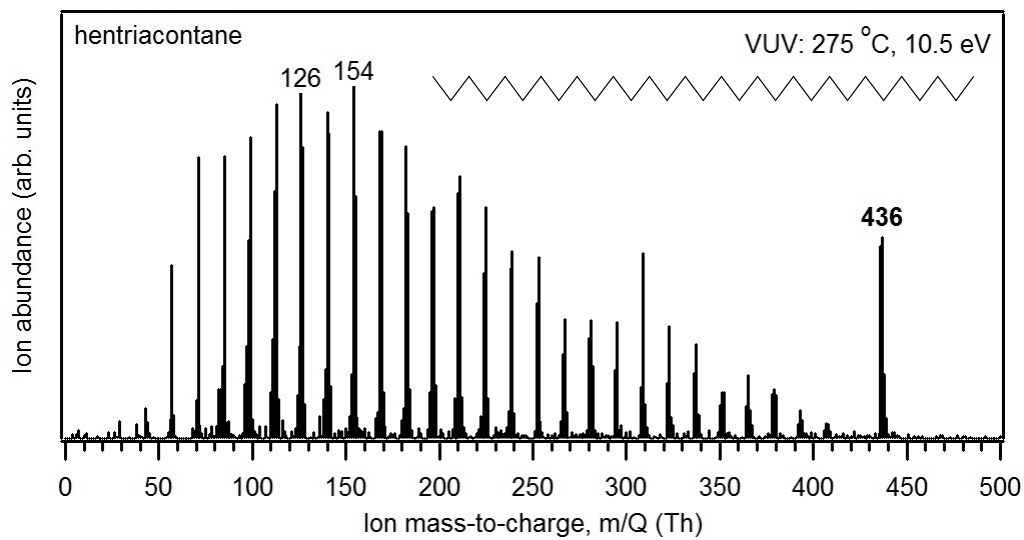


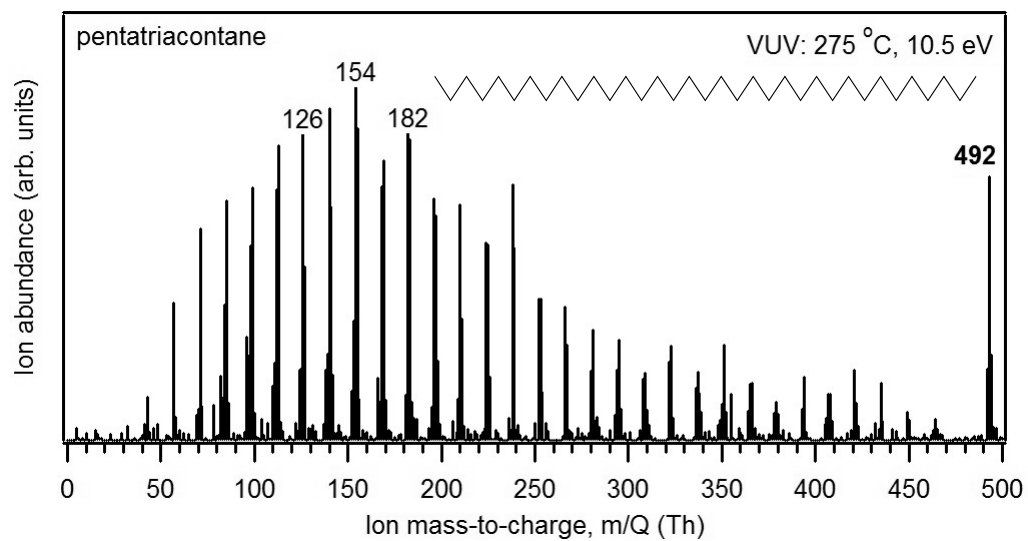
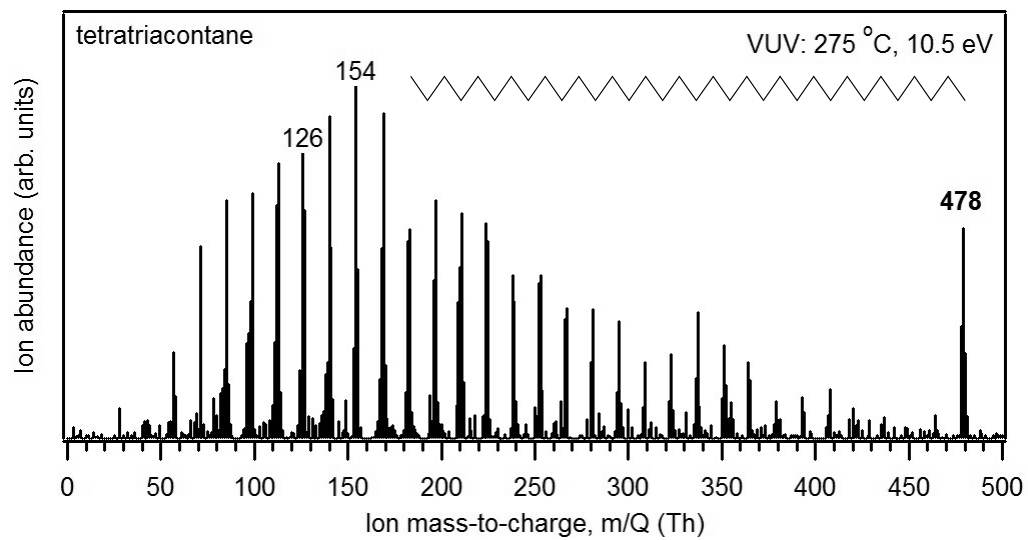




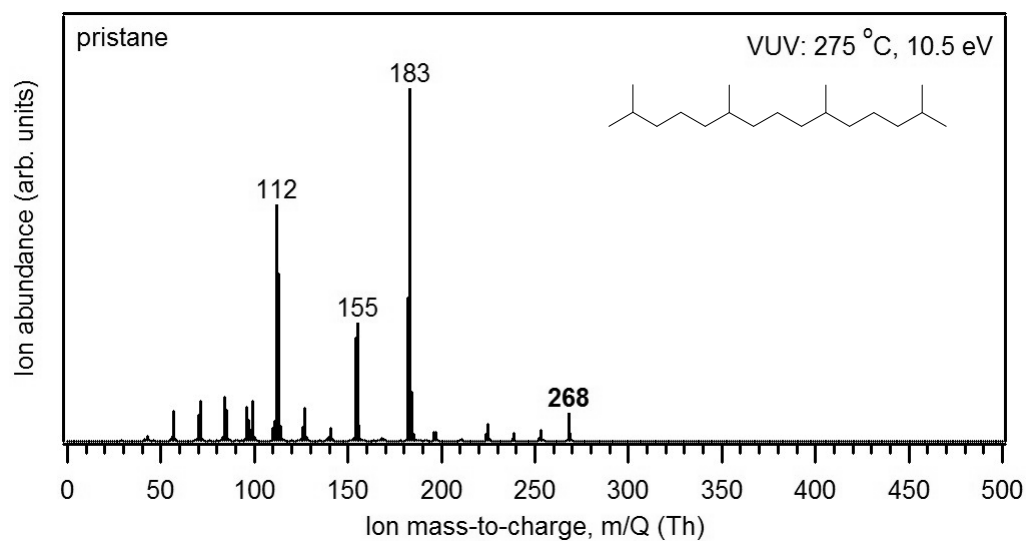
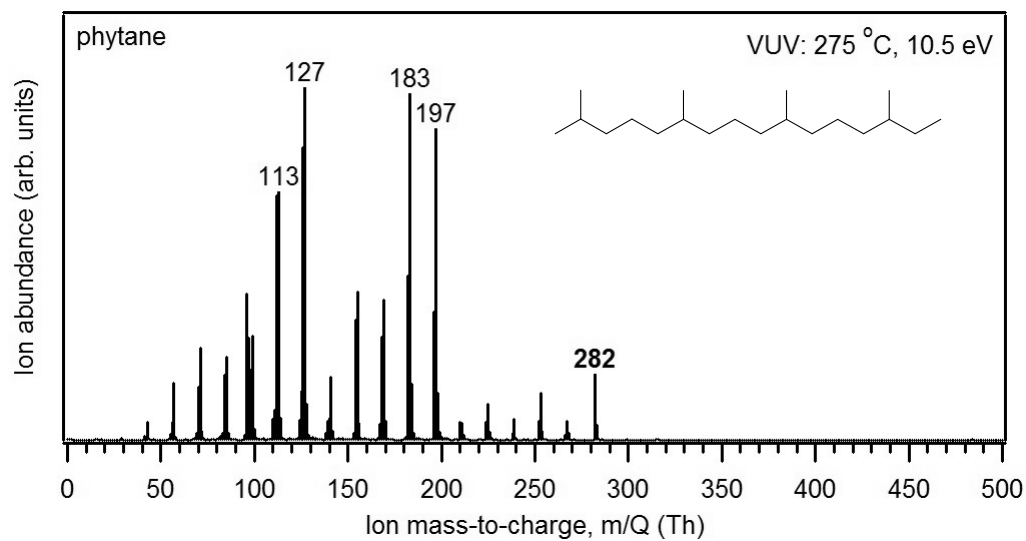


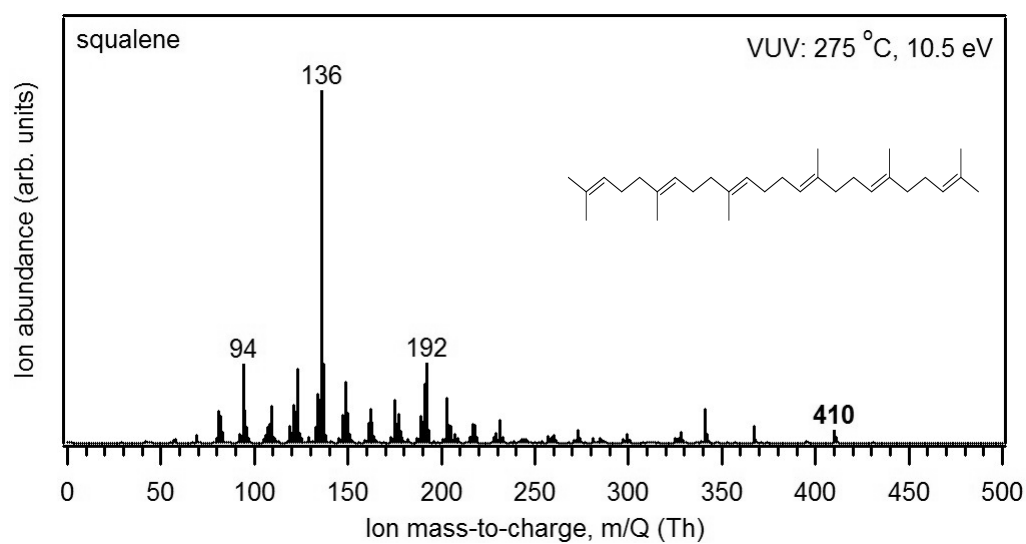
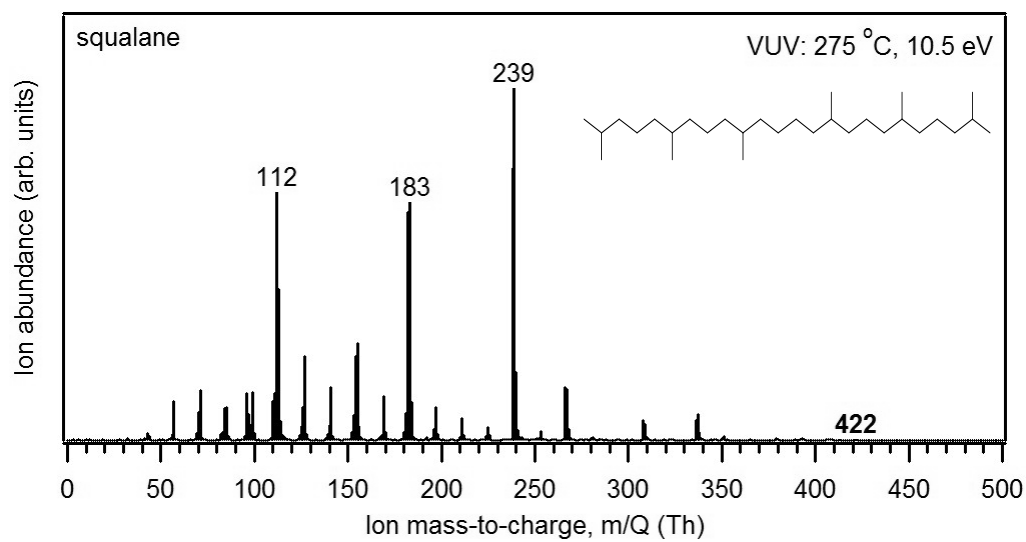




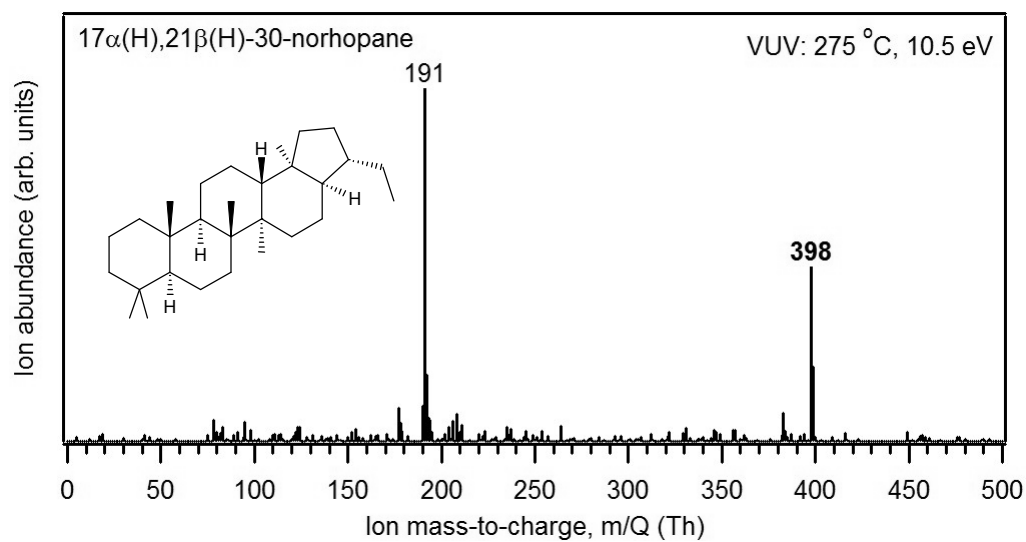
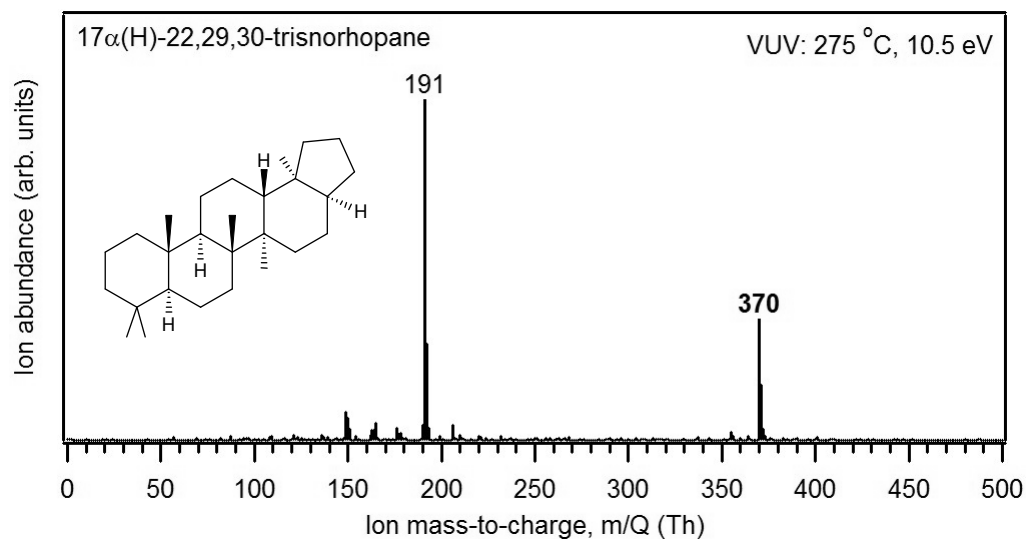


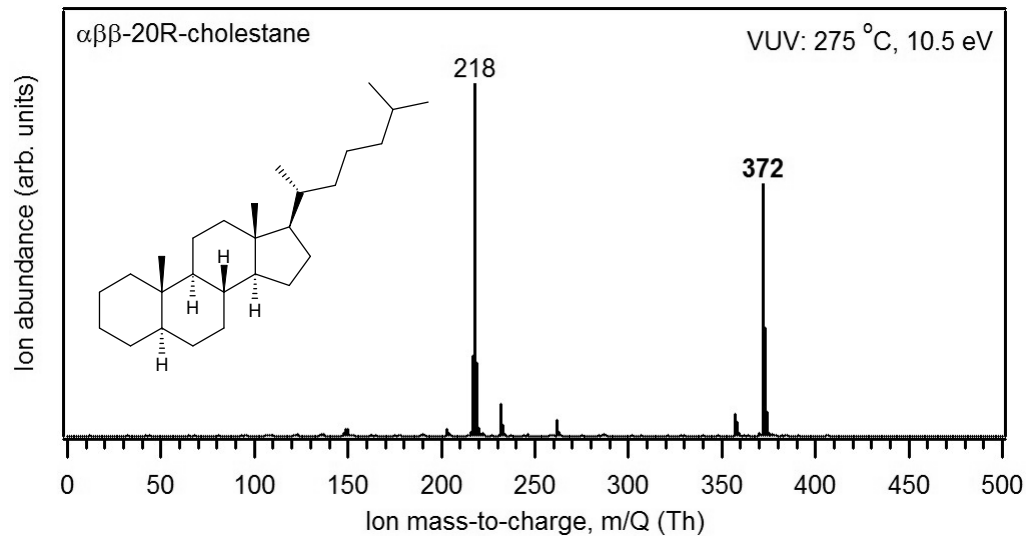
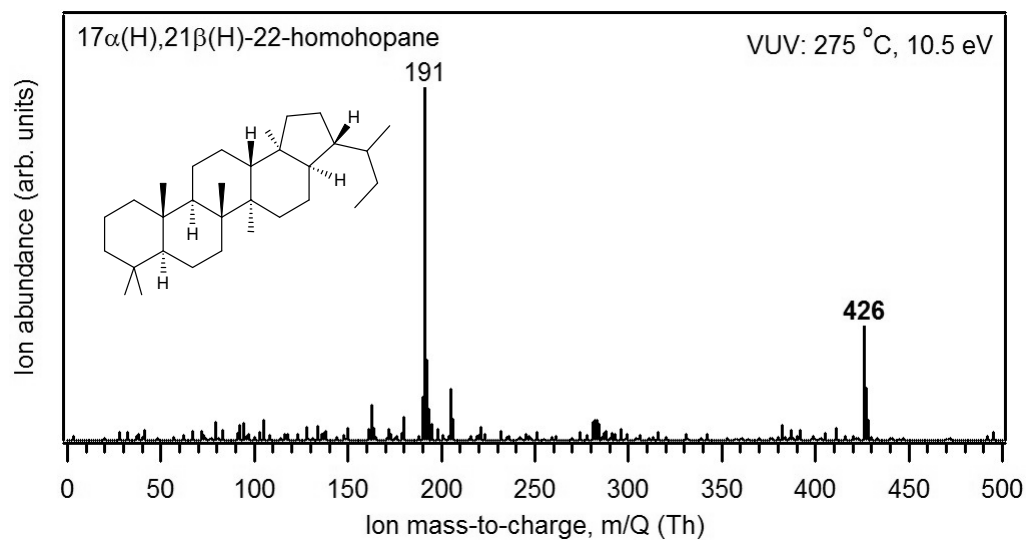
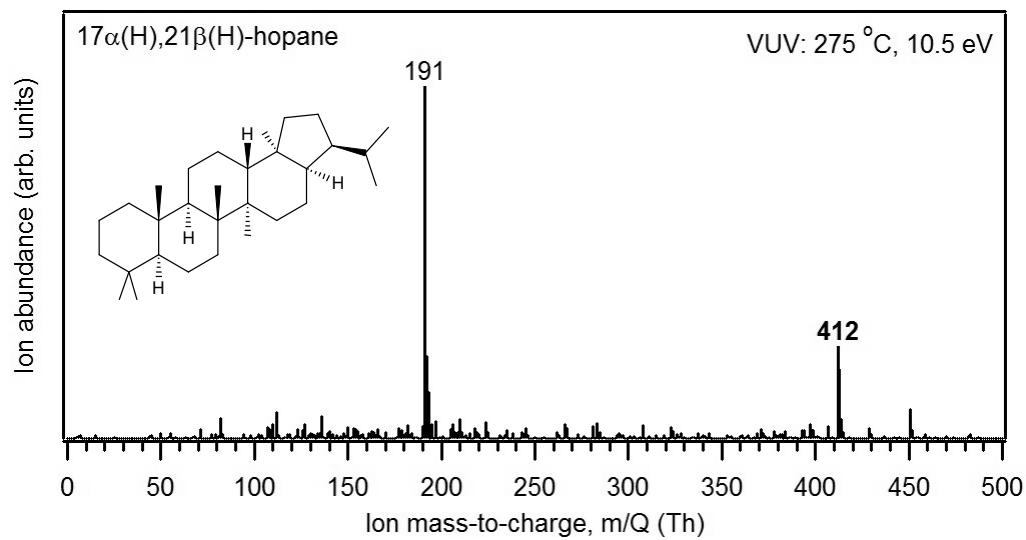
S.2.2. Branched aliphatic hydrocarbons

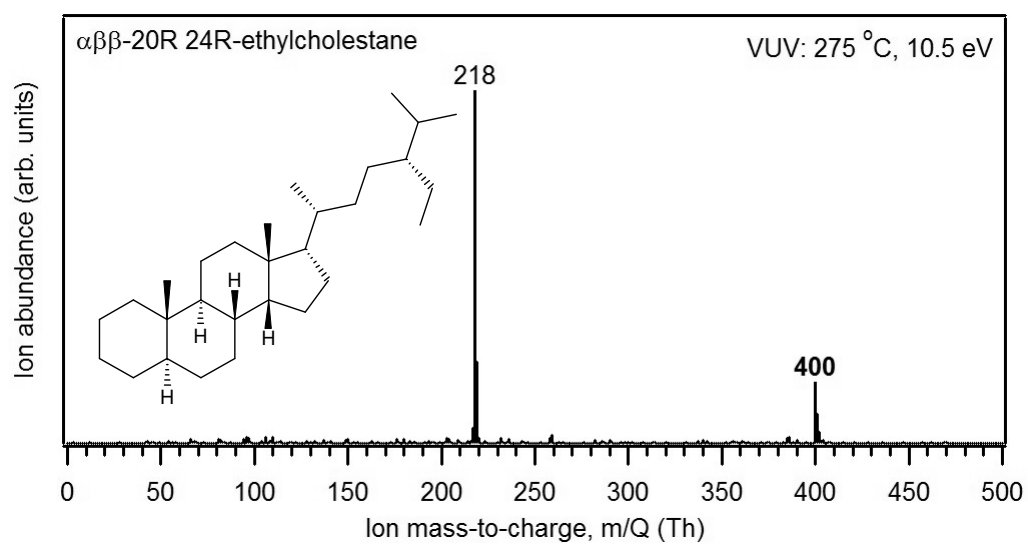
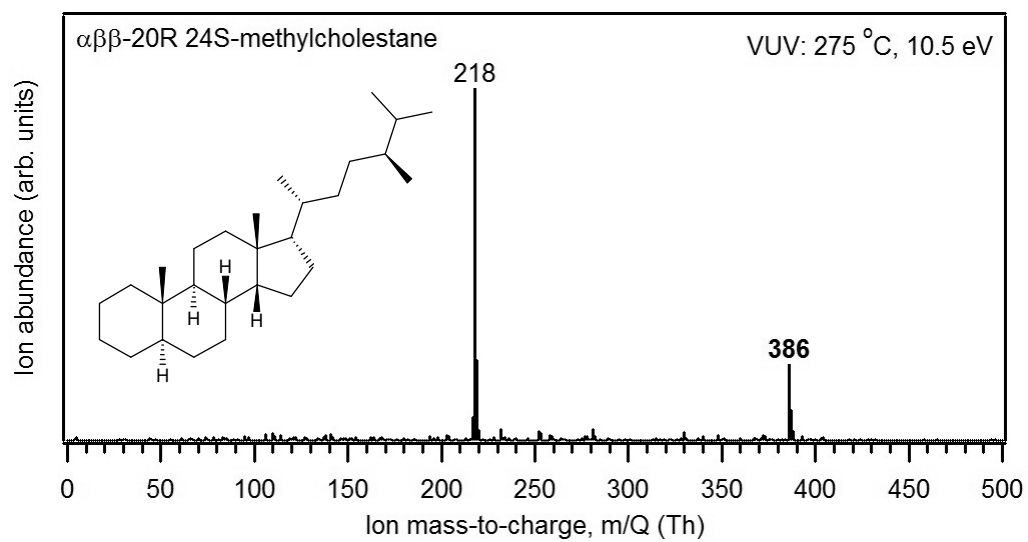




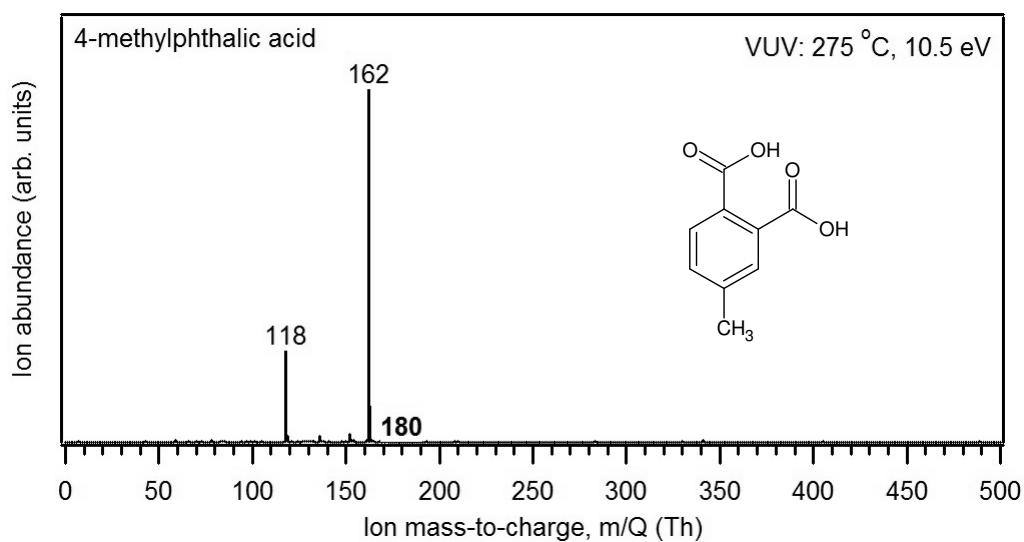
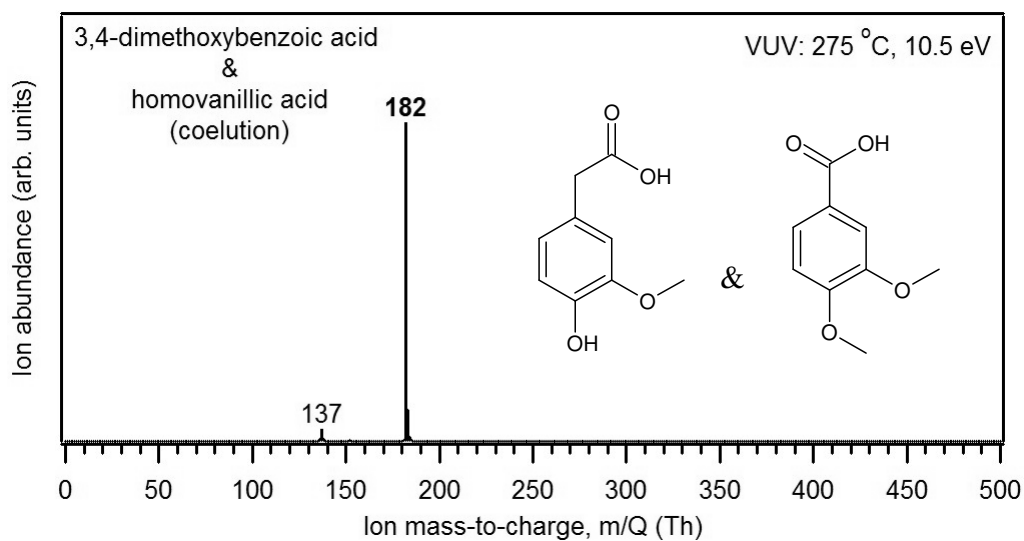
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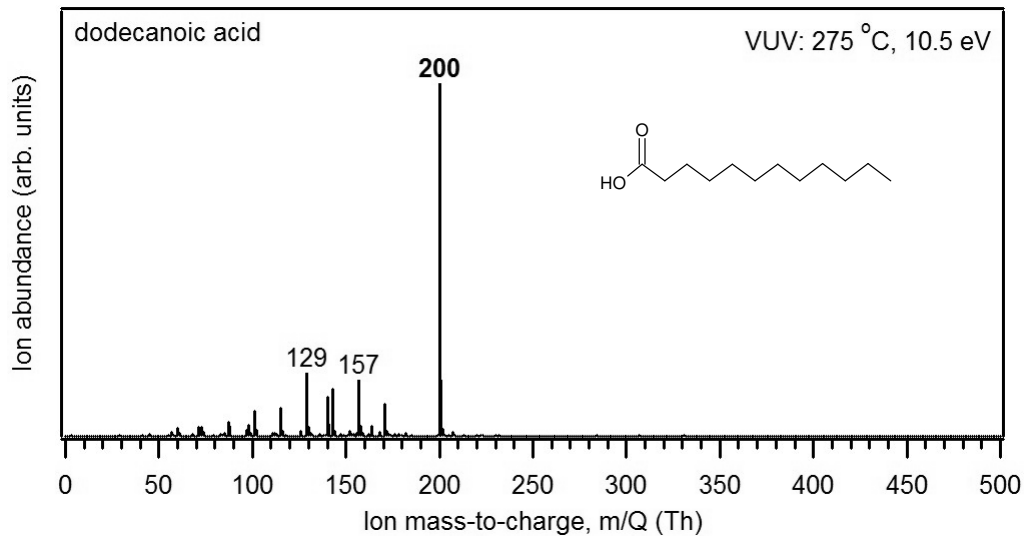
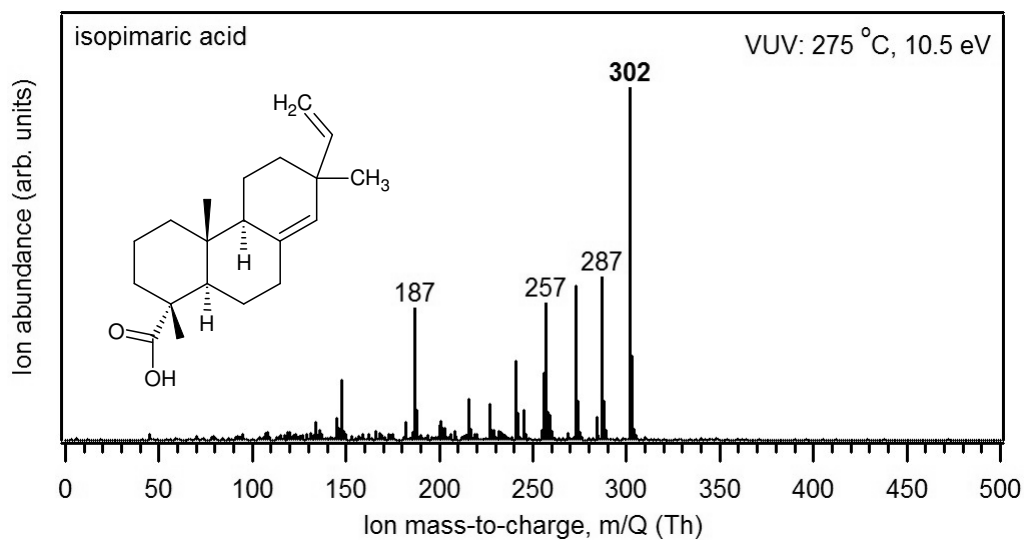
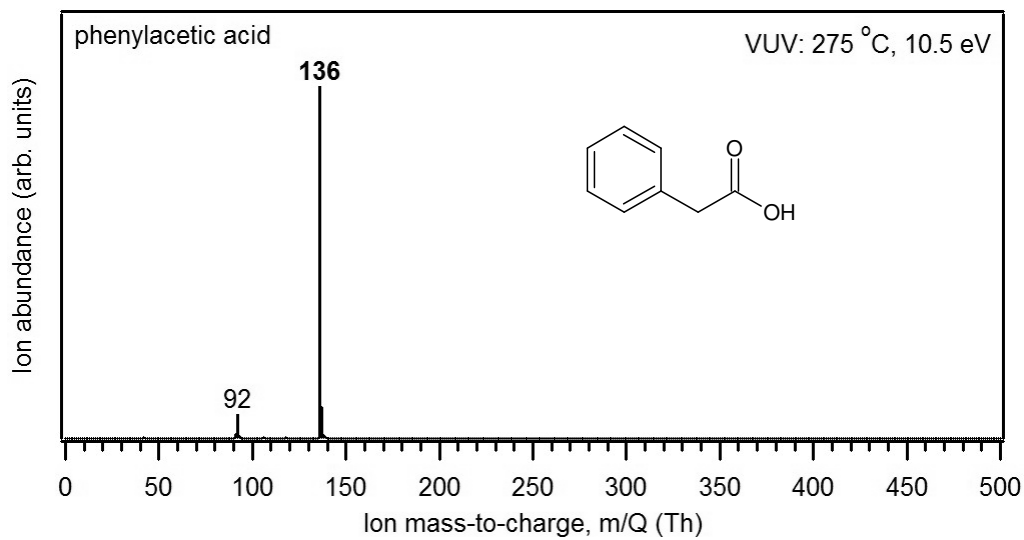


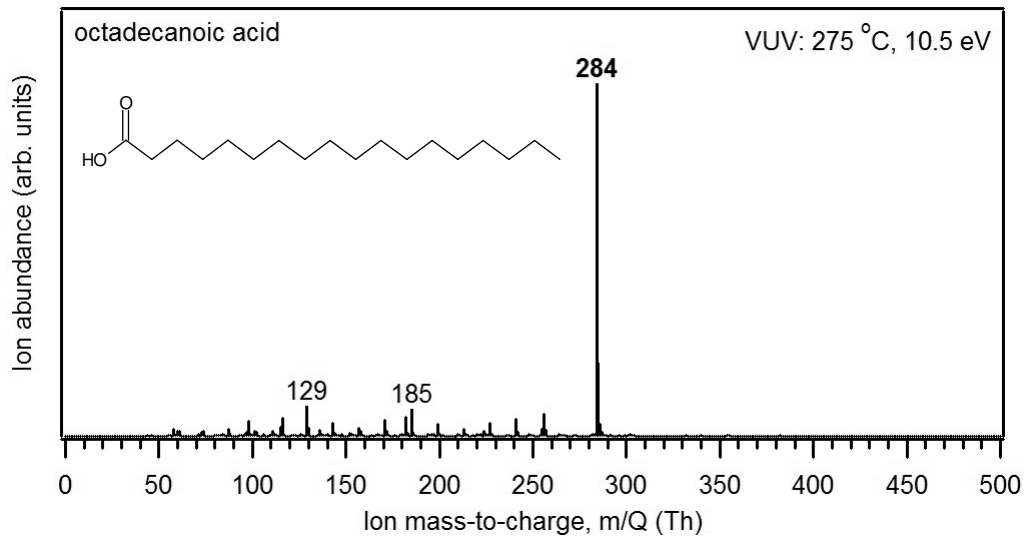
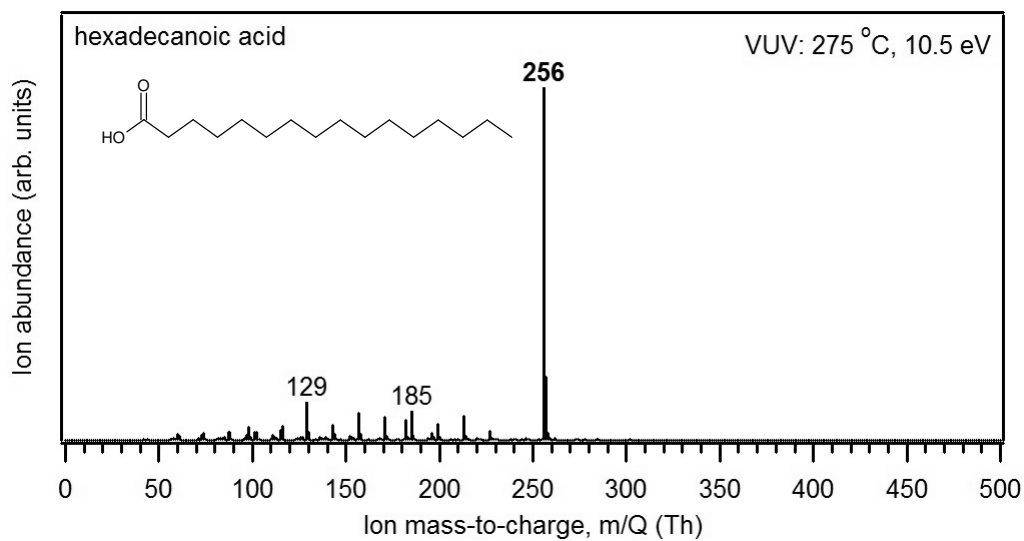
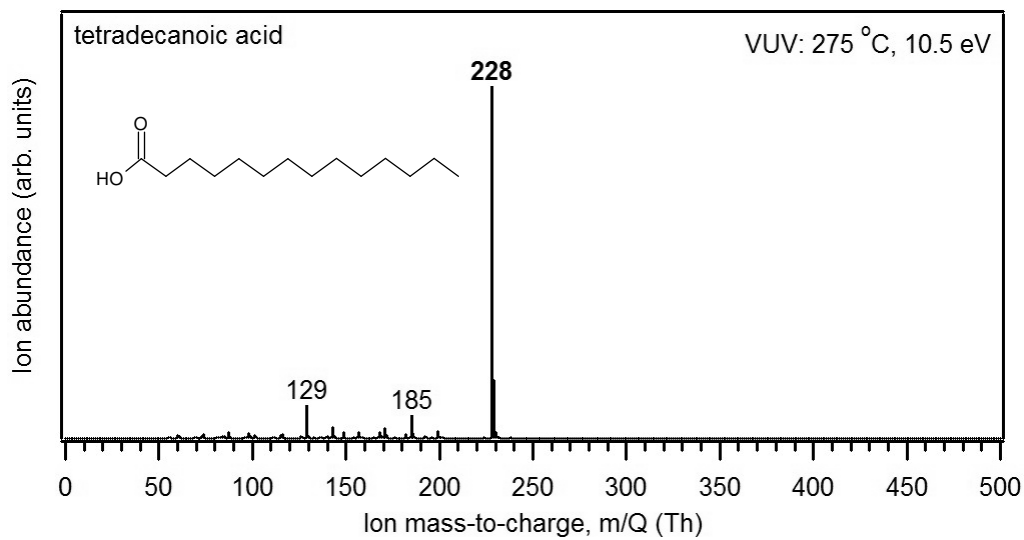


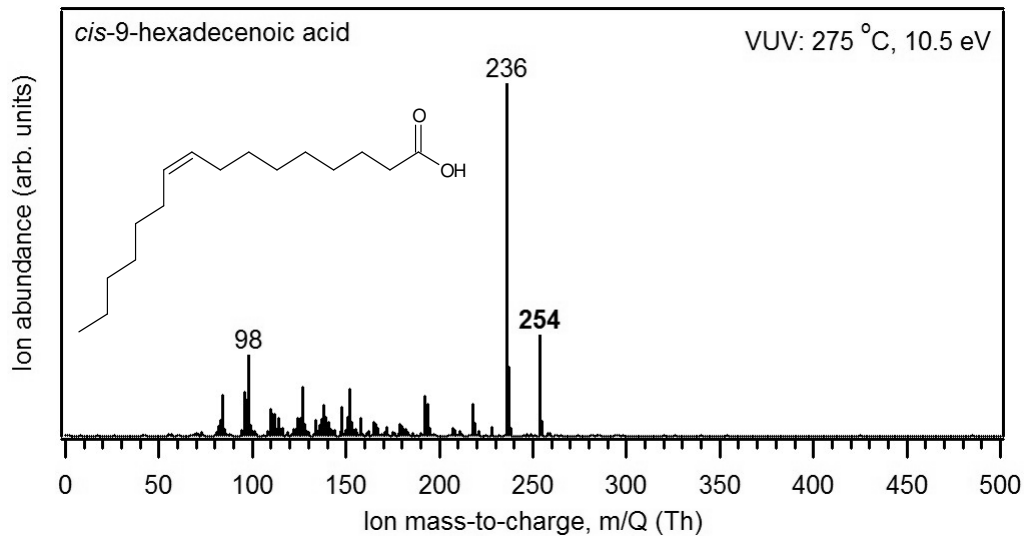
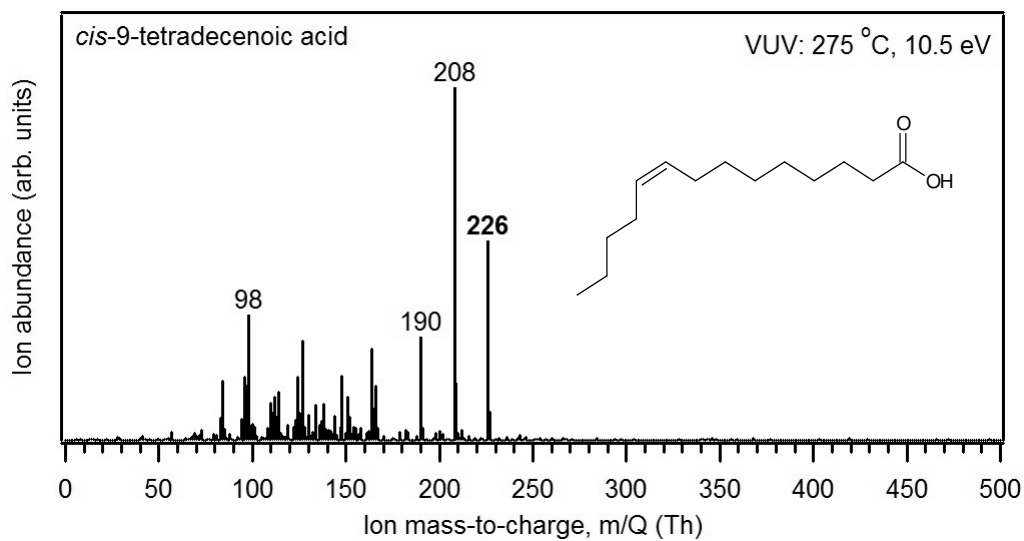
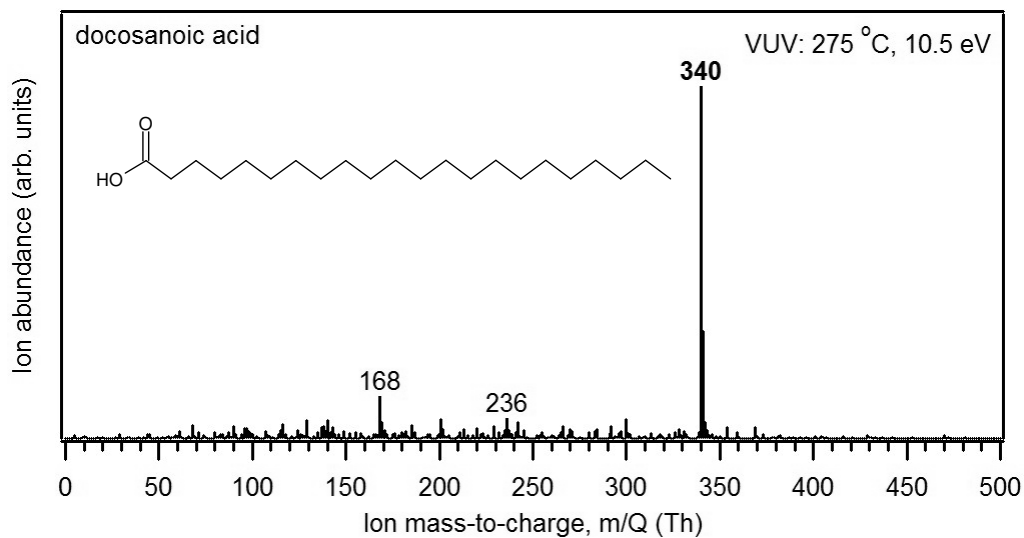


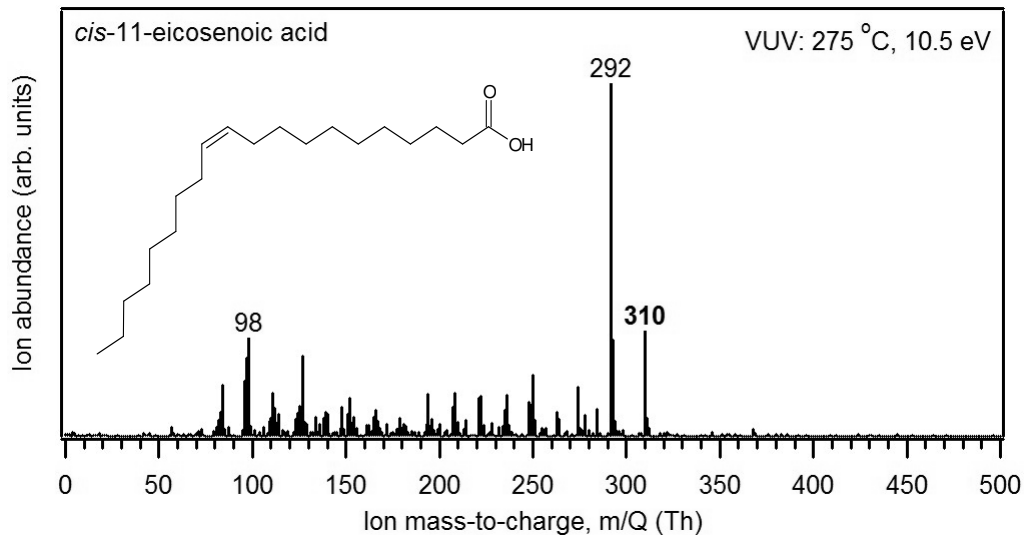
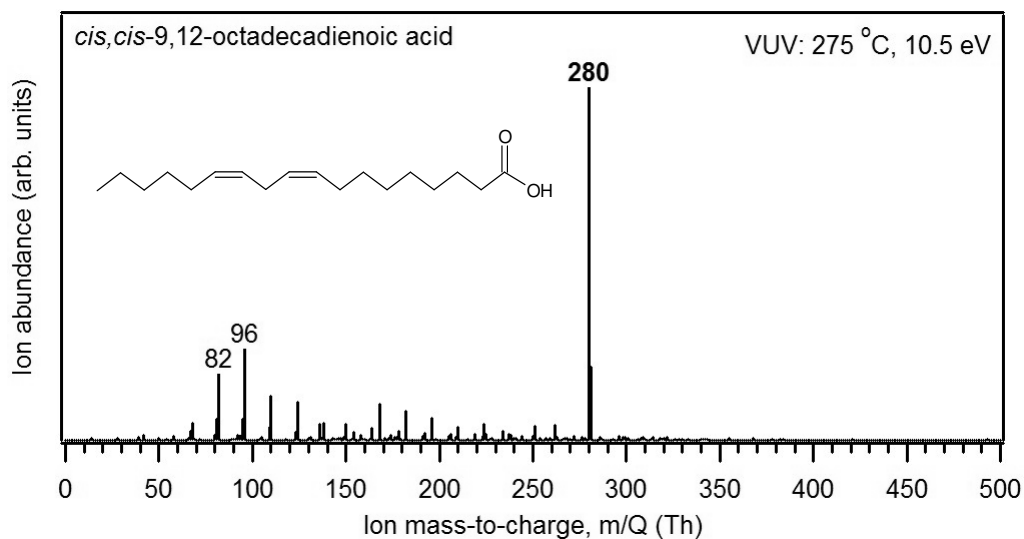
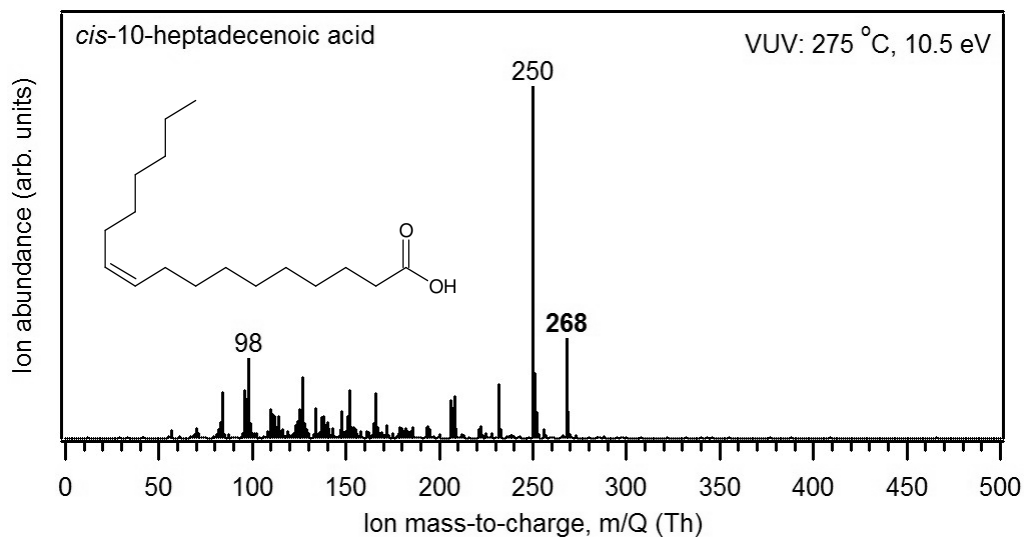
S.2.4. Acids

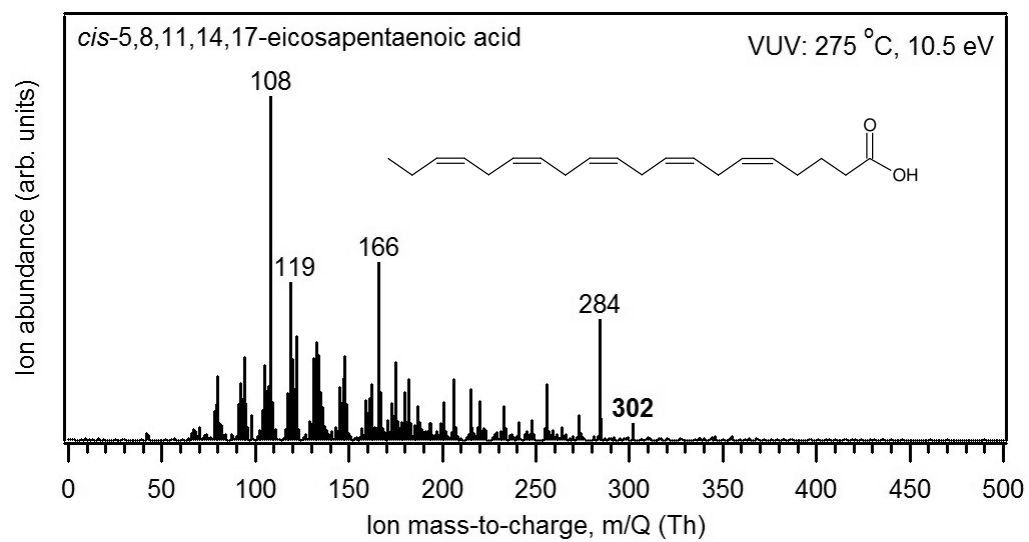




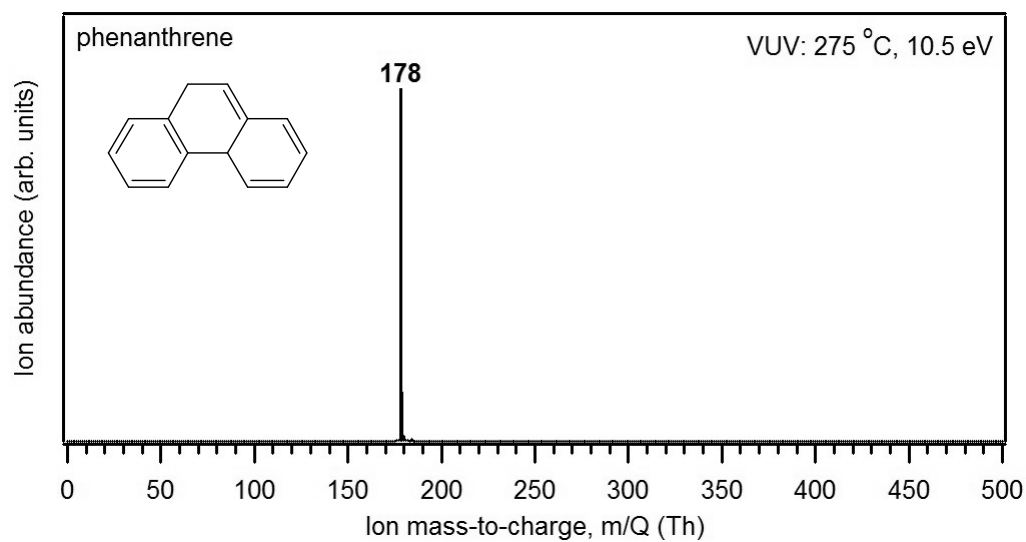
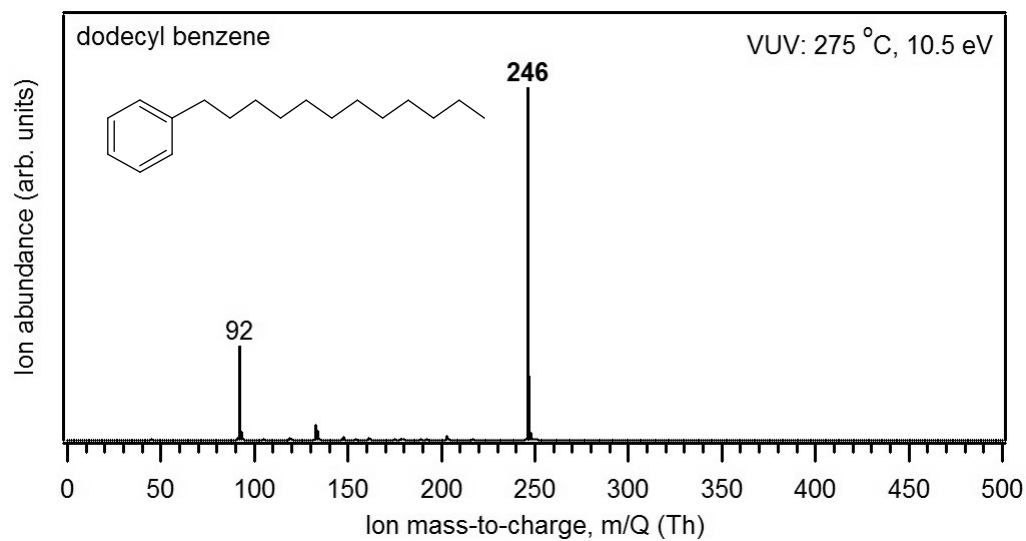


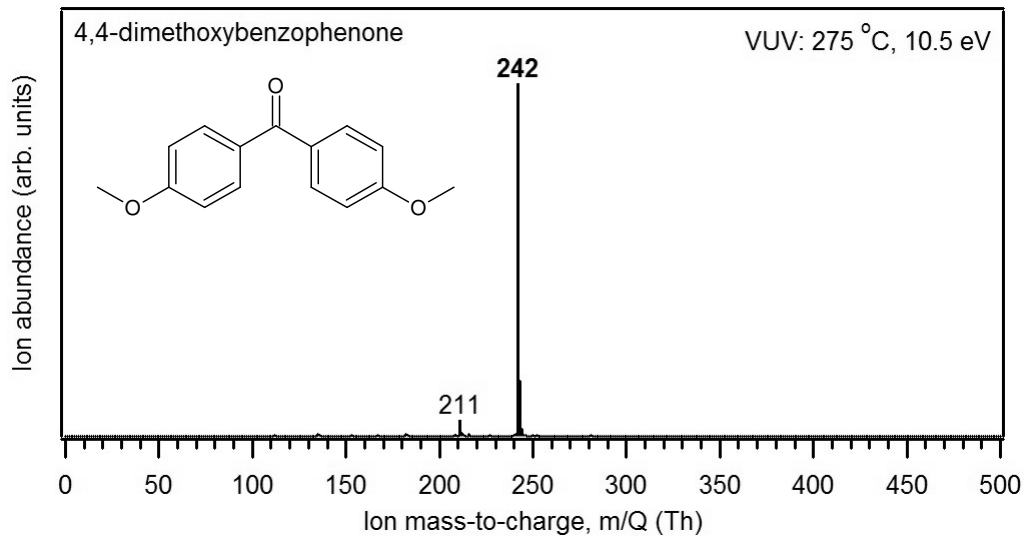
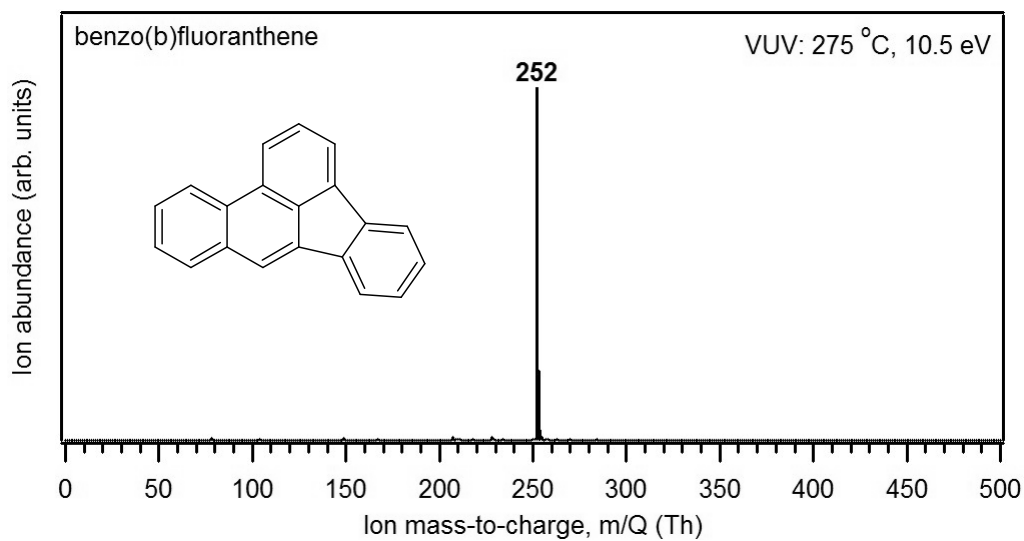
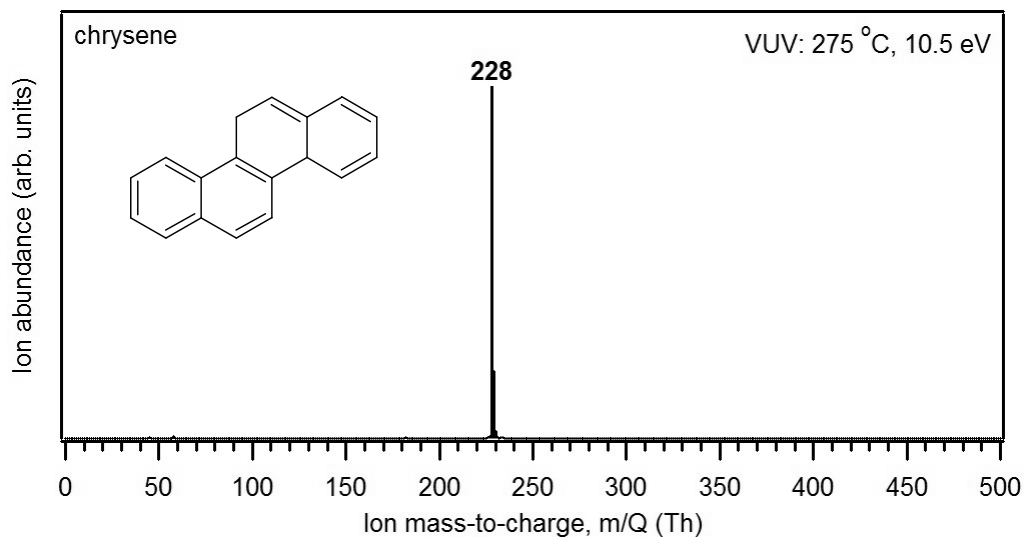


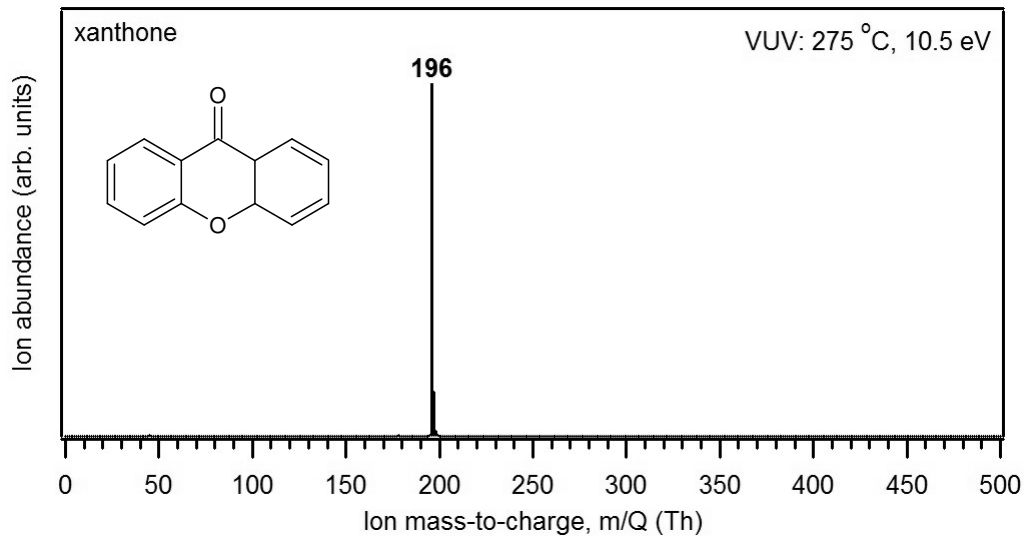
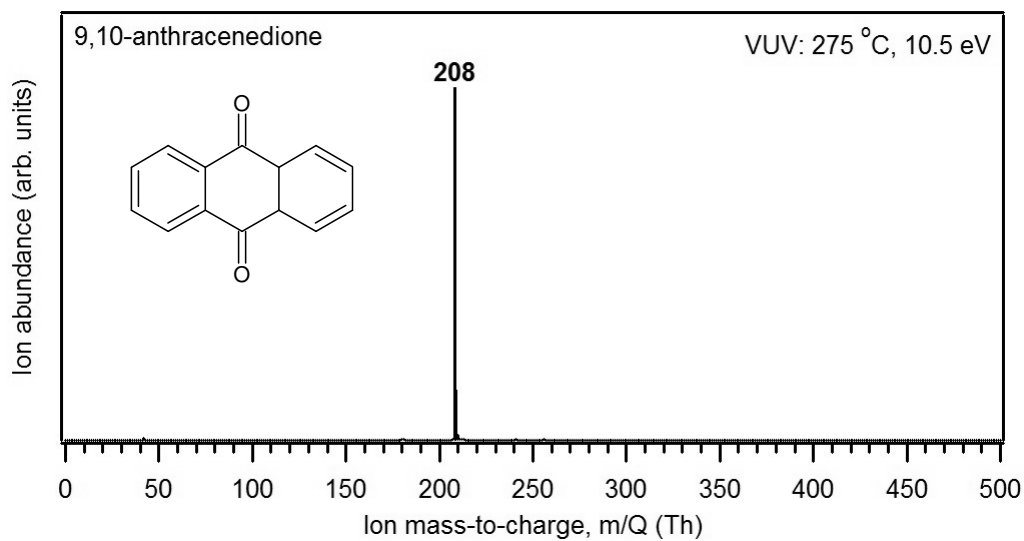
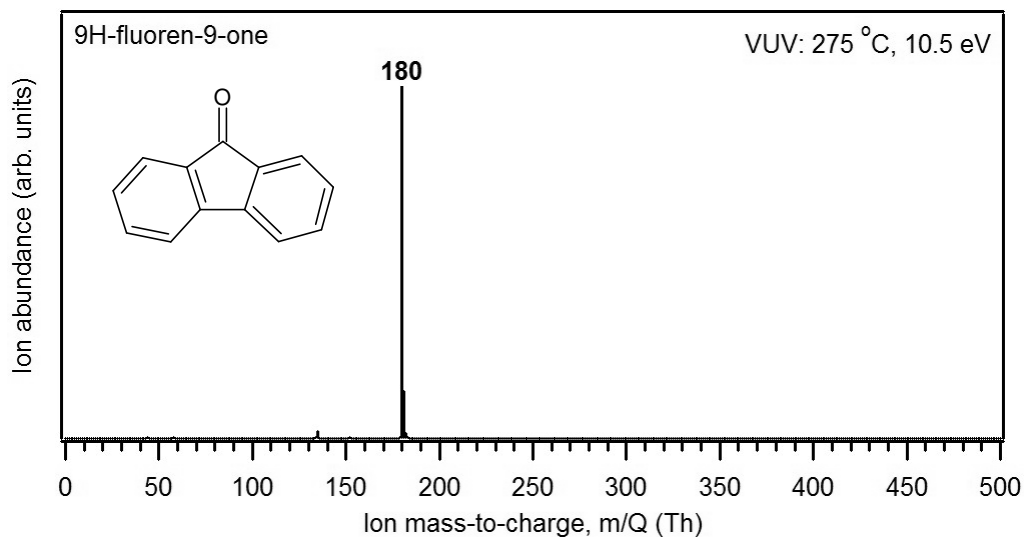




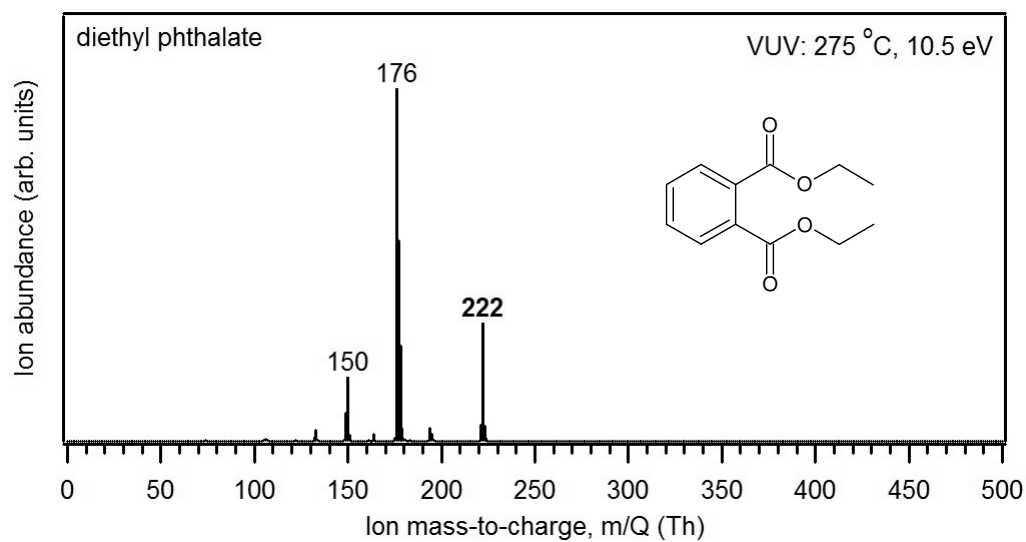
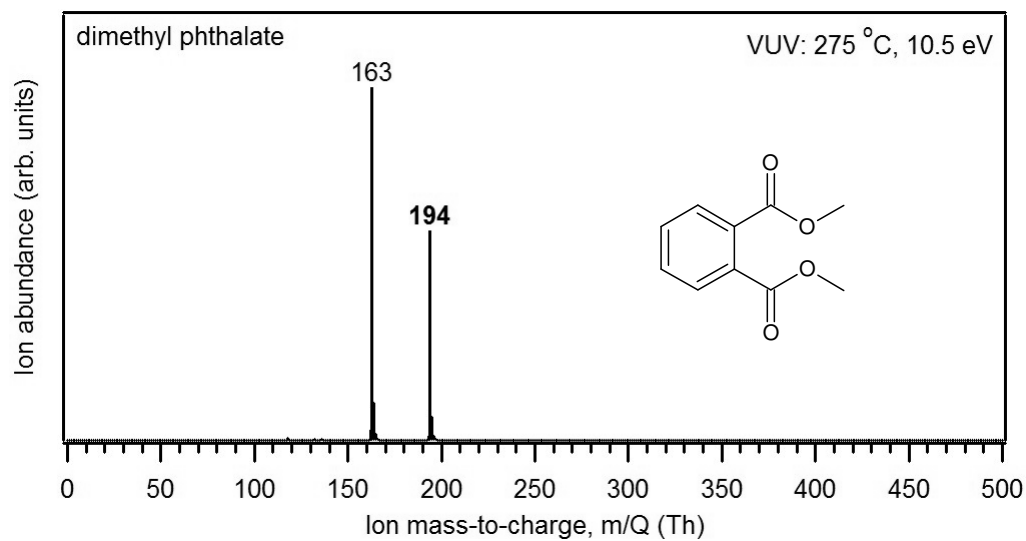
S.2.5. Aromatics and oxygenated polycyclic aromatic hydrocarbons

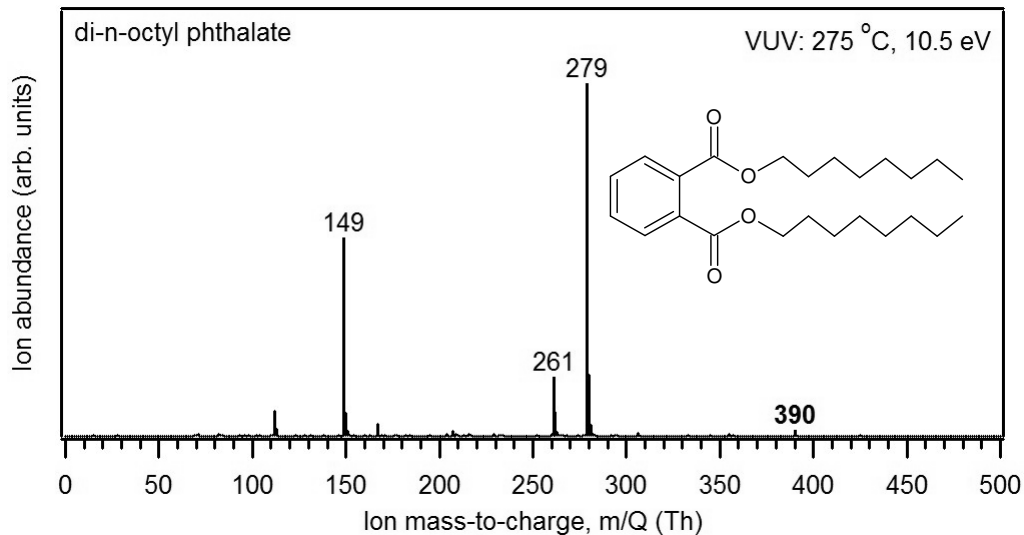
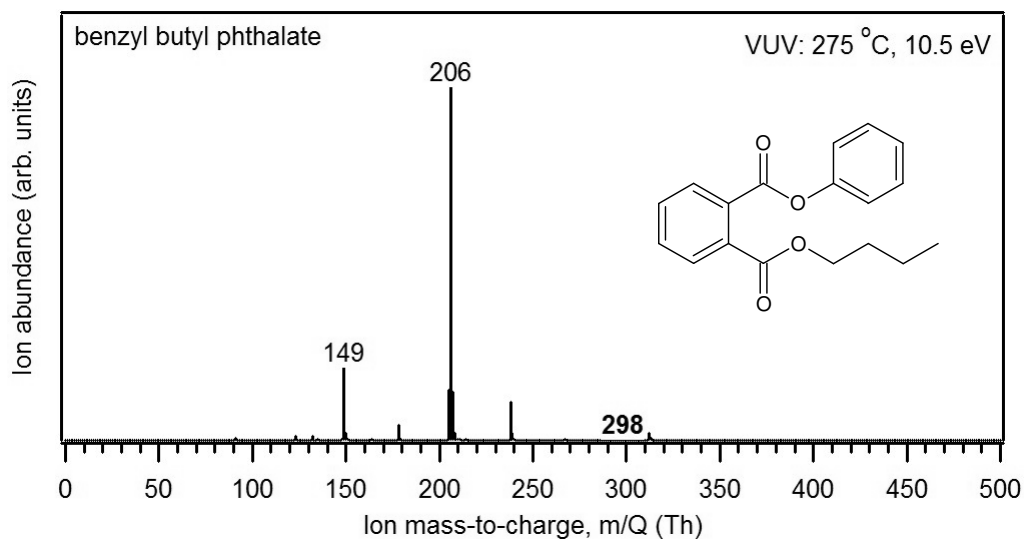
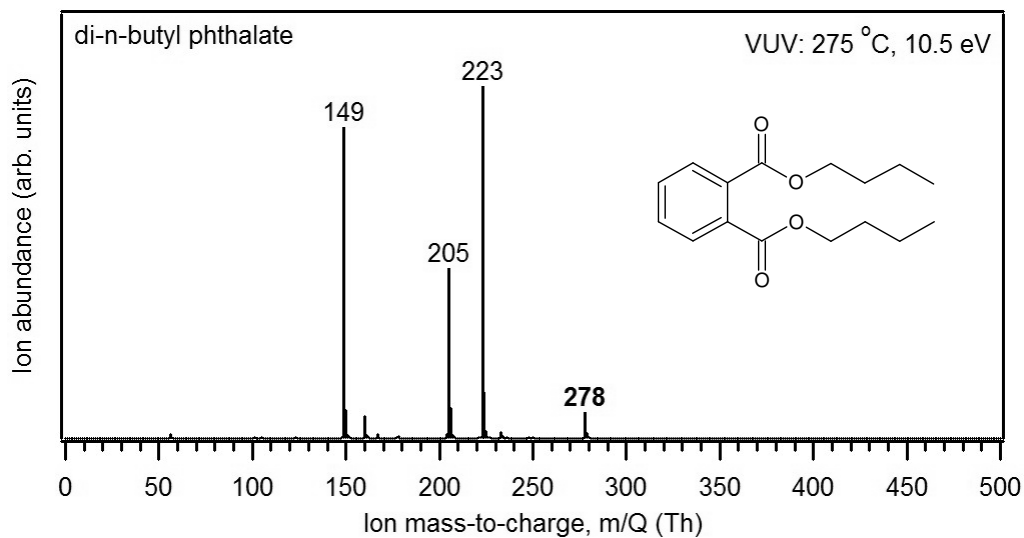


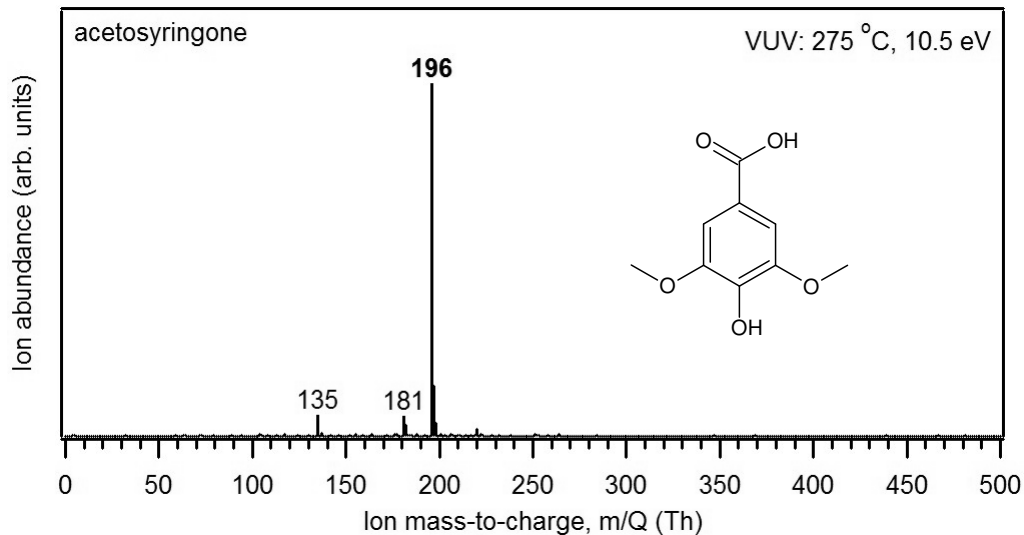
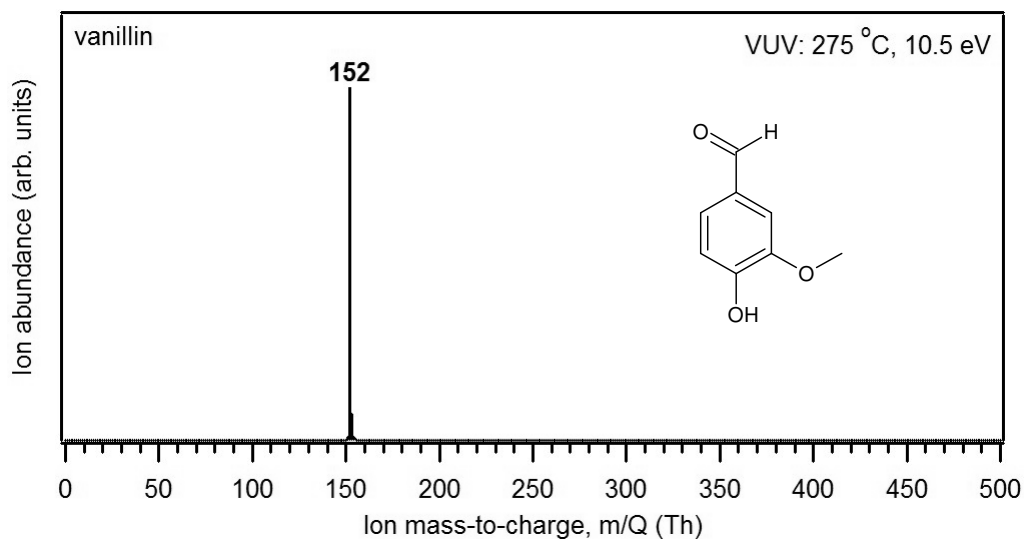
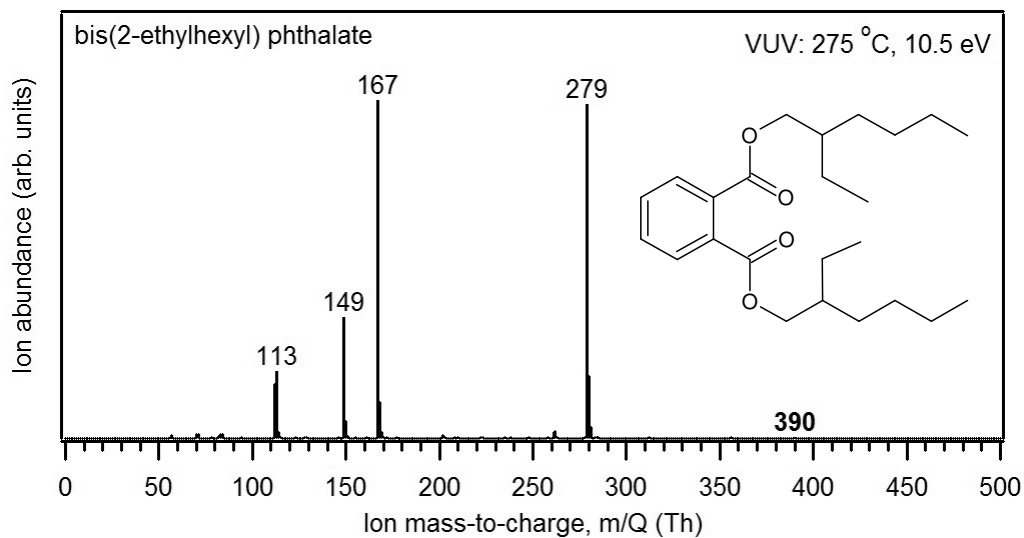




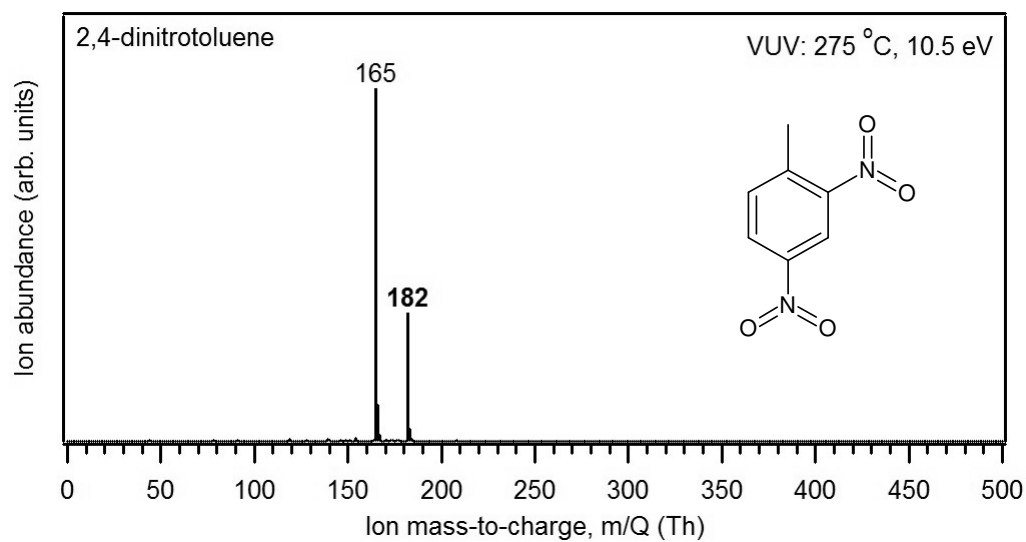
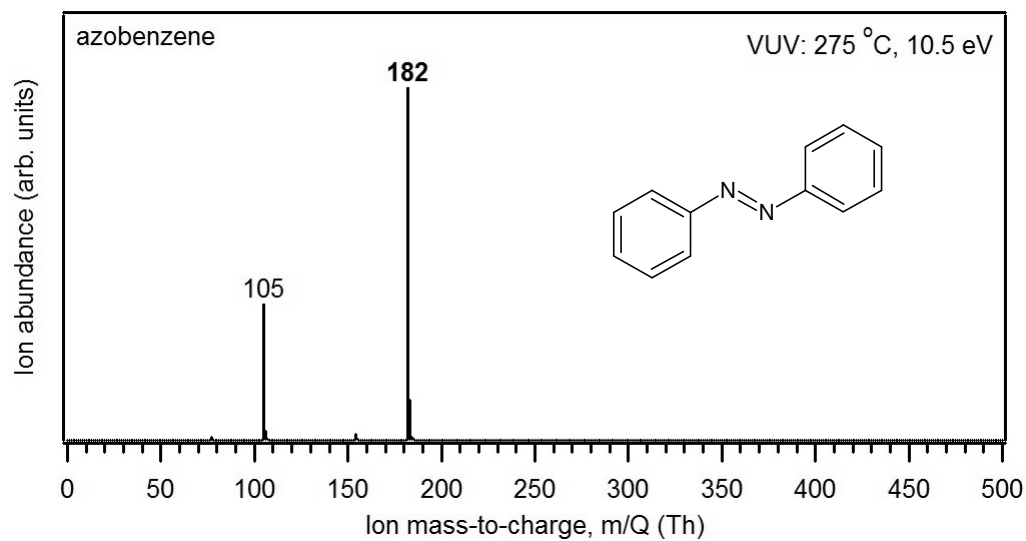
S.2.6. Phthalates and other oxygenated aromatics

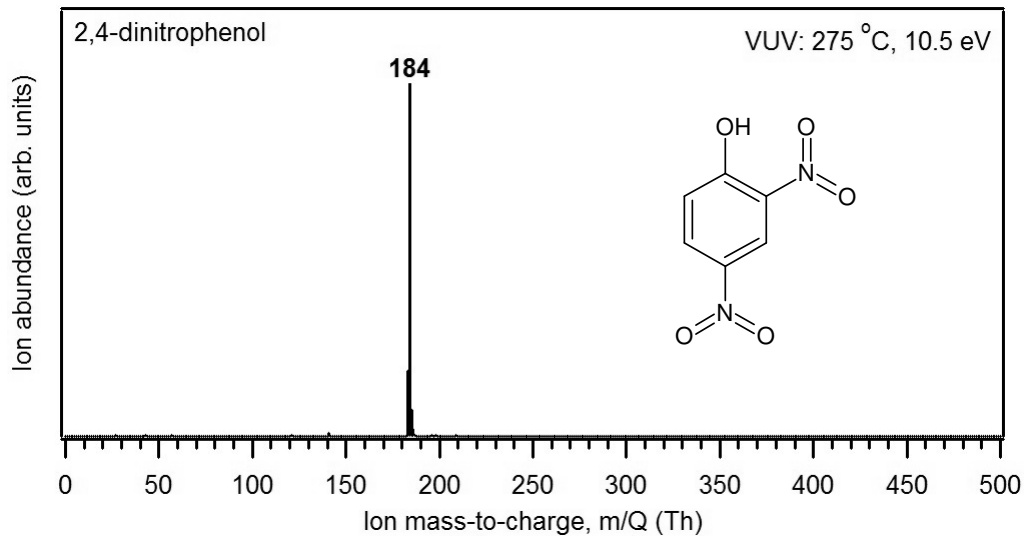
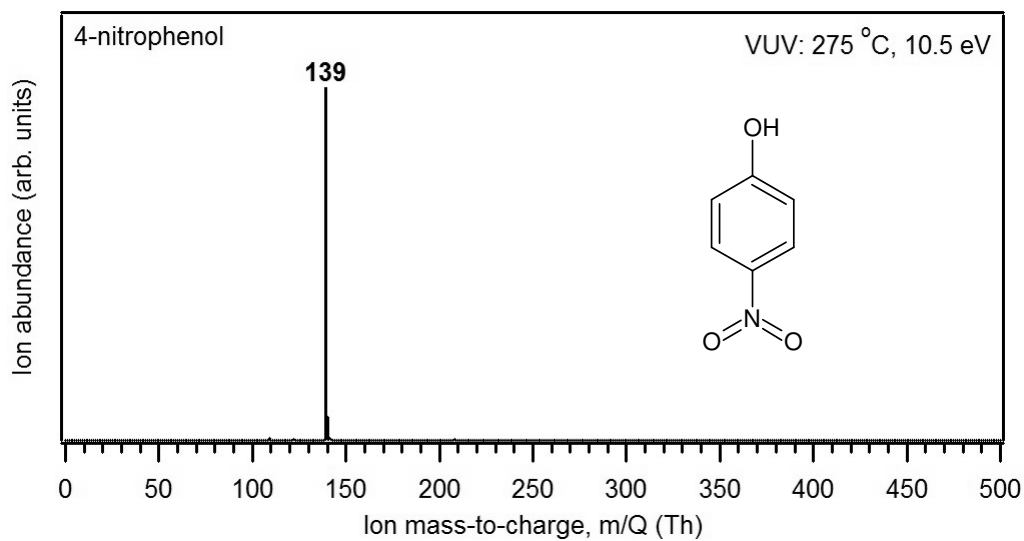
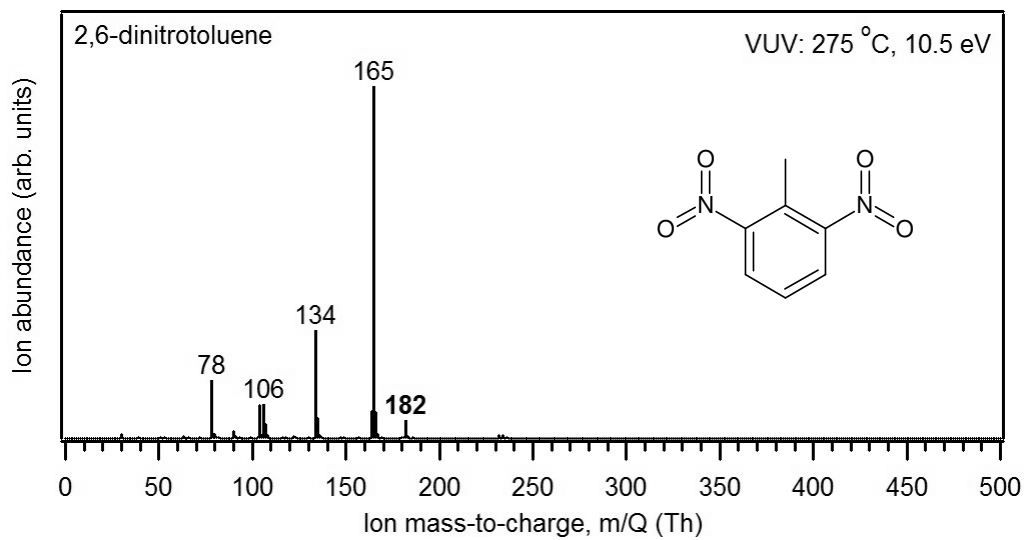


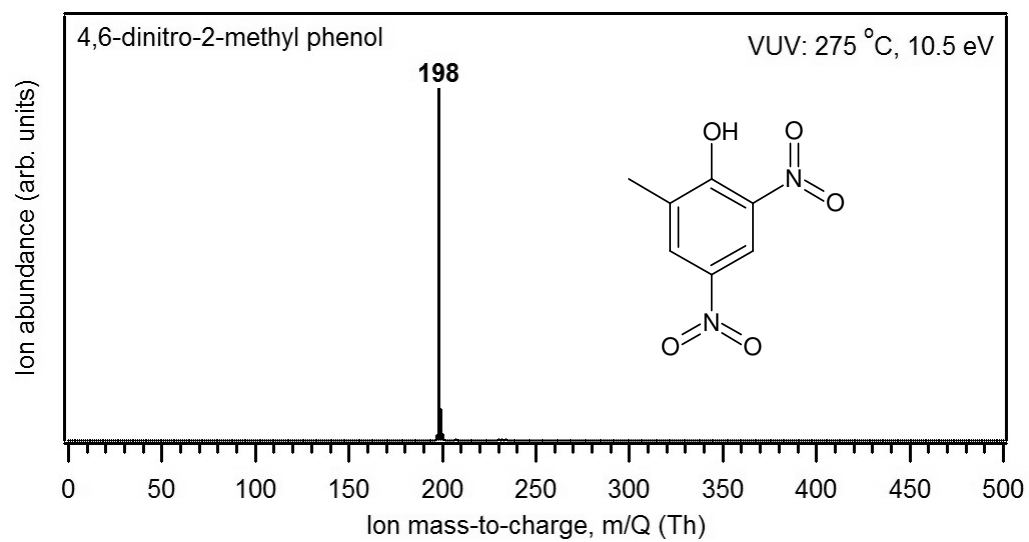




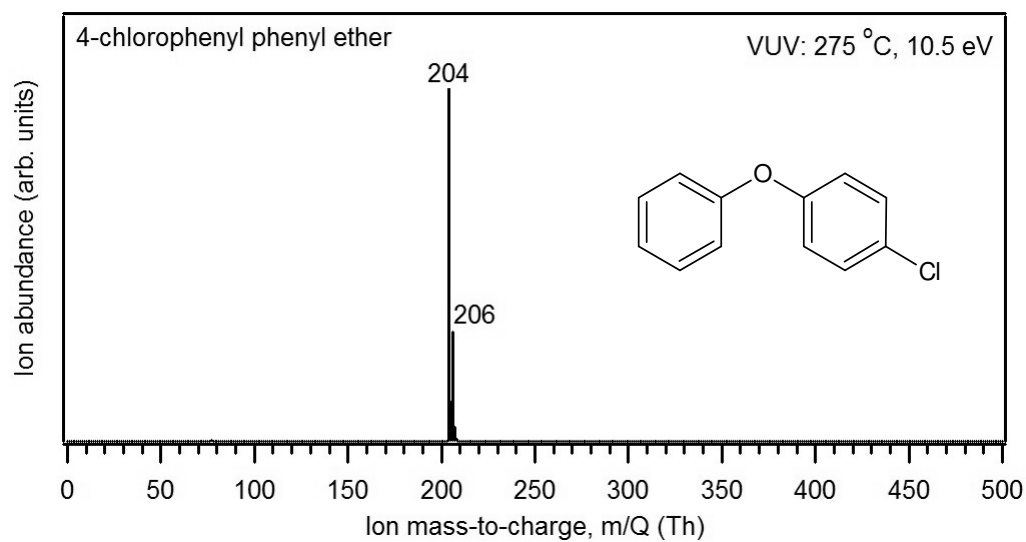
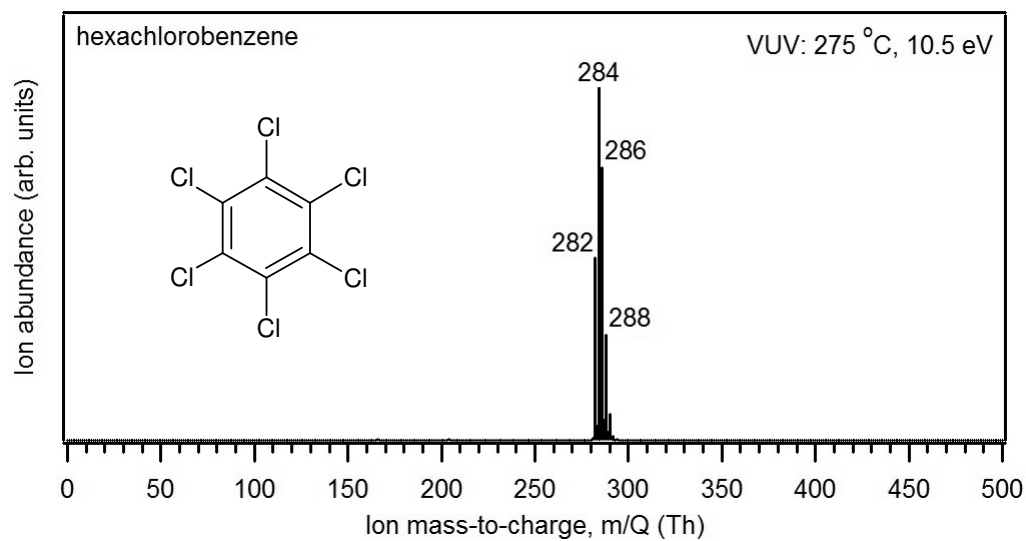
S.2.7. Nitrogenated aromatics

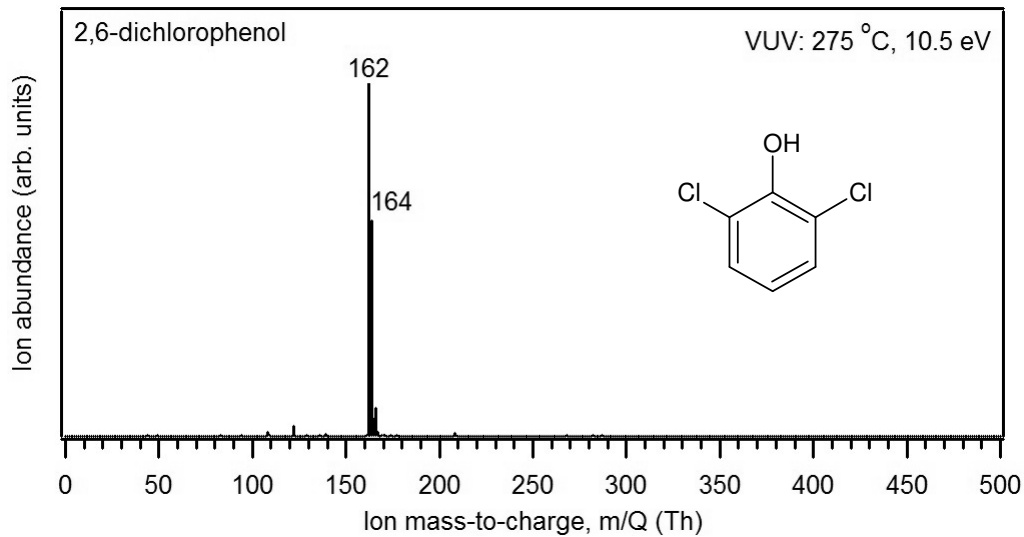
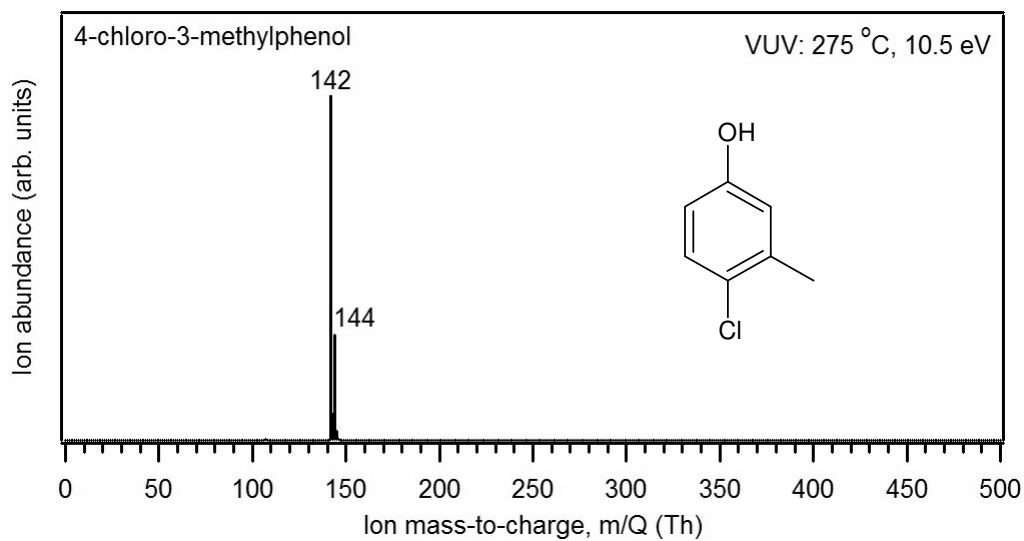
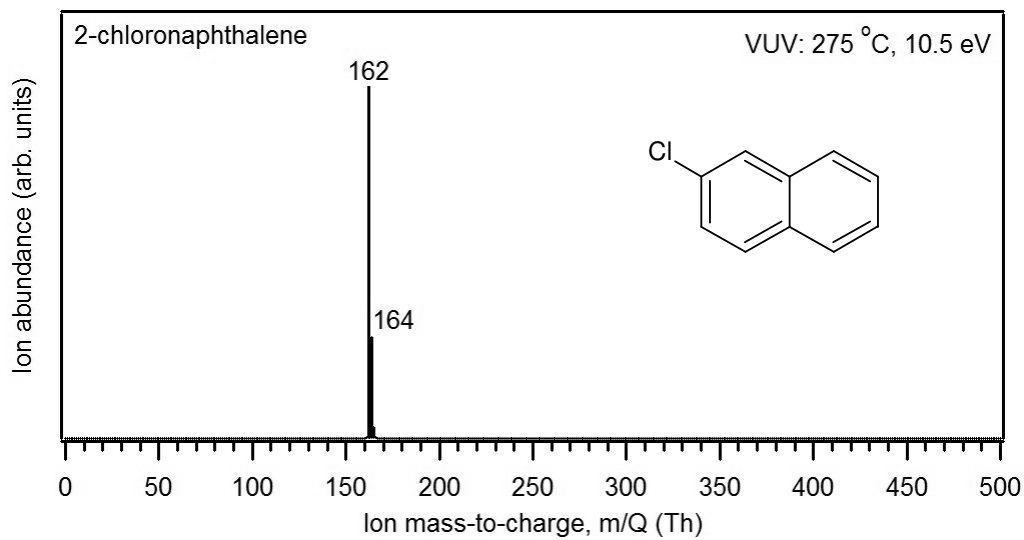


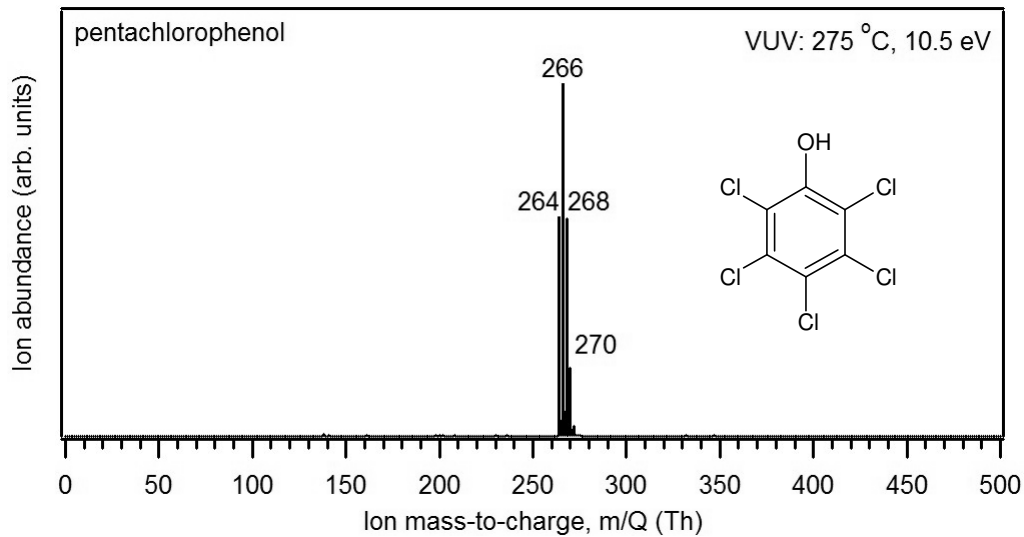
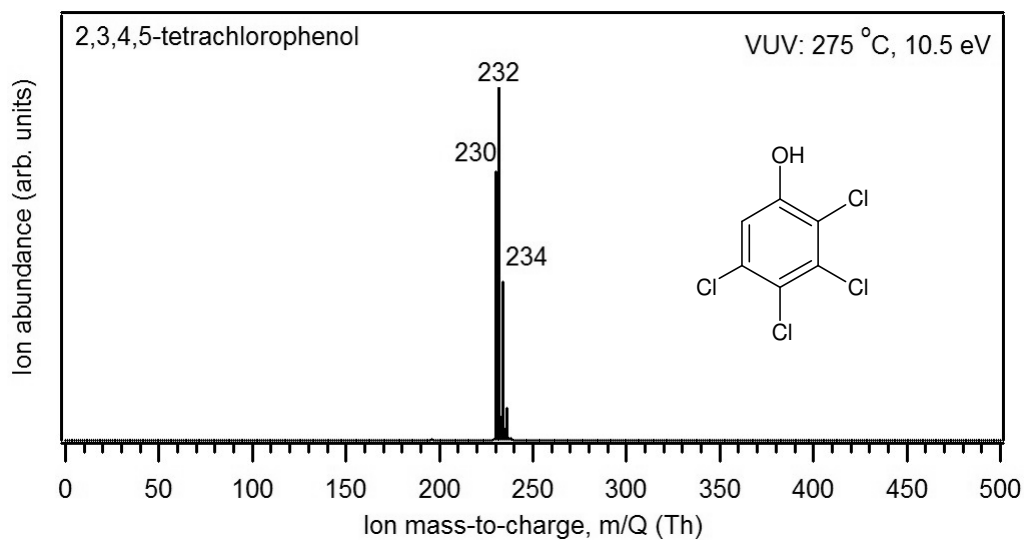
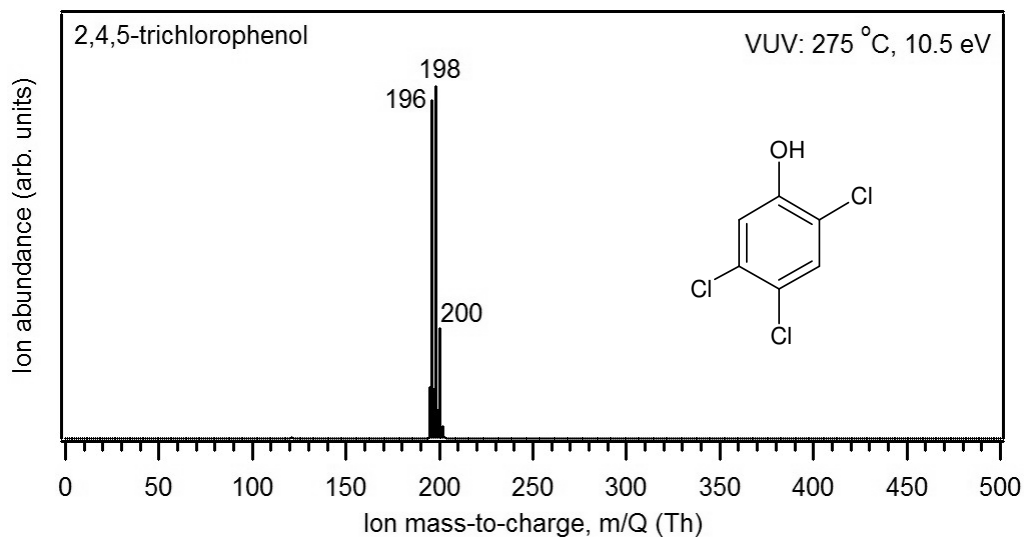




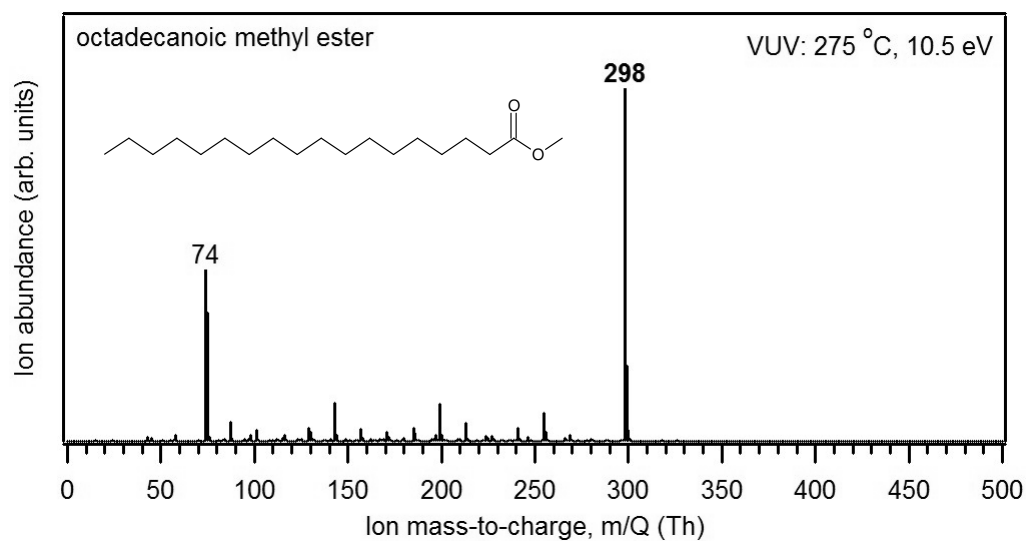
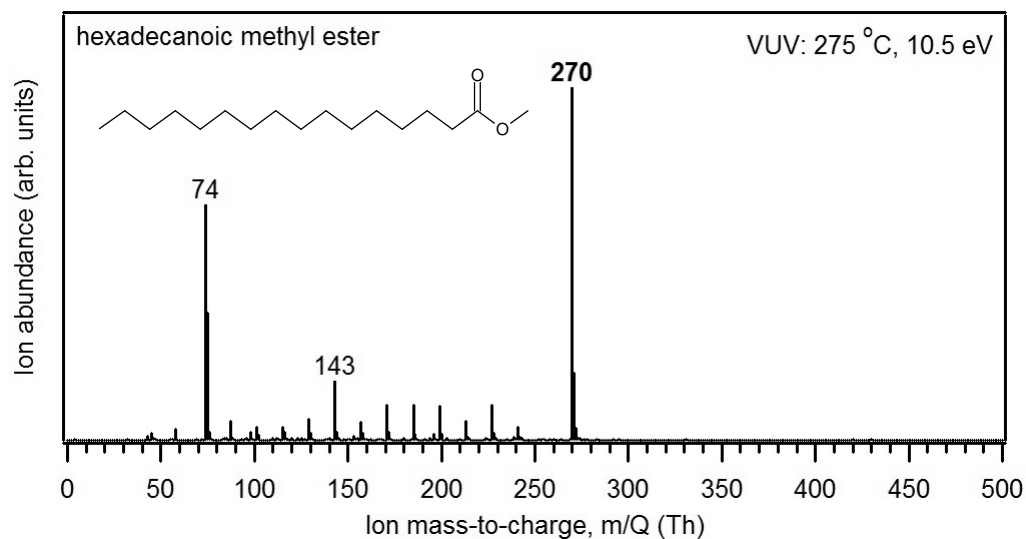
S.2.8. Chlorinated aromatics

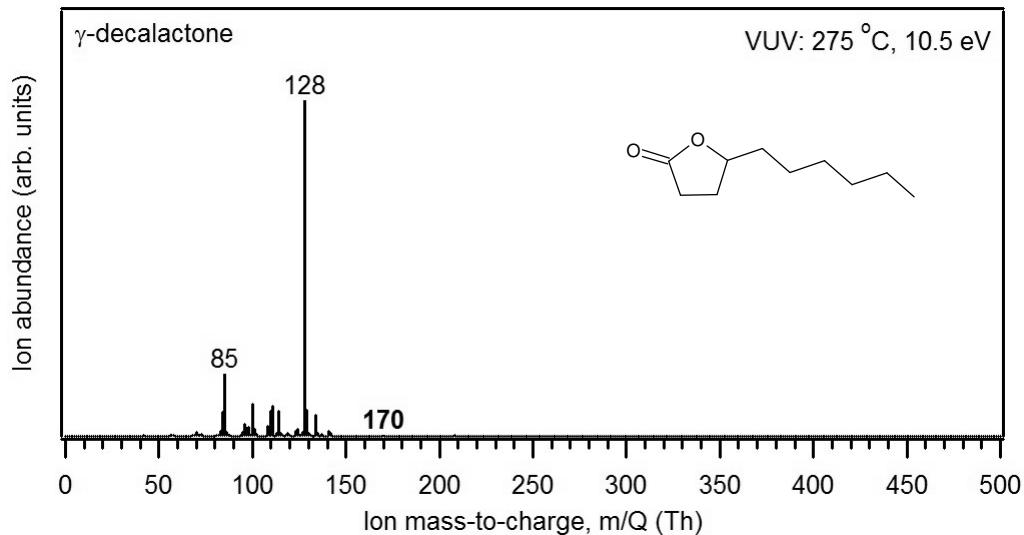
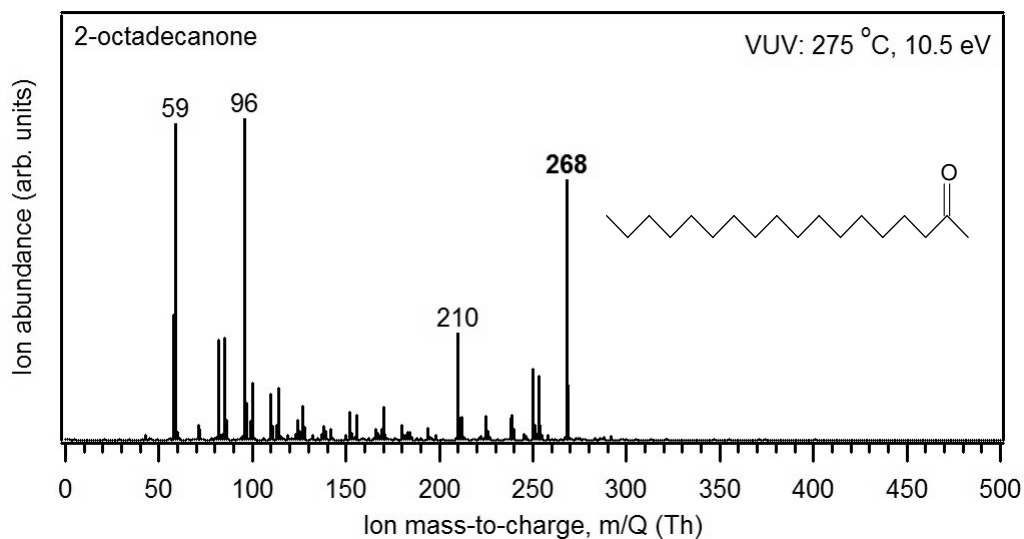
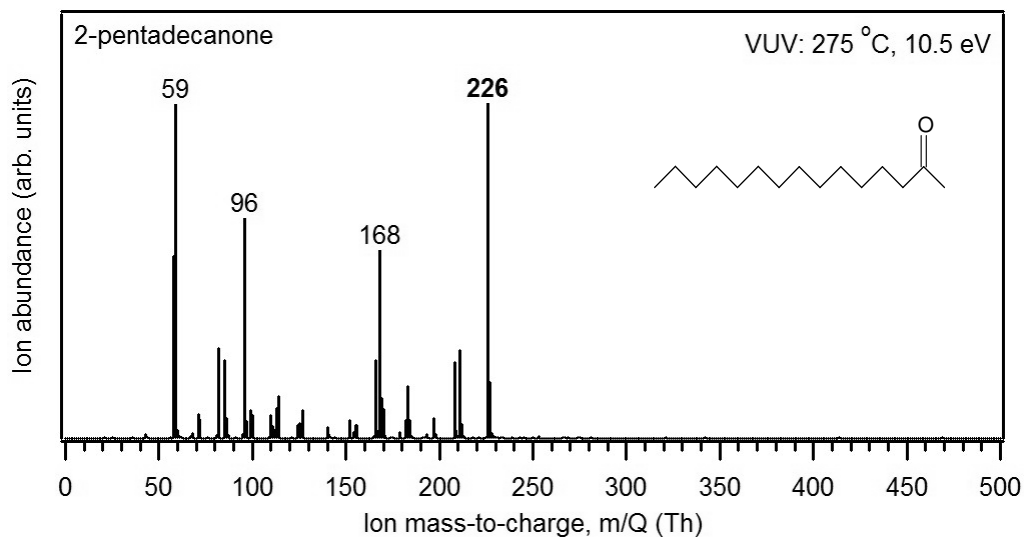


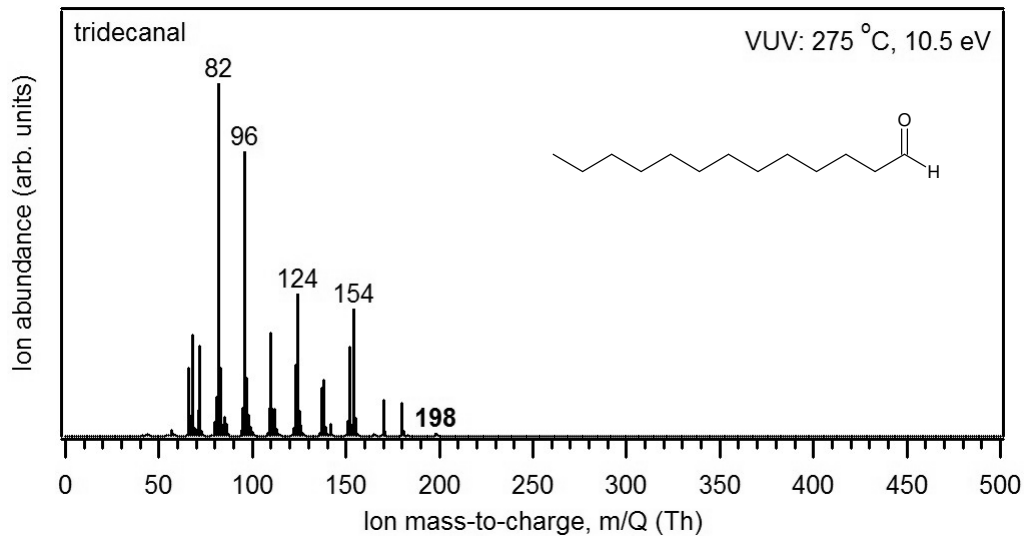
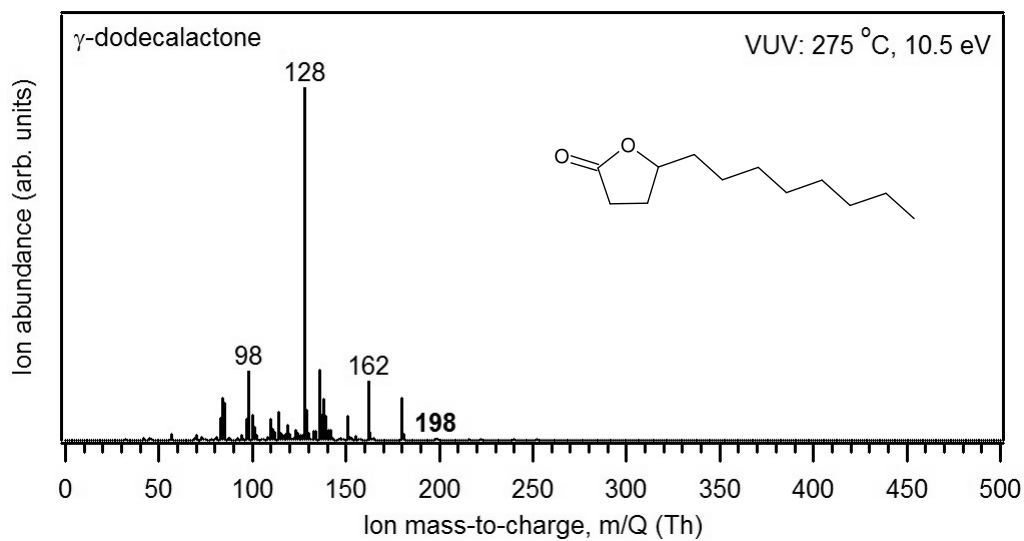
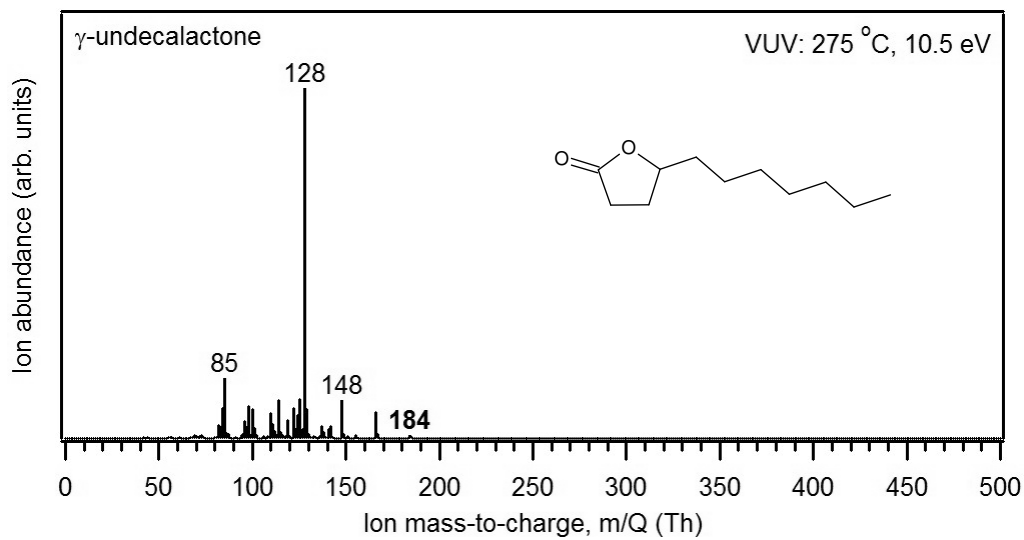




S.2.9. Oxygenated aliphatic compounds (ketones, esters, aldehydes)







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