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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This supplementary information contains the mass spectra of known compounds using vacuum ultraviolet (VUV) ionization at transfer temperatures of 150 ^{o}C (38 compounds) and 275 ^{o}C (84 compounds). Parent ion is shown in bold (not shown for chlorinated compounds because the prevalence of both ^{35}Cl and ^{37}Cl 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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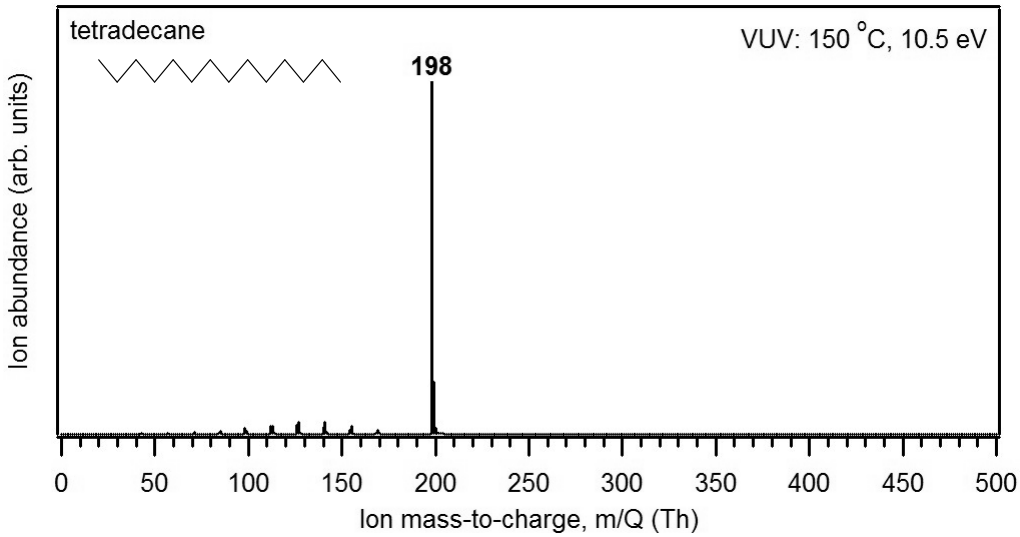
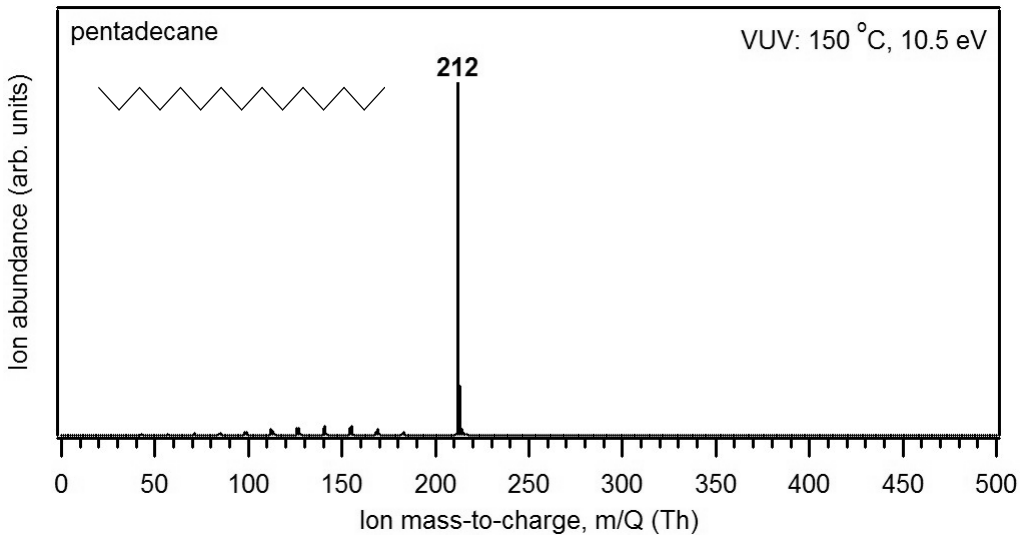
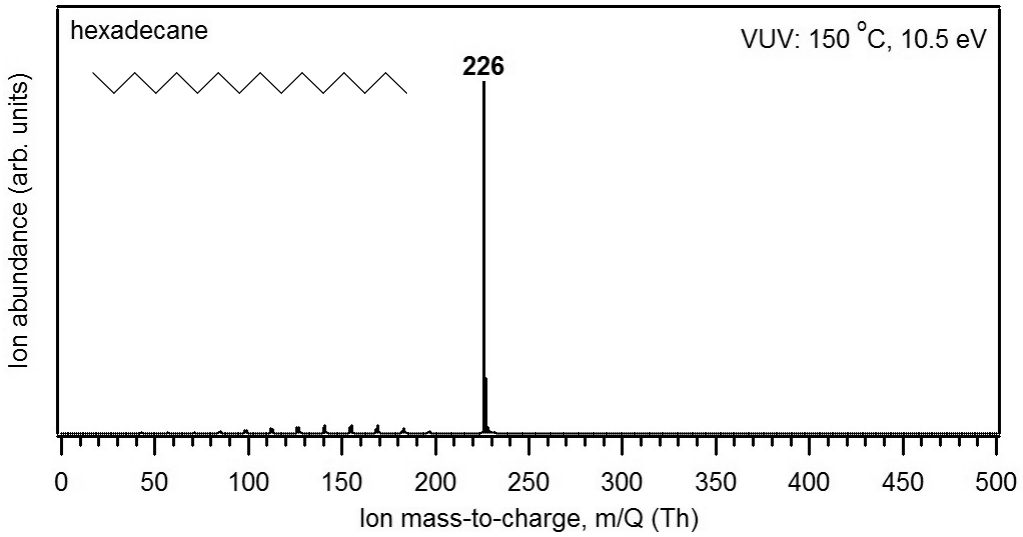
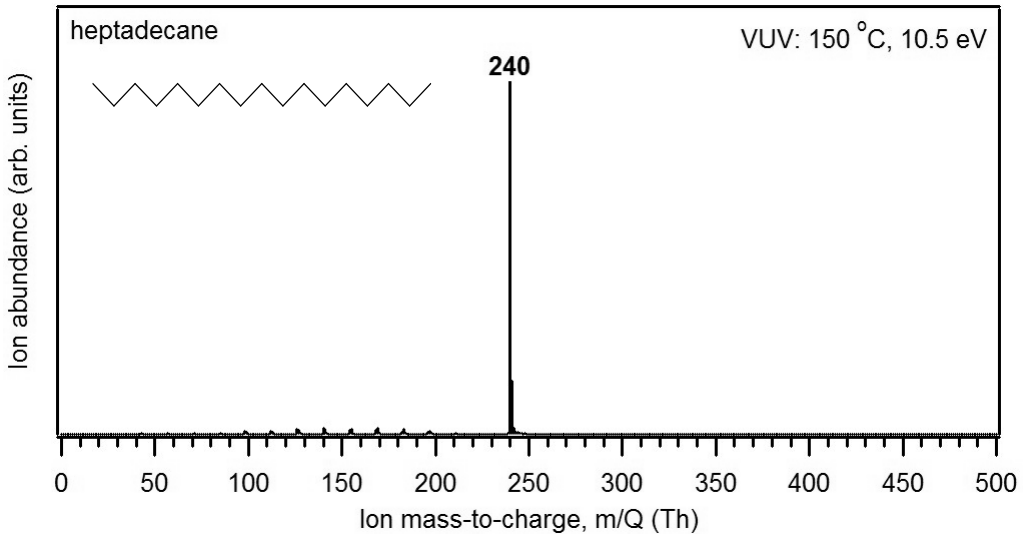
S.1. Spectra at a transfer temperature of 150 °C

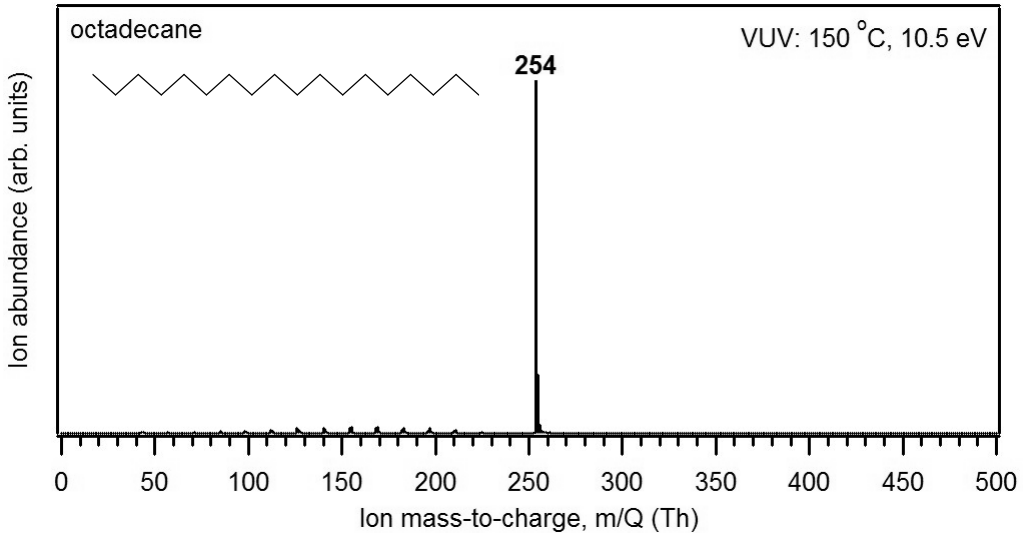
S.1.1. Normal alkanes

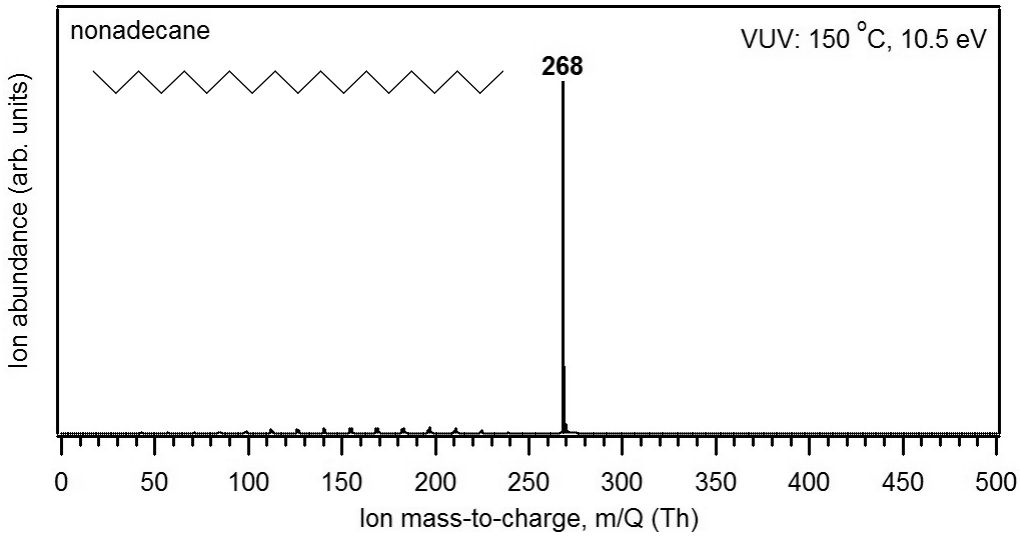


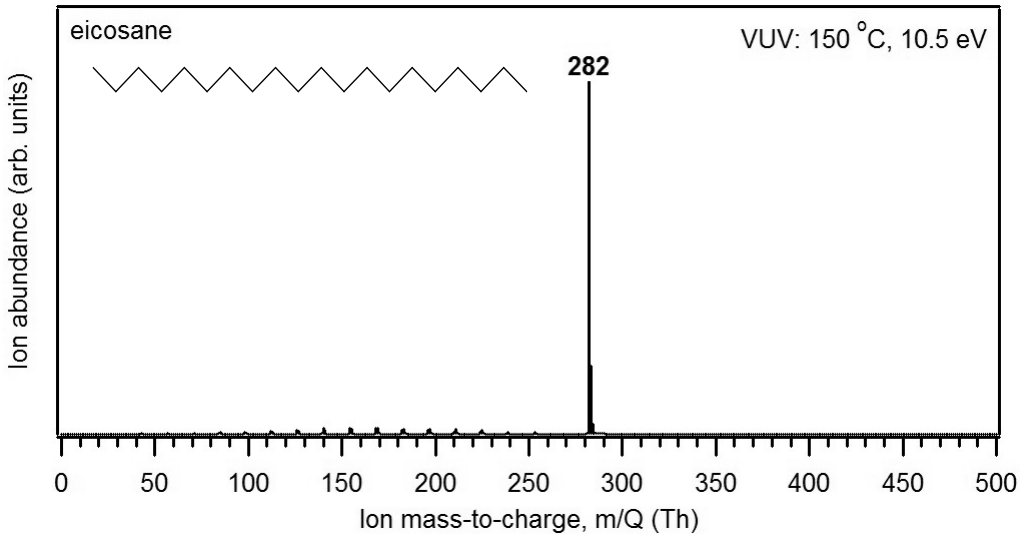


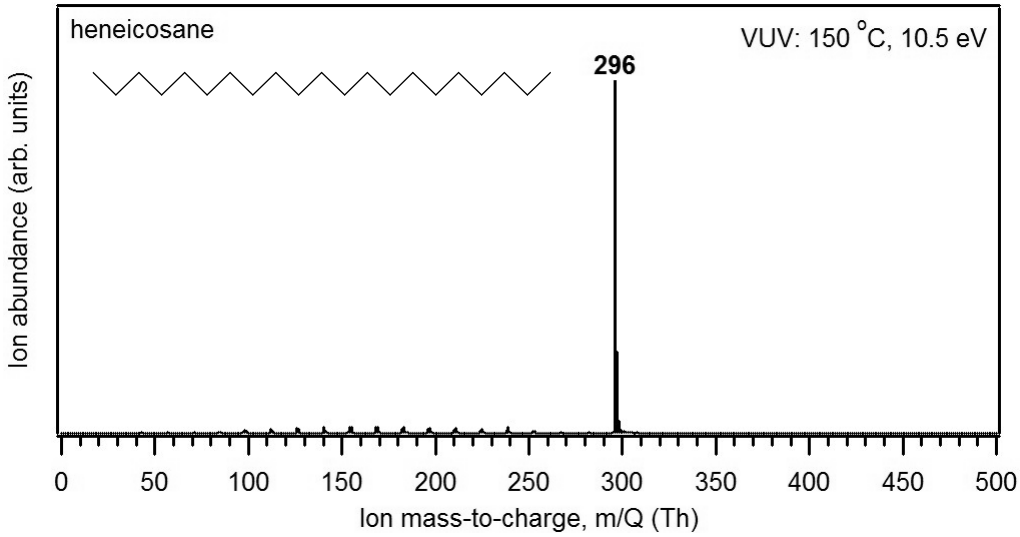

hexadecane
VUV: 150 °C, 10.5 eV
226
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

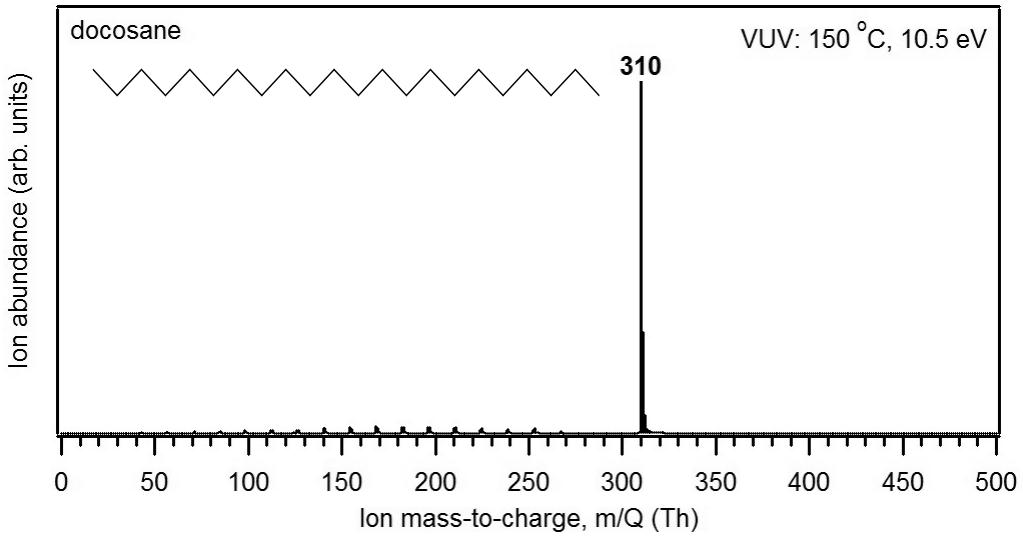

heptadecane
VUV: 150 °C, 10.5 eV
240
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

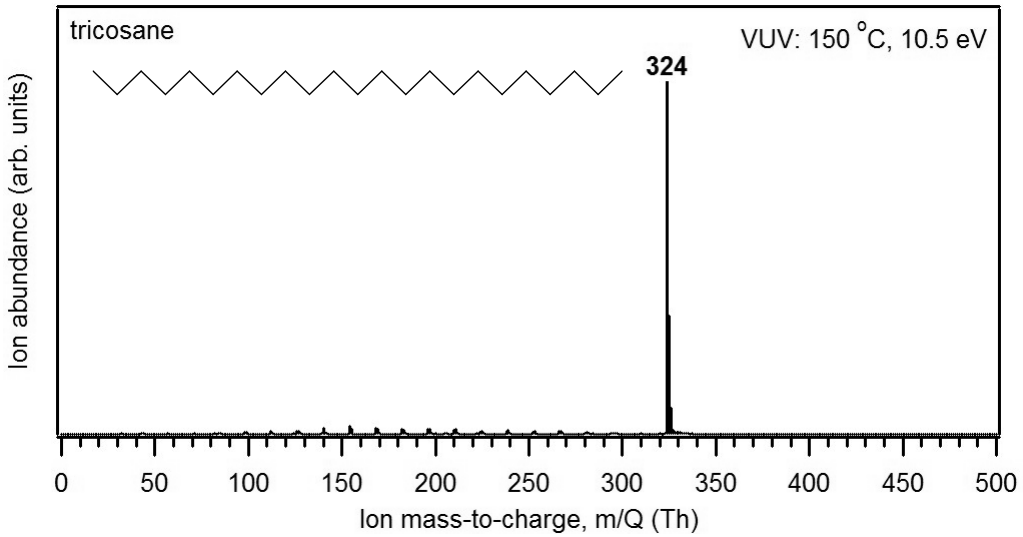

octadecane
VUV: 150 °C, 10.5 eV
254
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

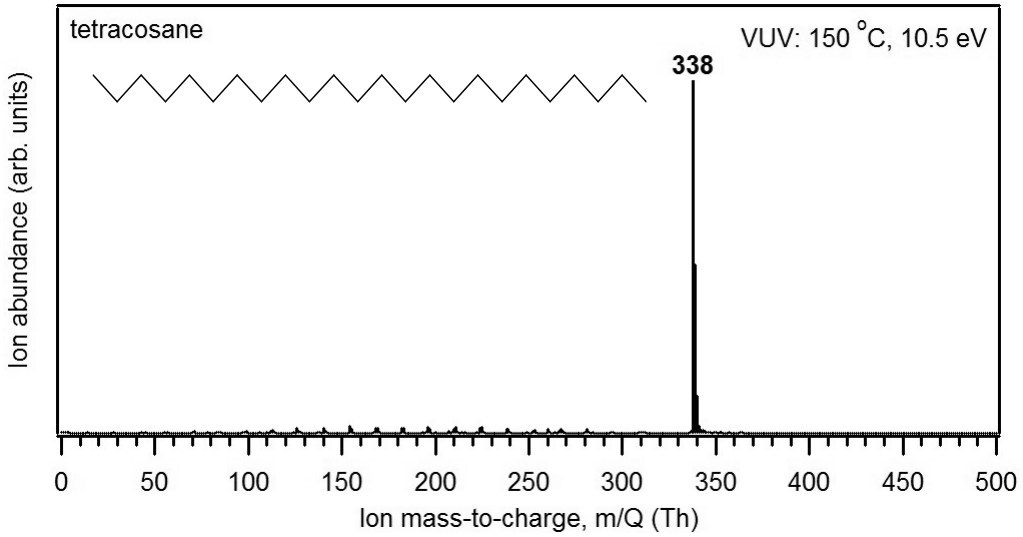

nonadecane
VUV: 150 °C, 10.5 eV
268
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

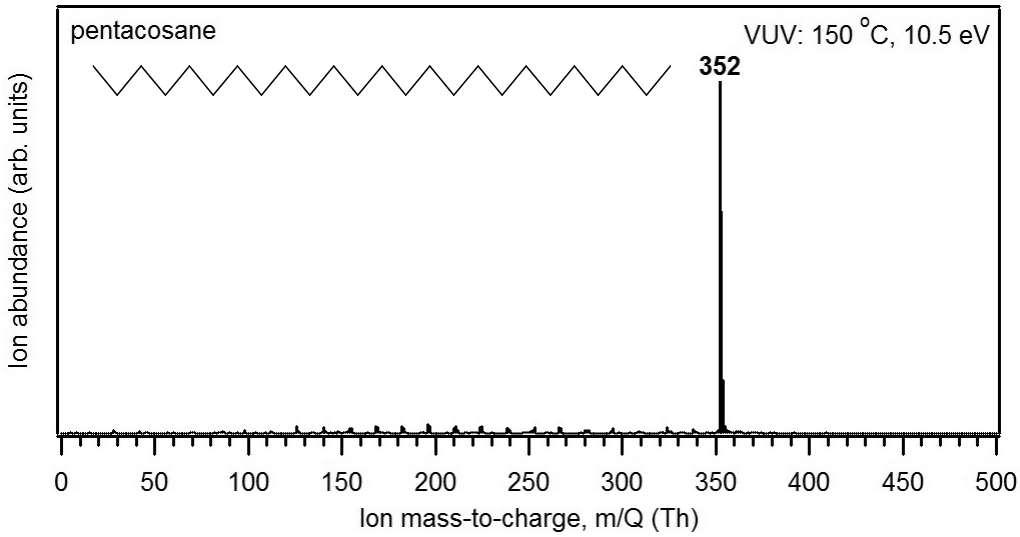

eicosane
VUV: 150 °C, 10.5 eV
282
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

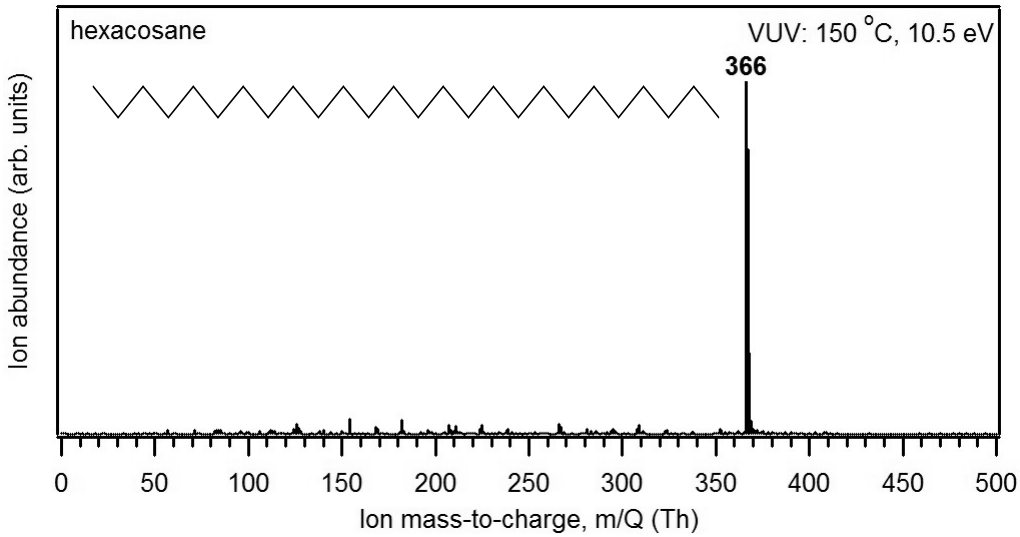

heneicosane
VUV: 150 °C, 10.5 eV
296
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)


docosane
VUV: 150 °C, 10.5 eV
310
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

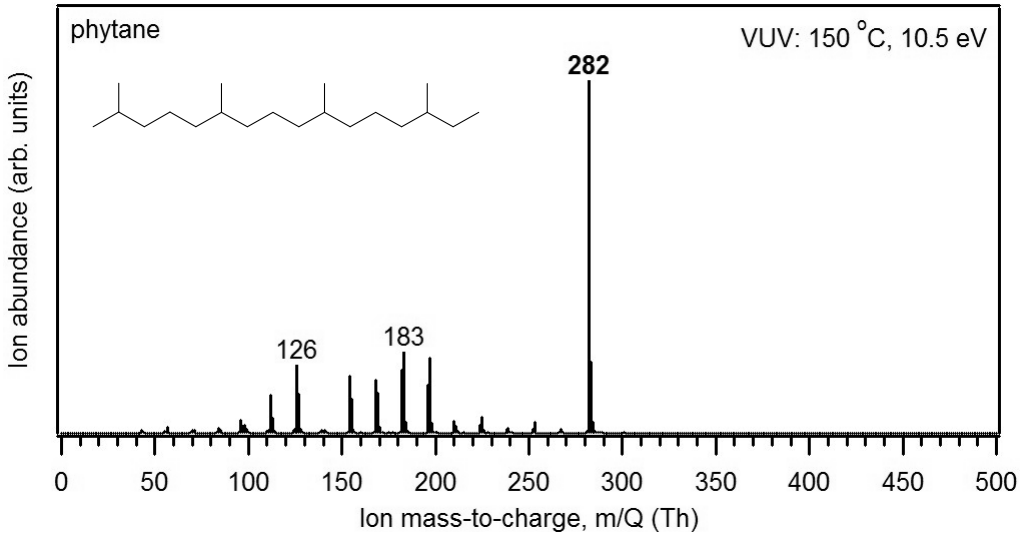

tricosane
VUV: 150 °C, 10.5 eV
324
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

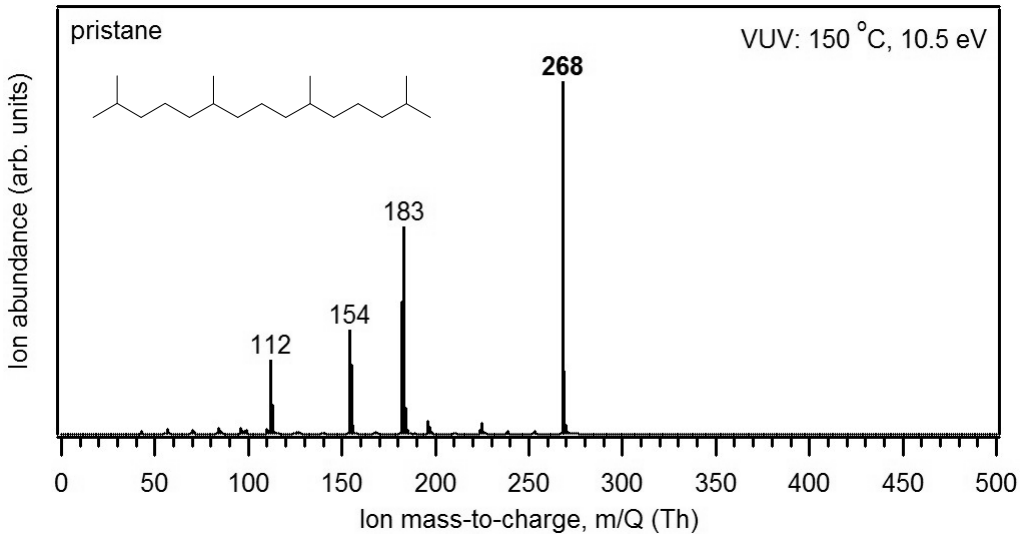

tetracosane
VUV: 150 °C, 10.5 eV
338
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

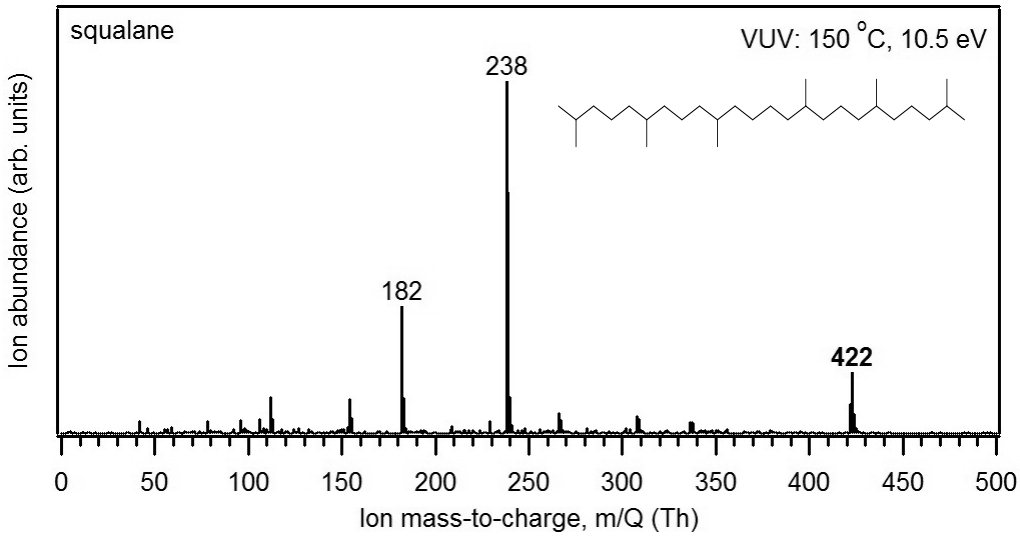

pentacosane
VUV: 150 °C, 10.5 eV
352
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

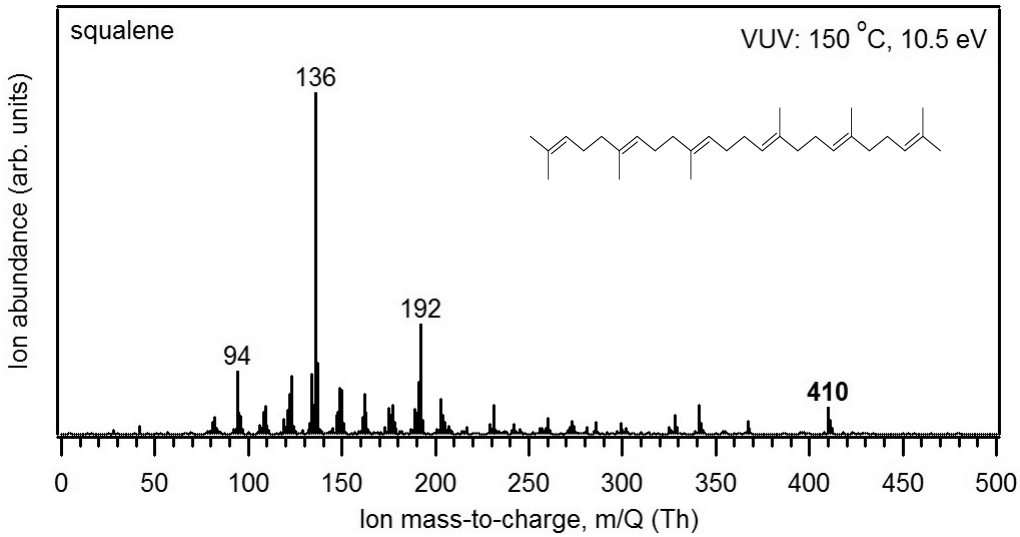

hexacosane
VUV: 150 °C, 10.5 eV
366
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

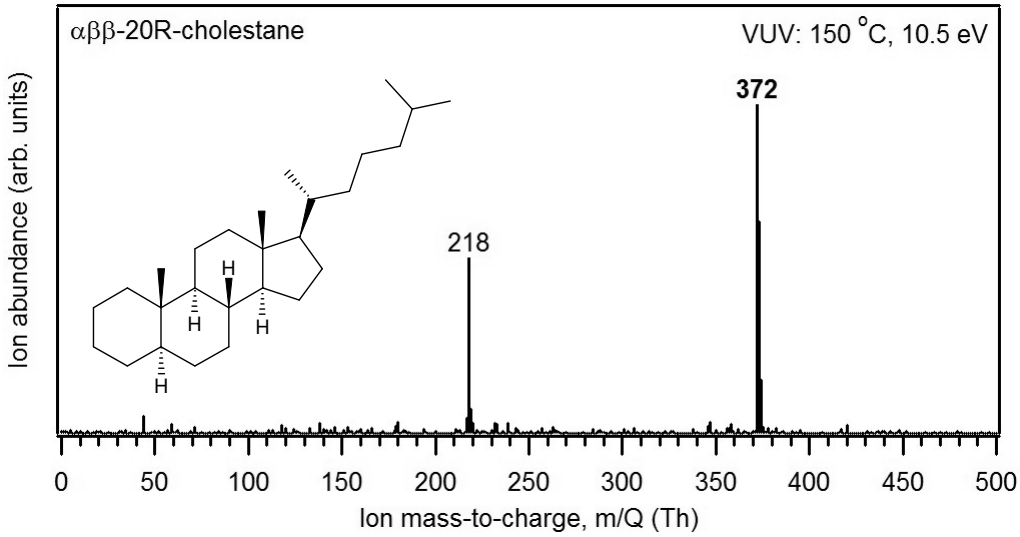
S.1.2. Branched aliphatic hydrocarbons



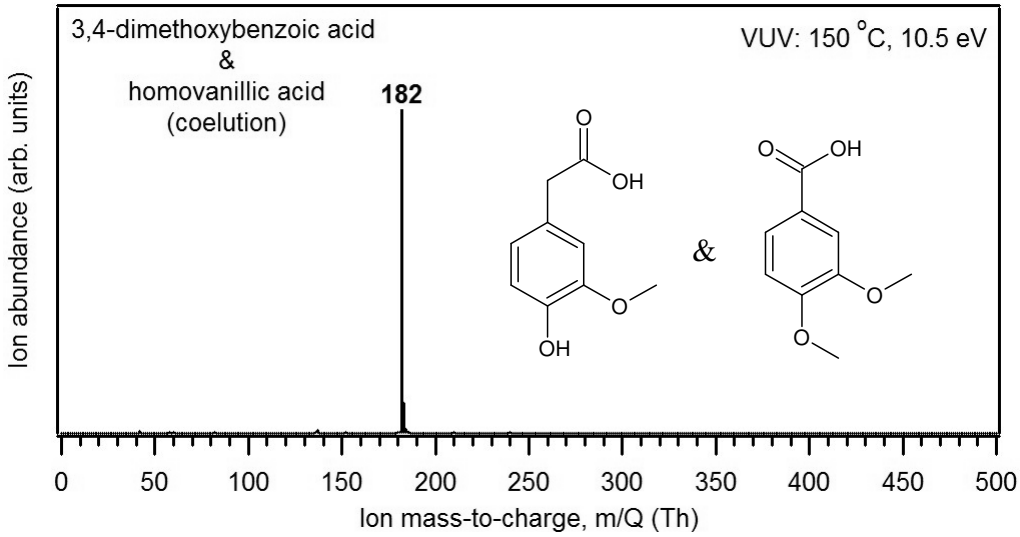


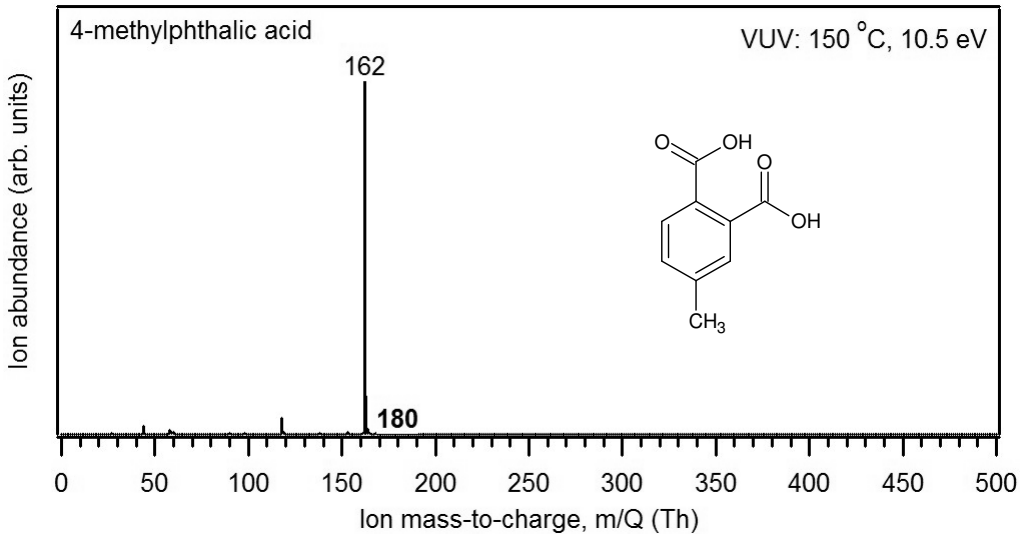

squalane
VUV: 150 °C, 10.5 eV
238
182
422
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

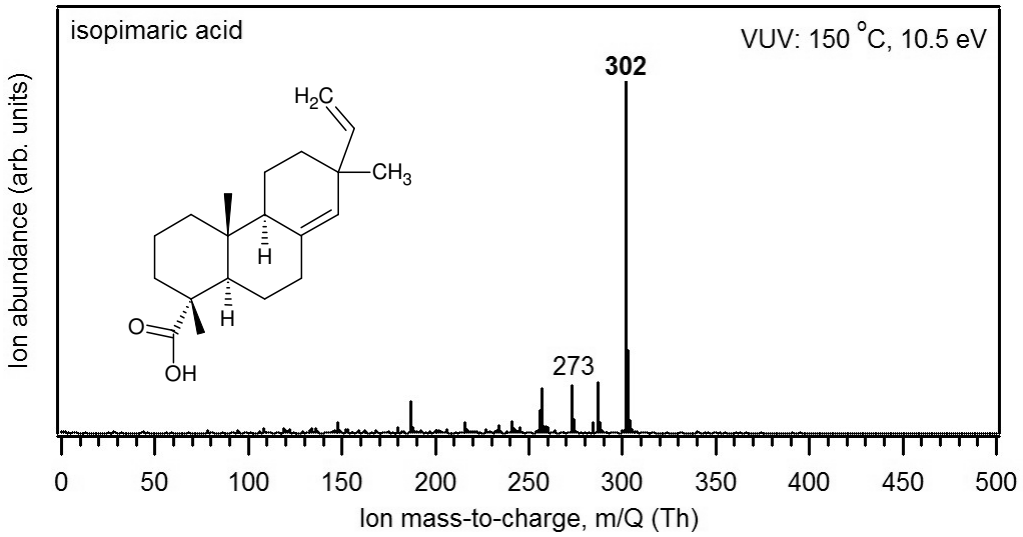

squalene
VUV: 150 °C, 10.5 eV
136
192
94
410
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

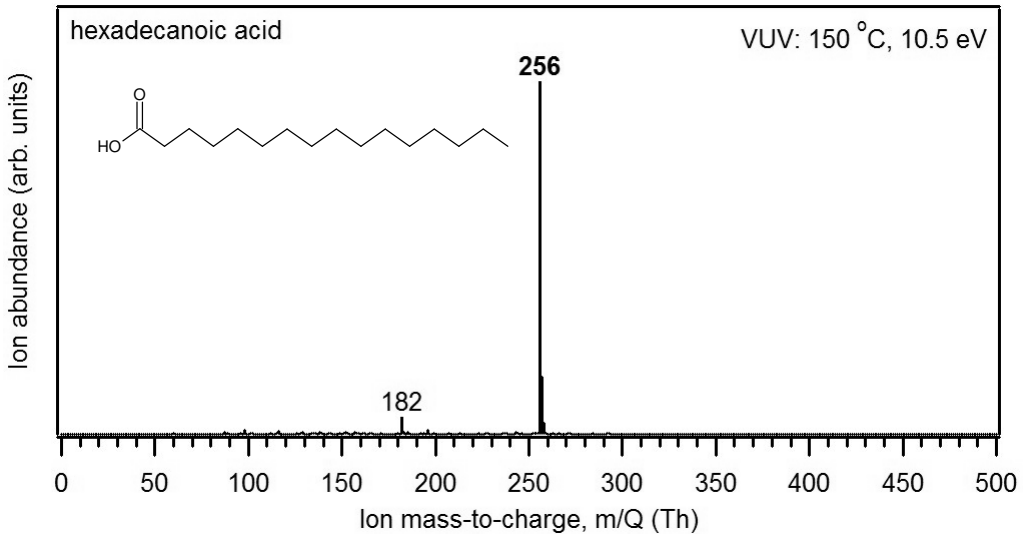

αββ-20R-cholestane
VUV: 150 °C, 10.5 eV
372
218
H
H
H
H
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

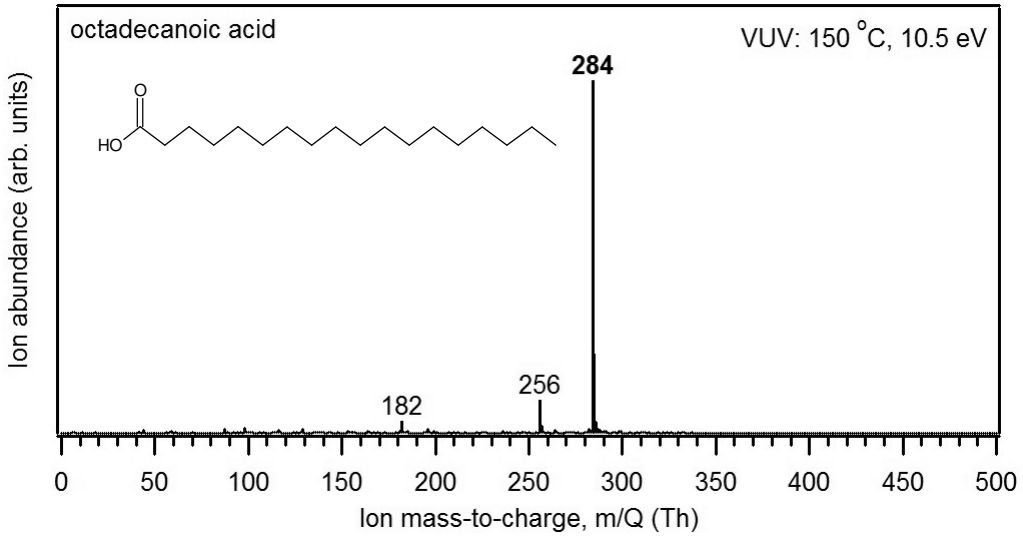
S.1.3. Acids

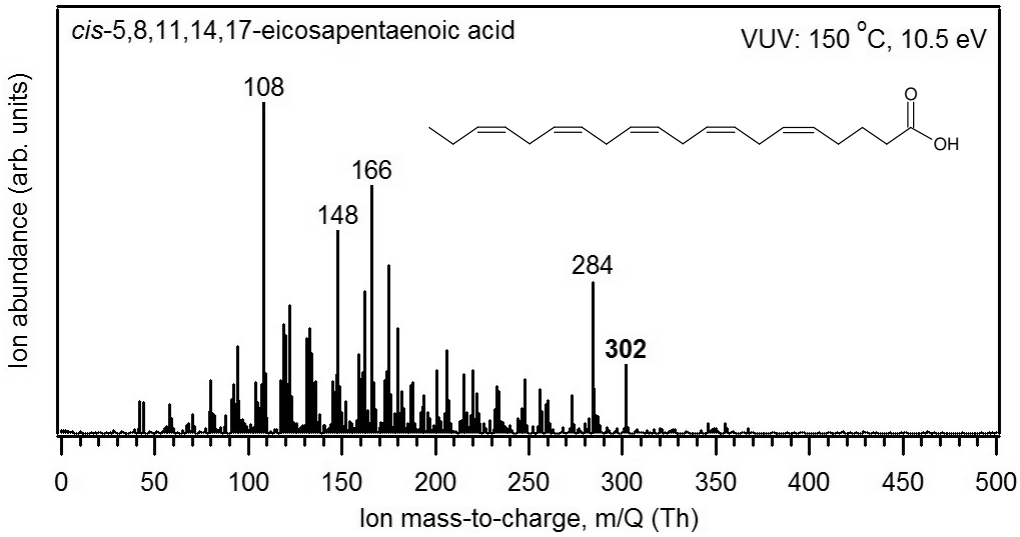

3,4-dimethoxybenzoic acid
&
homovanillic acid
(coelution)
VUV: 150 °C, 10.5 eV
182
Ion abundance (arb. units)
Ion mass-to-charge, m/Q (Th)
0
50
100
150
200
250
300
350
400
450
500


4-methylphthalic acid
VUV: 150 °C, 10.5 eV
162
180
Ion abundance (arb. units)
Ion mass-to-charge, m/Q (Th)
0
50
100
150
200
250
300
350
400
450
500

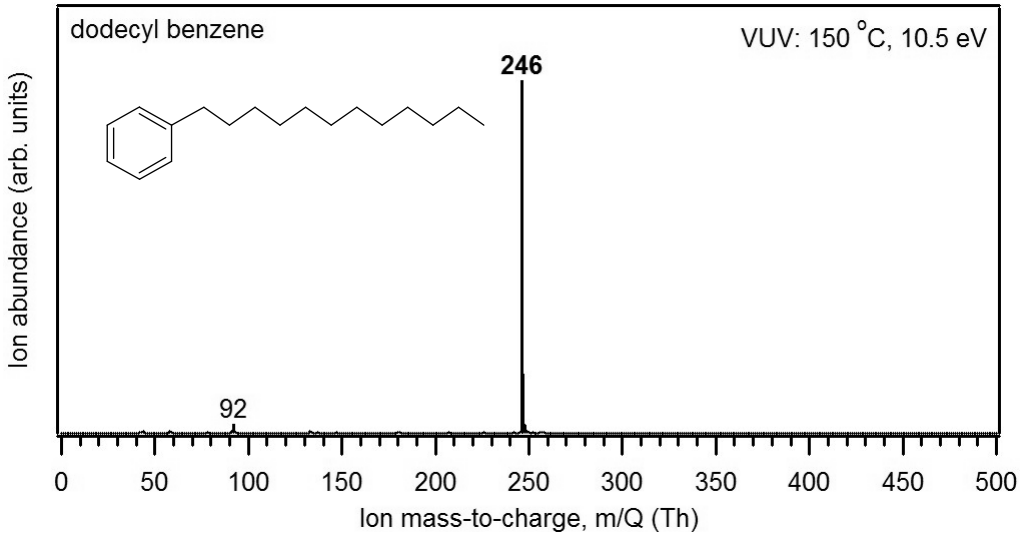

isopimaric acid
VUV: 150 °C, 10.5 eV
302
273
H2C
CH3
H
H
O
OH
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

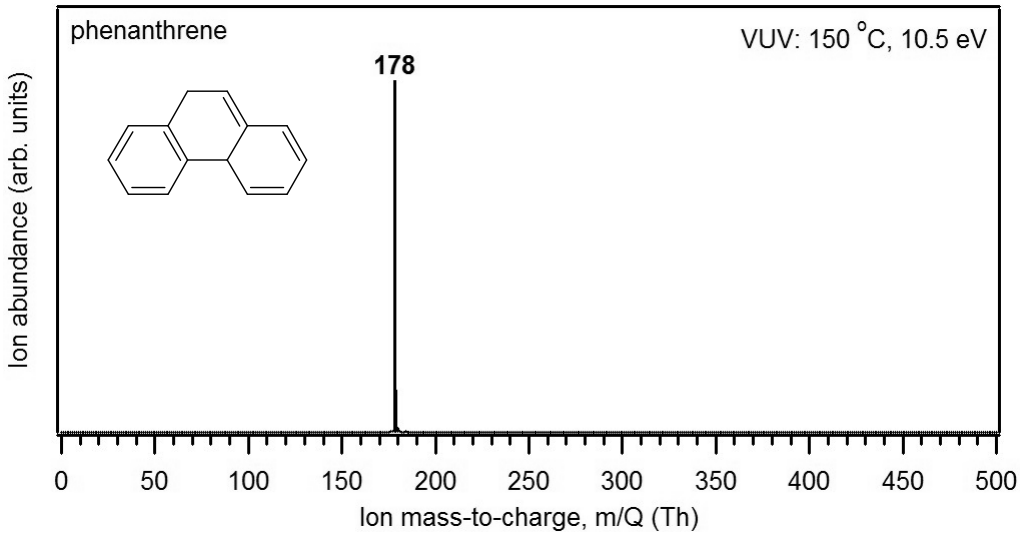

hexadecanoic acid
VUV: 150 °C, 10.5 eV
256
182
O
HO
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

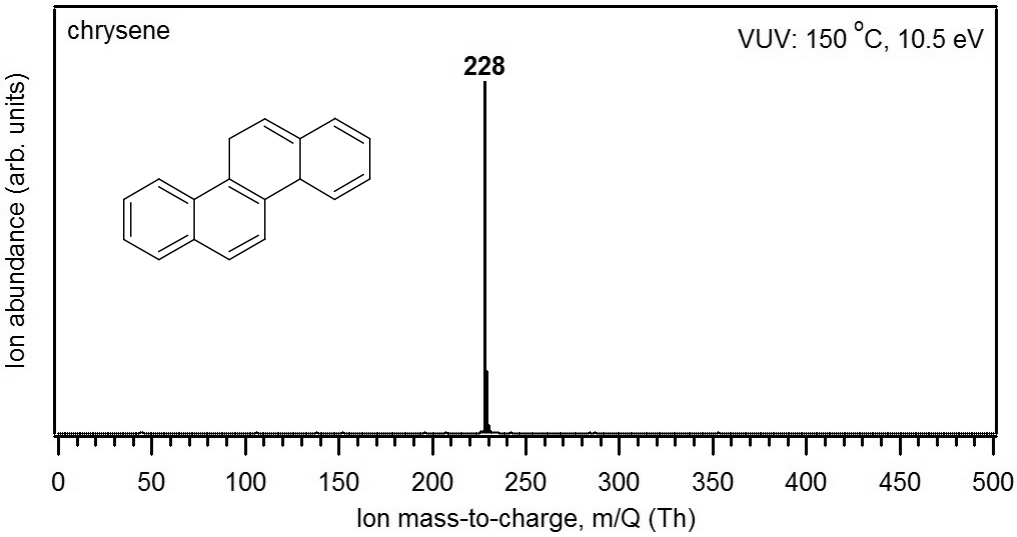

octadecanoic acid
VUV: 150 °C, 10.5 eV
284
256
182
O
HO
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

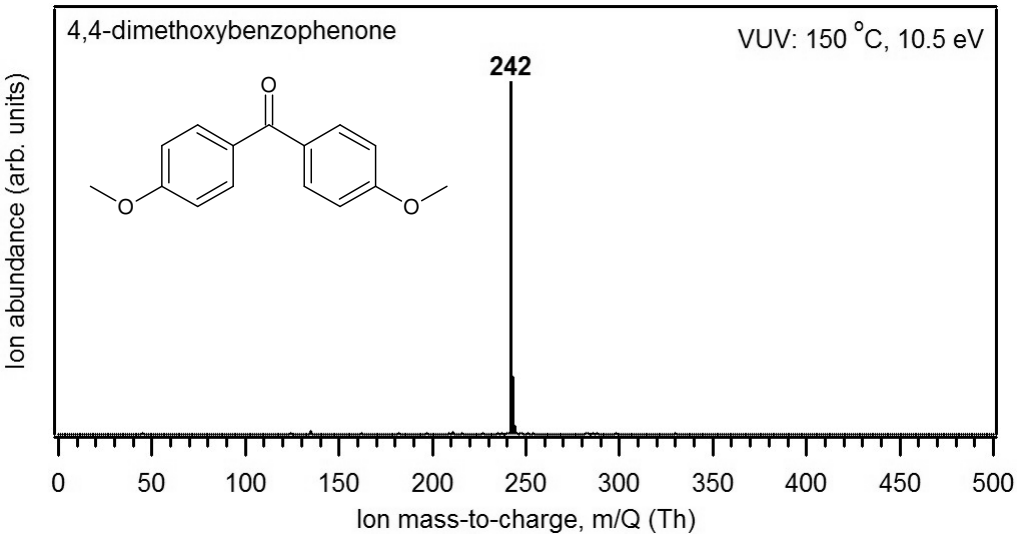

cis-5,8,11,14,17-eicosapentaenoic acid
VUV: 150 °C, 10.5 eV
108
166
148
284
302
O
OH
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

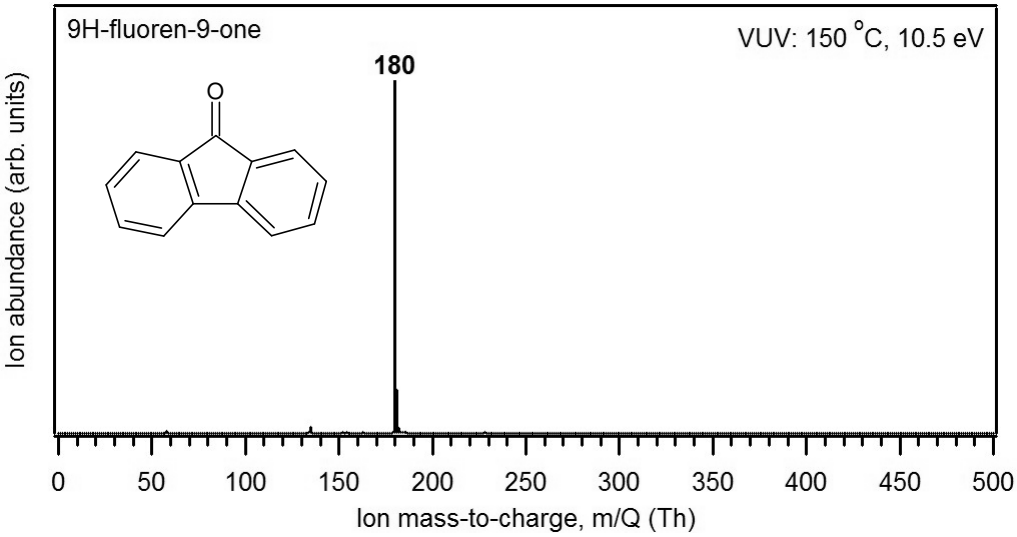
S.1.4. Aromatics and oxygenated polycyclic aromatic hydrocarbons

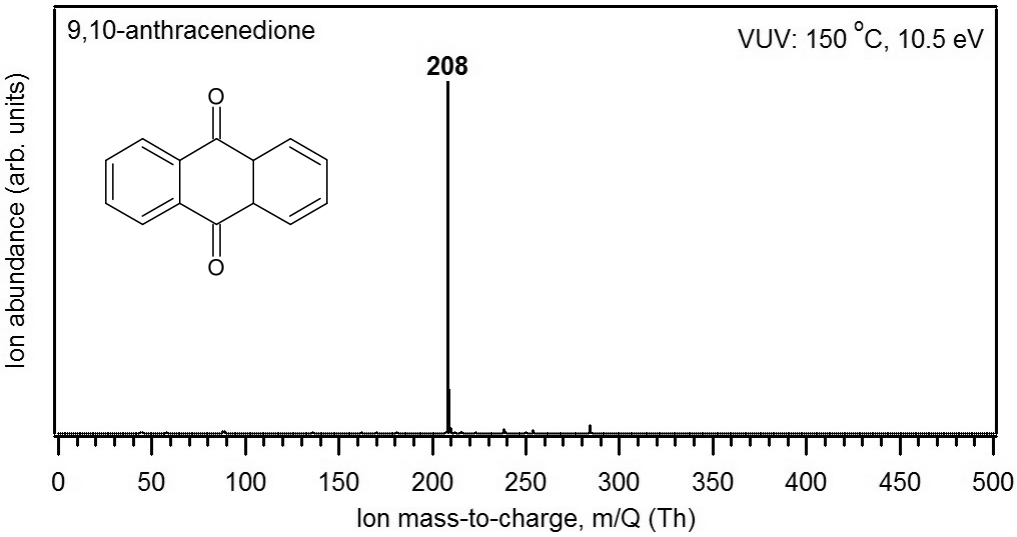


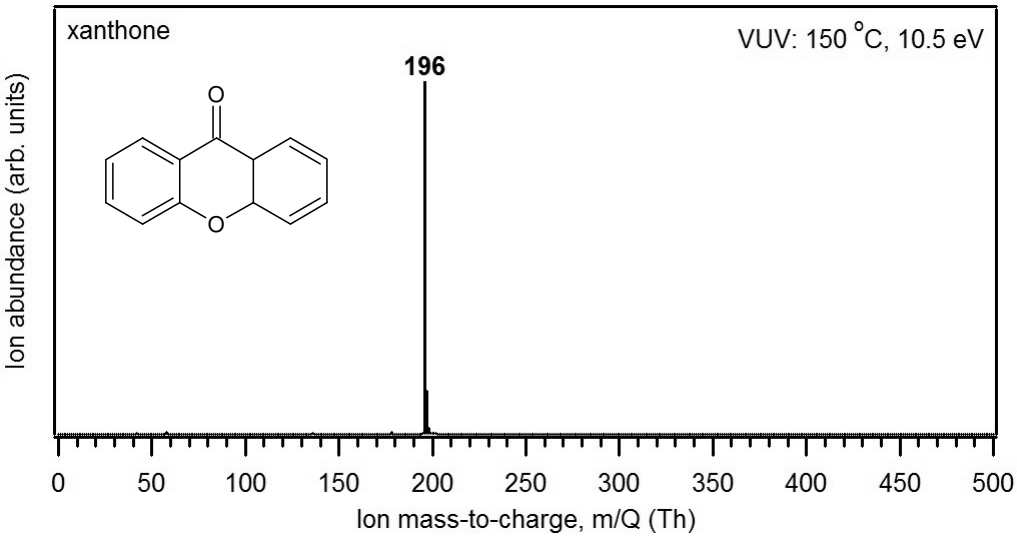



chrysene
VUV: 150 °C, 10.5 eV
228
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

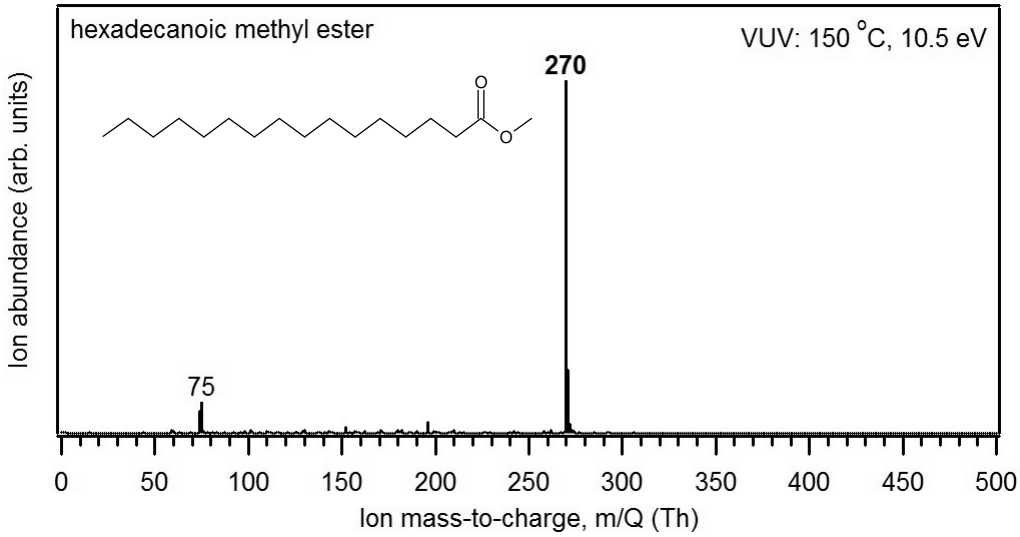

4,4-dimethoxybenzophenone
VUV: 150 °C, 10.5 eV
242
O
O
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

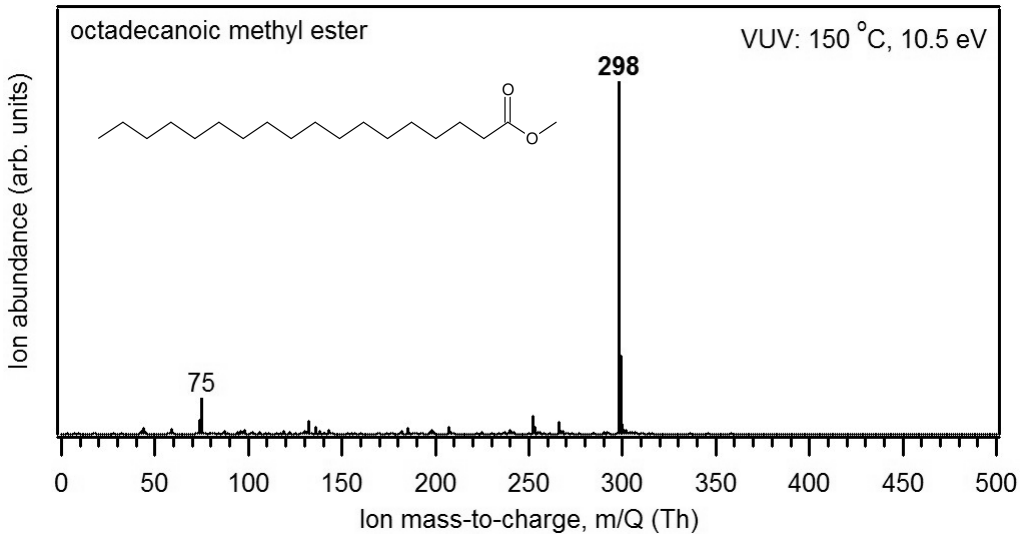

9H-fluoren-9-one
VUV: 150 °C, 10.5 eV
180
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

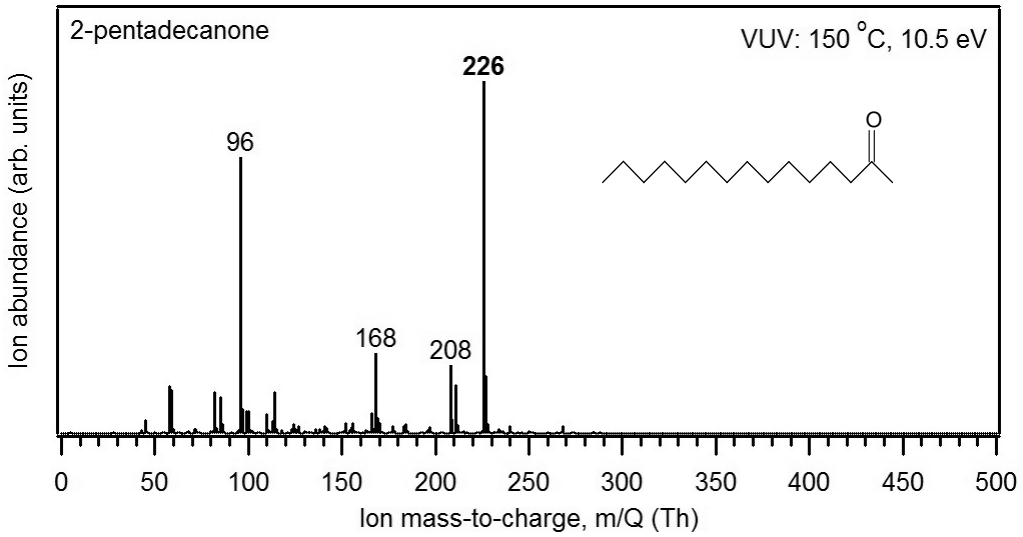

9,10-anthracenedione
VUV: 150 °C, 10.5 eV
208
O
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

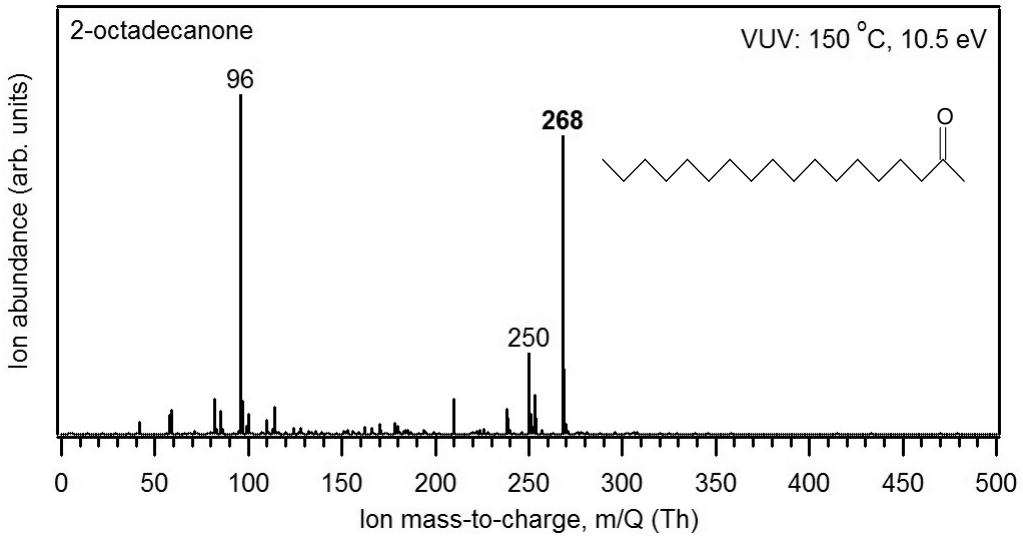

xanthone
VUV: 150 °C, 10.5 eV
196
O
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

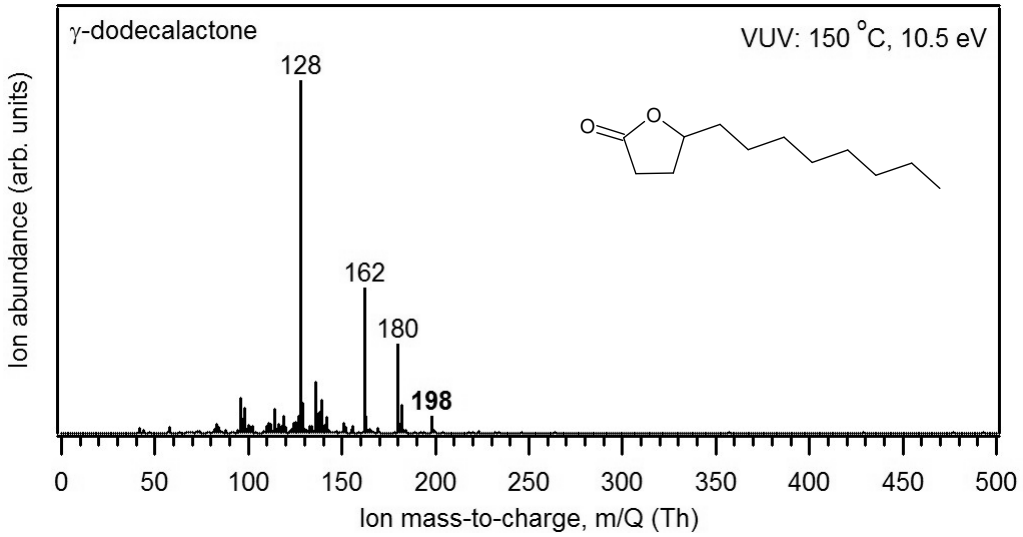
S.1.5. Other oxygenated compounds (ketones, esters, aldehydes)

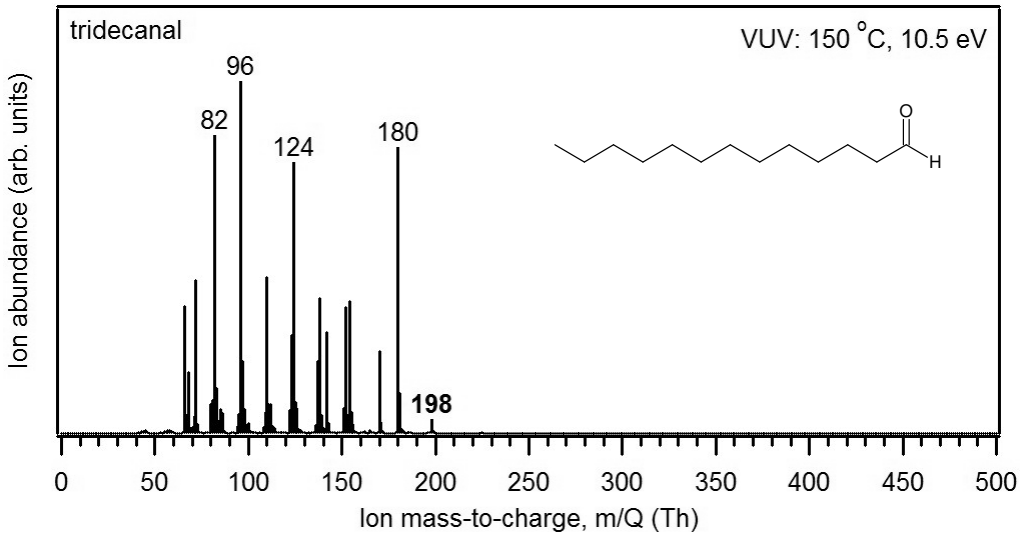


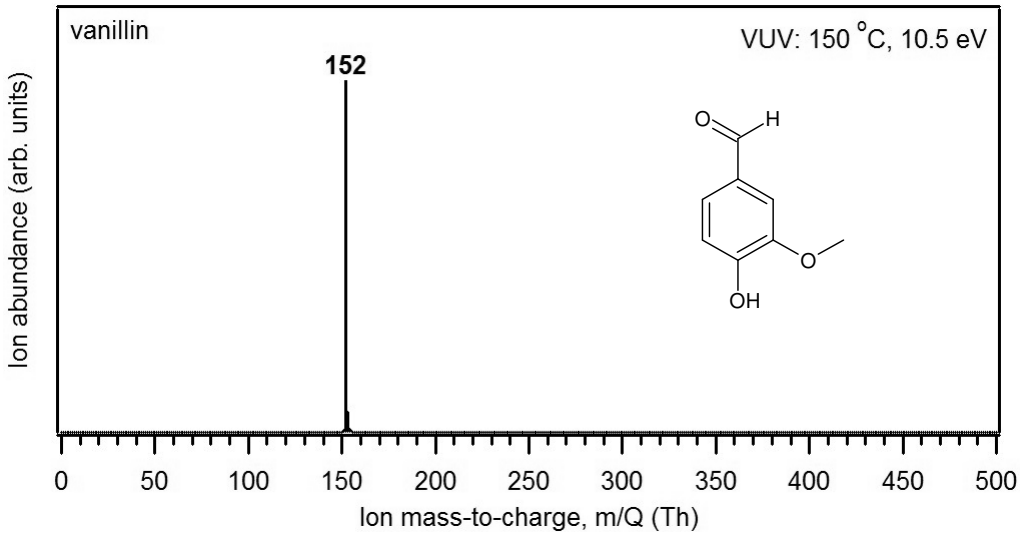



2-pentadecanone
VUV: 150 °C, 10.5 eV
226
96
168
208
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)


2-octadecanone
VUV: 150 °C, 10.5 eV
96
268
250
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

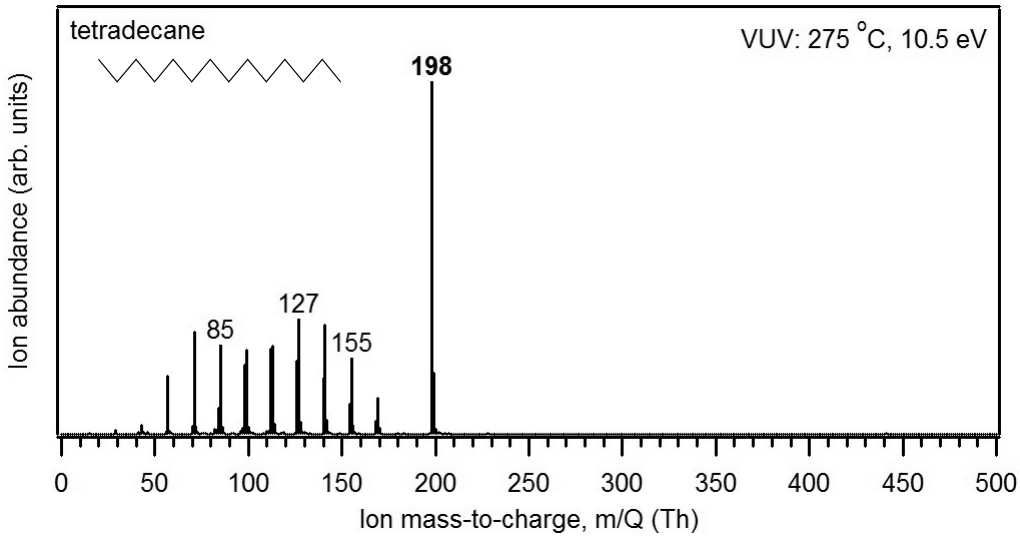

γ-dodecalactone
VUV: 150 °C, 10.5 eV
128
162
180
198
O
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

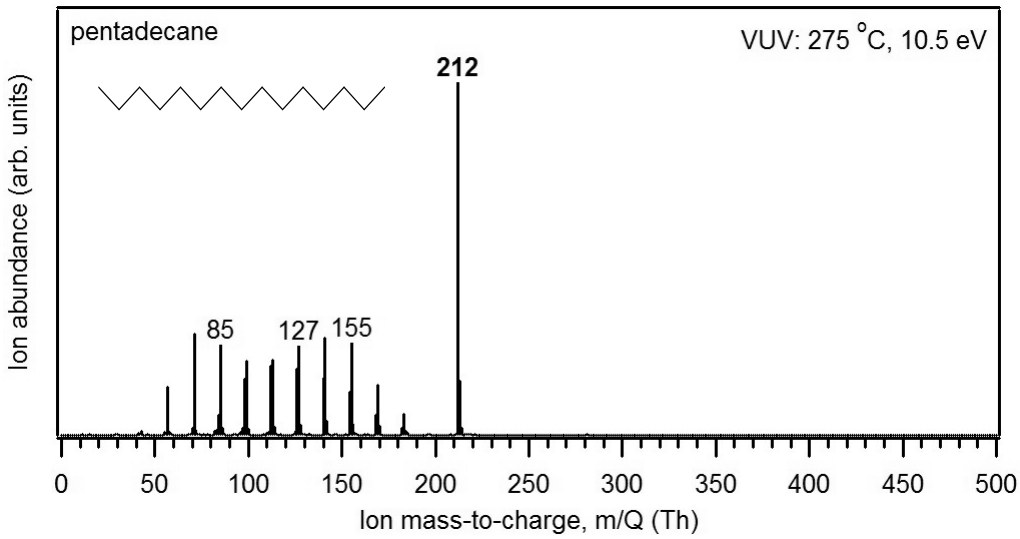

tridecanal
VUV: 150 °C, 10.5 eV
96
82
124
180
198
O
H
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

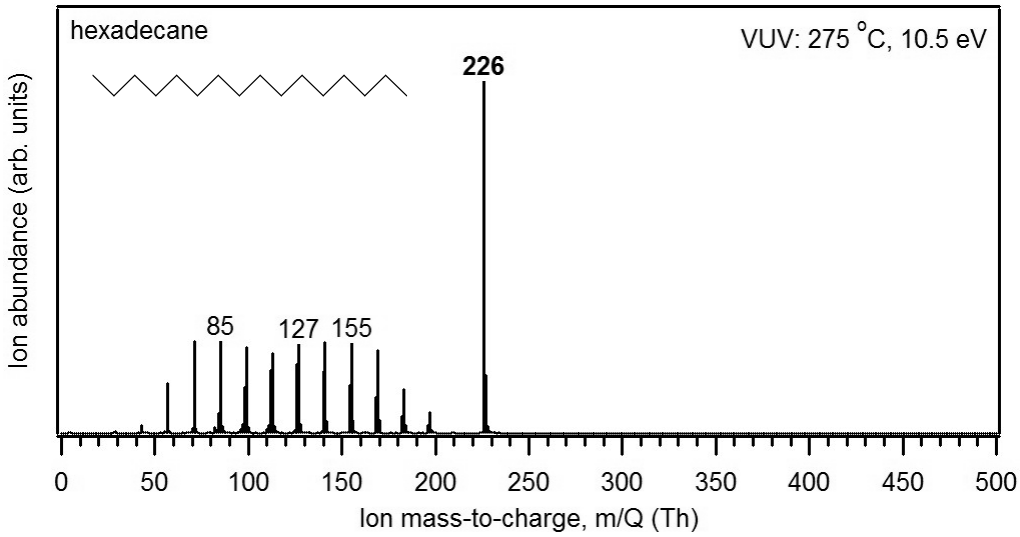

vanillin
VUV: 150 °C, 10.5 eV
152
O
H
O
OH
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

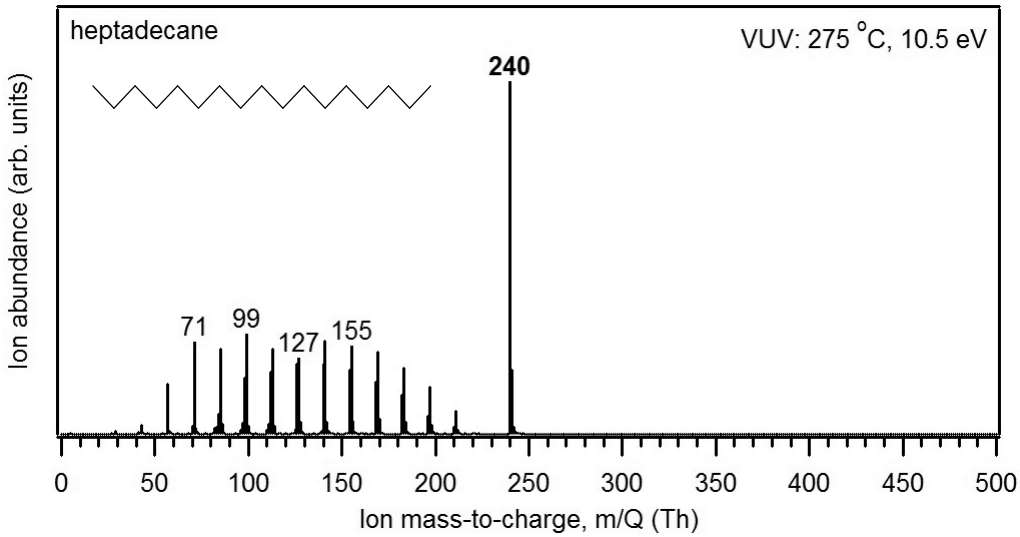
S.2. Spectra at a transfer temperature of 275 °C

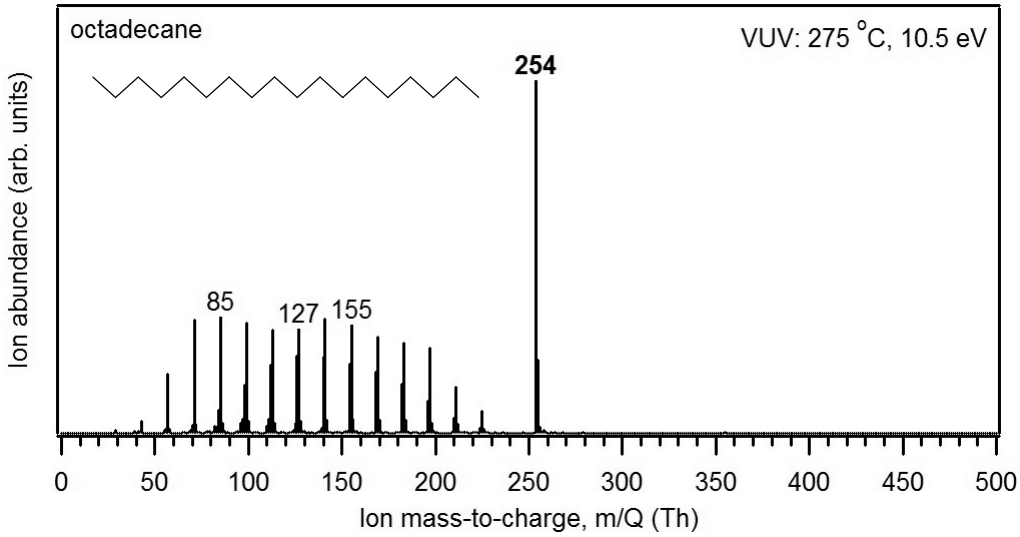
S.2.1. Normal alkanes

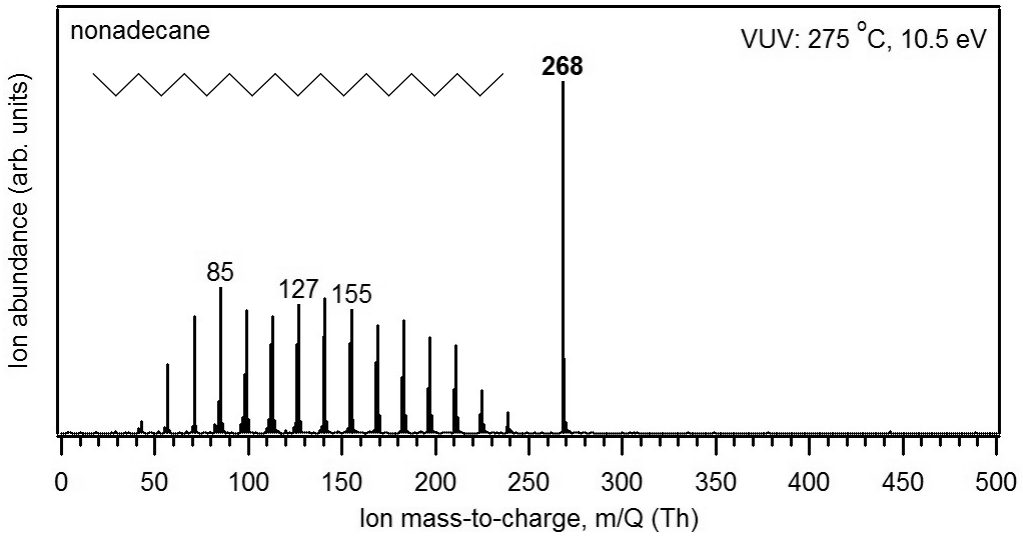


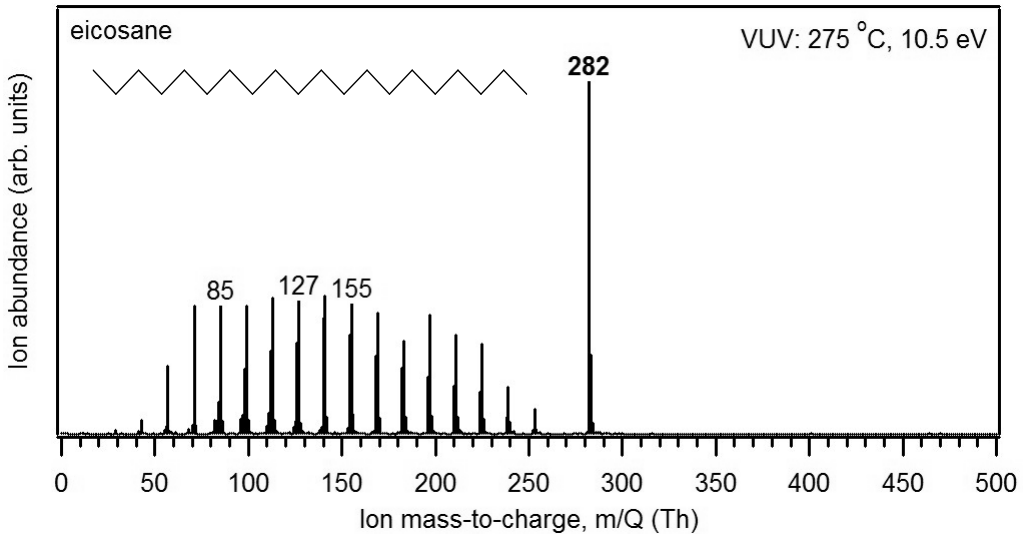


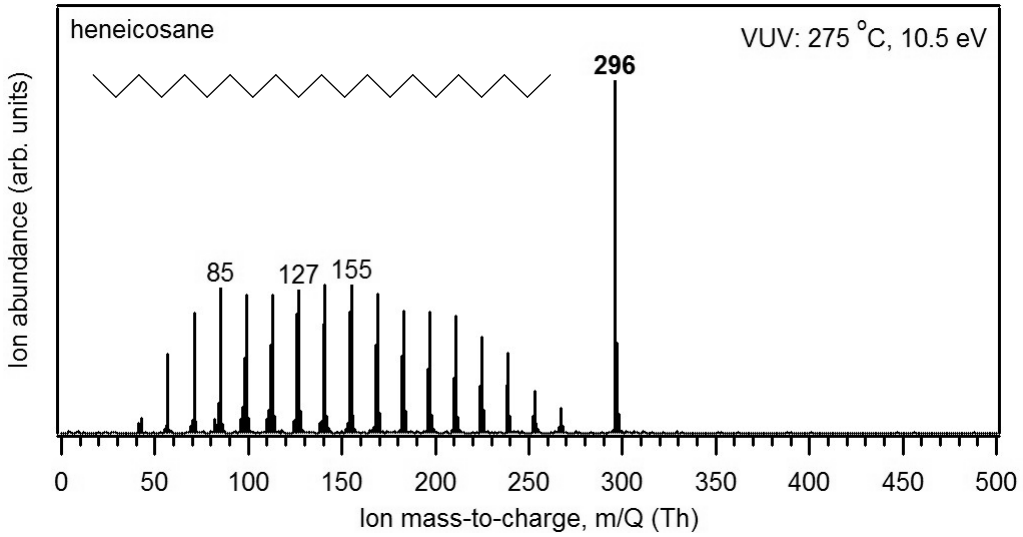

hexadecane
VUV: 275 °C, 10.5 eV
226
85
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

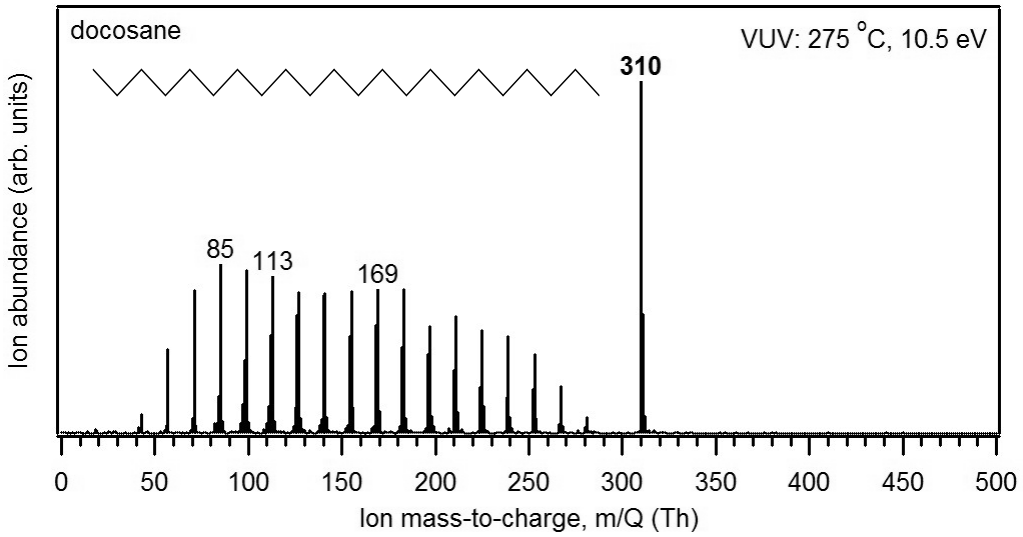

heptadecane
VUV: 275 °C, 10.5 eV
240
71
99
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

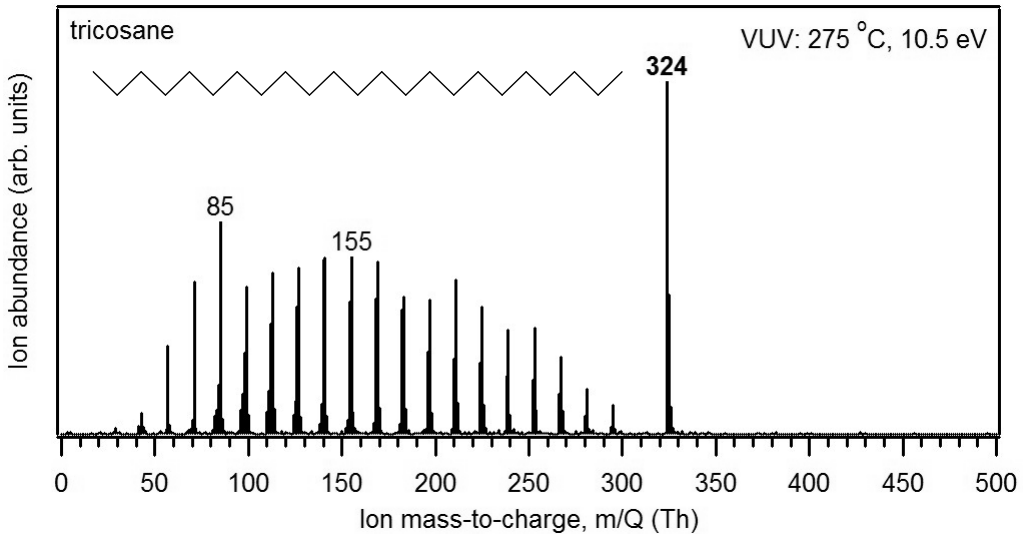

octadecane
VUV: 275 °C, 10.5 eV
254
85
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

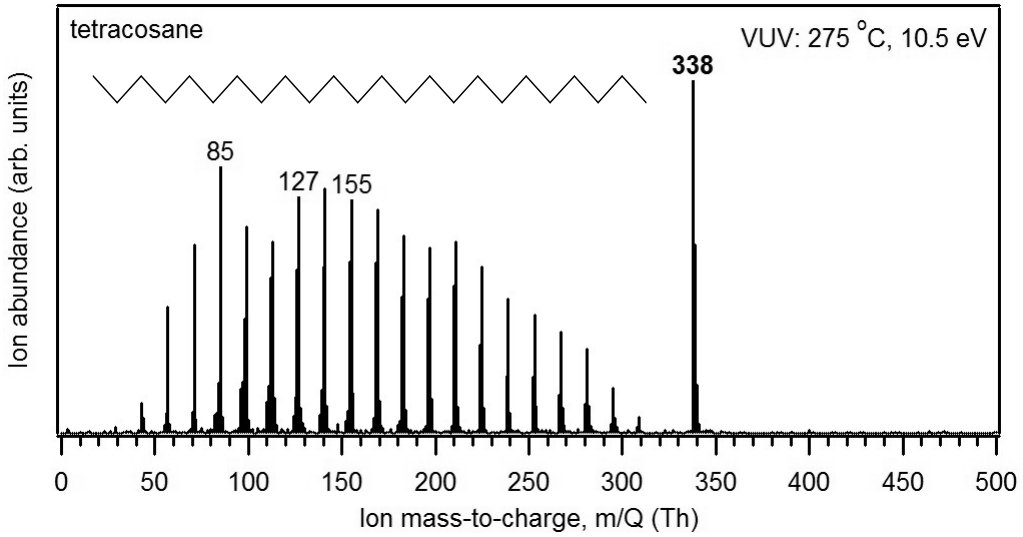

nonadecane
VUV: 275 °C, 10.5 eV
268
85
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

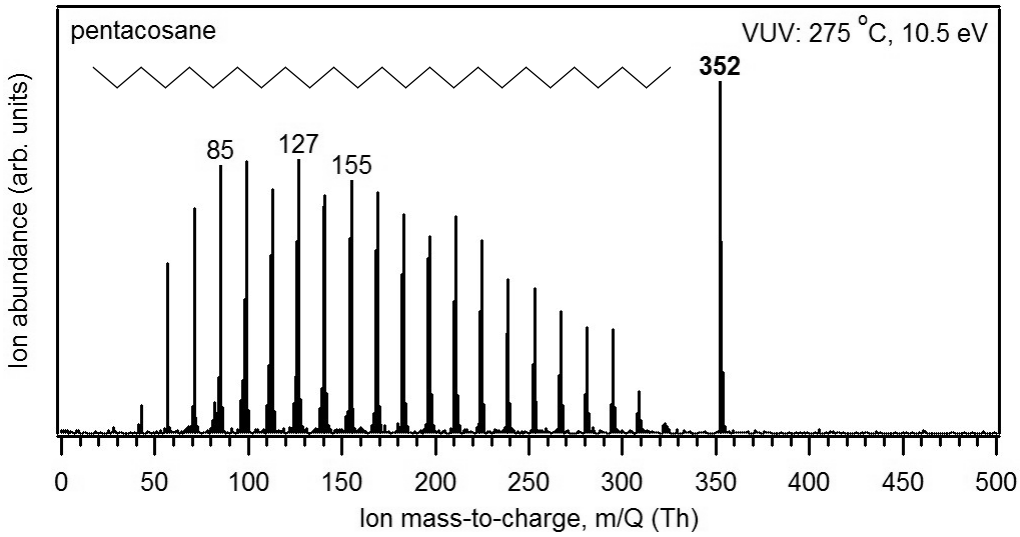

eicosane
VUV: 275 °C, 10.5 eV
282
85
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

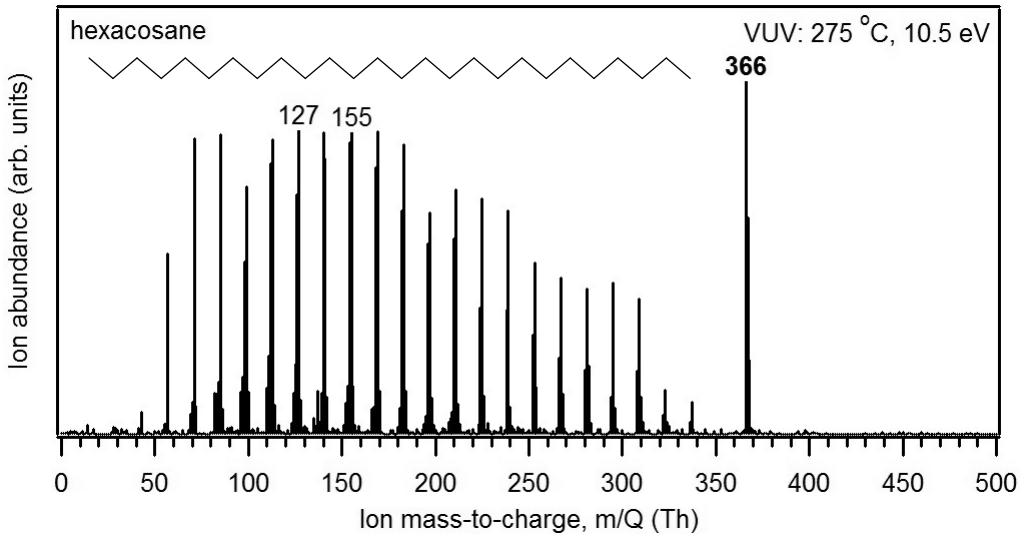

heneicosane
VUV: 275 °C, 10.5 eV
296
85
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

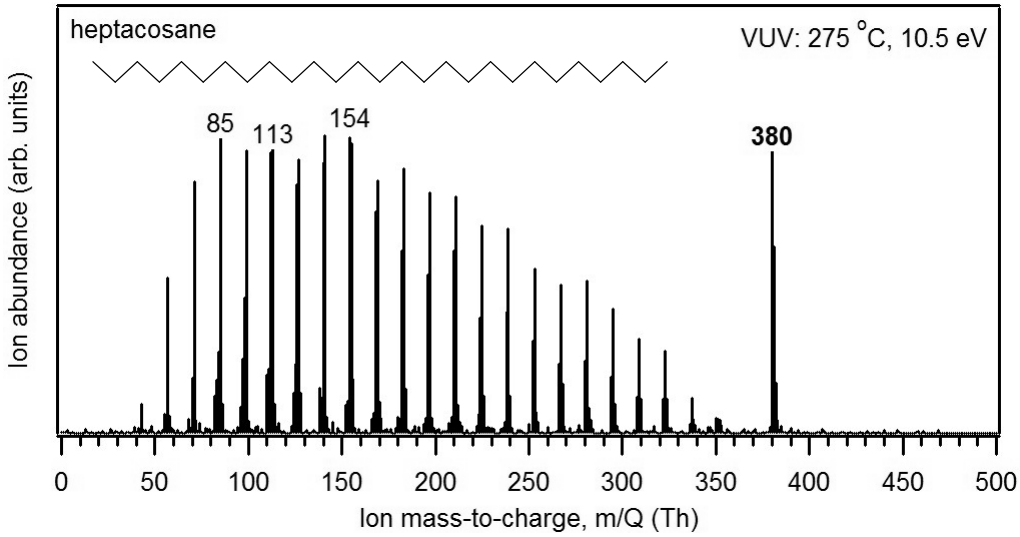

docosane
VUV: 275 °C, 10.5 eV
310
85
113
169
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

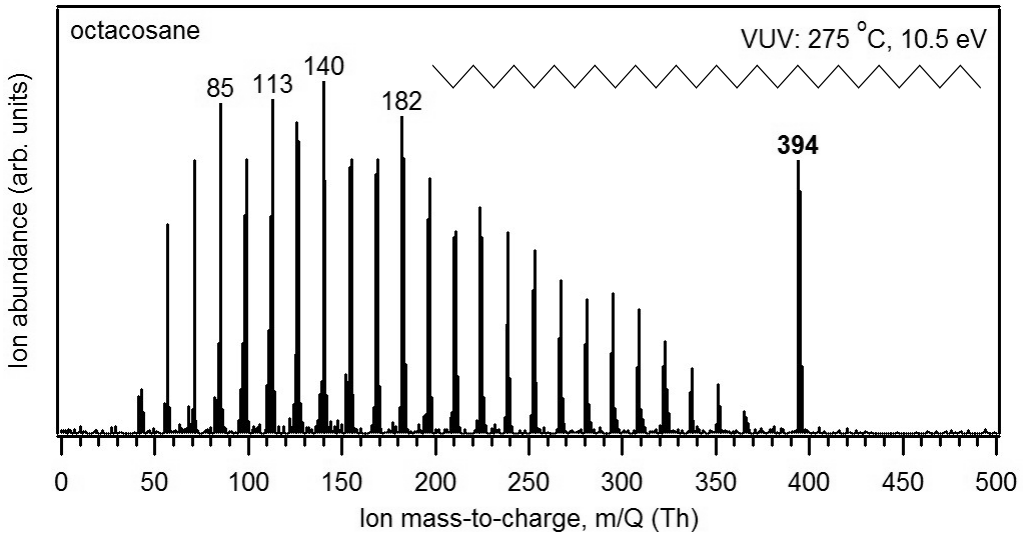

tricosane
VUV: 275 °C, 10.5 eV
324
85
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

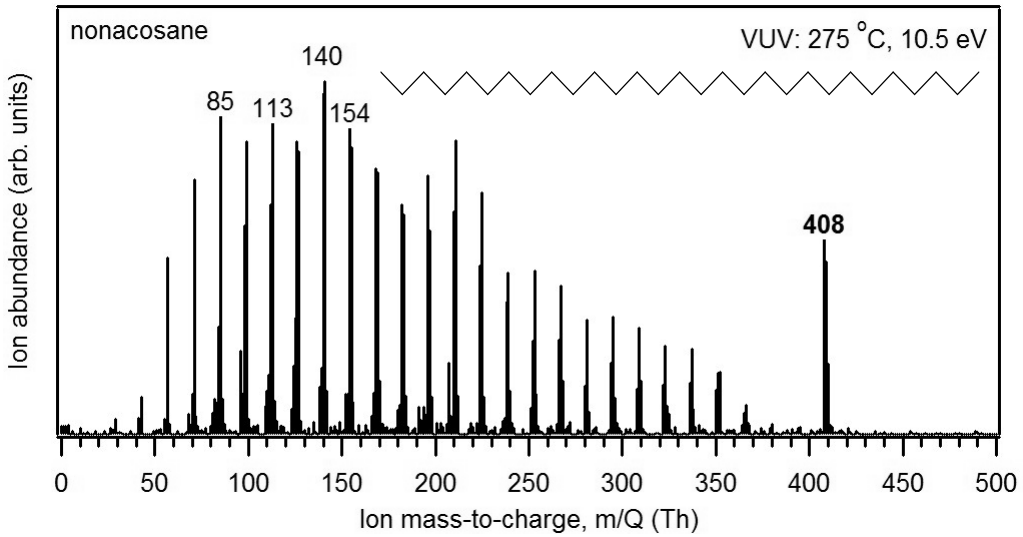

tetracosane
VUV: 275 °C, 10.5 eV
338
85
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

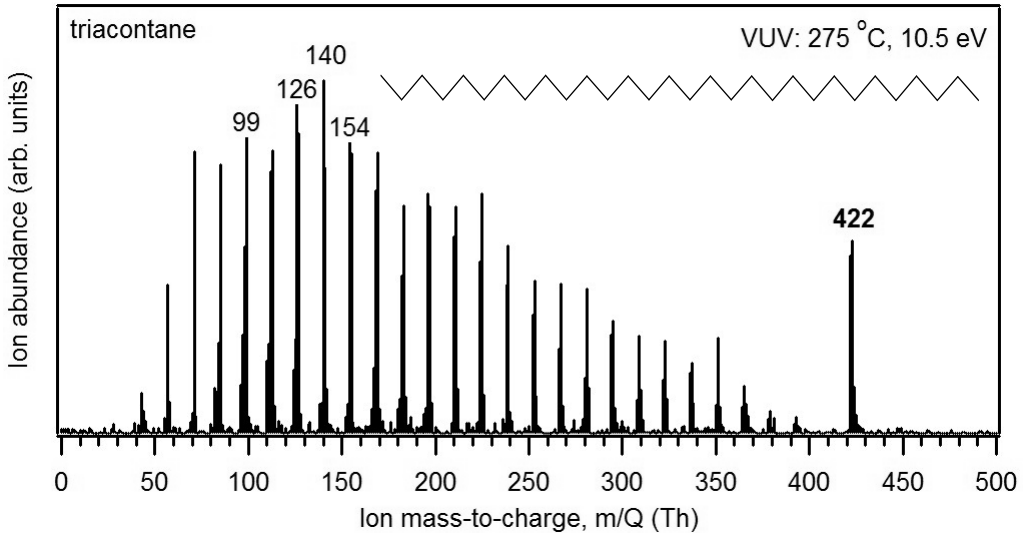

pentacosane
VUV: 275 °C, 10.5 eV
352
85
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

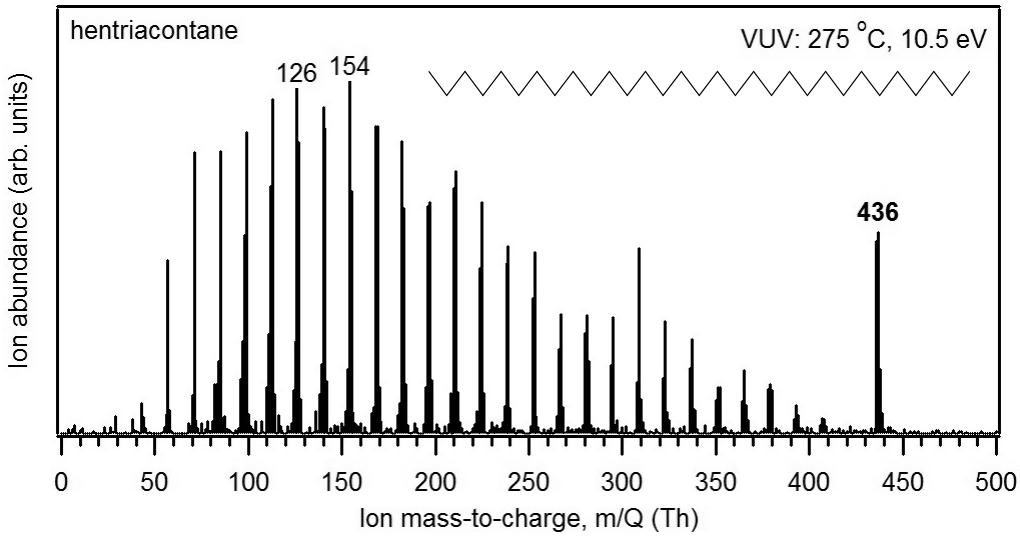

hexacosane
VUV: 275 °C, 10.5 eV
366
127
155
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

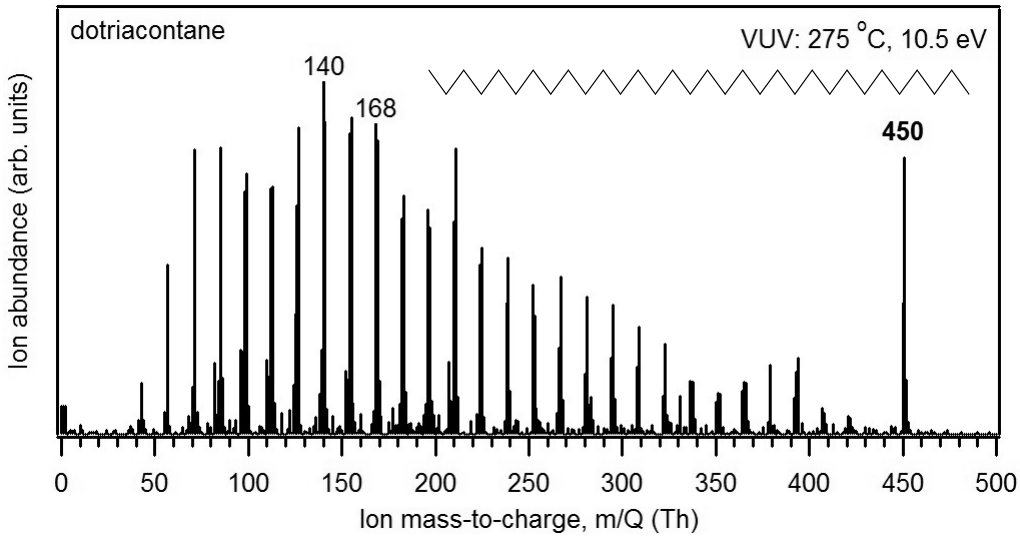

heptacosane
VUV: 275 °C, 10.5 eV
85
113
154
380
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

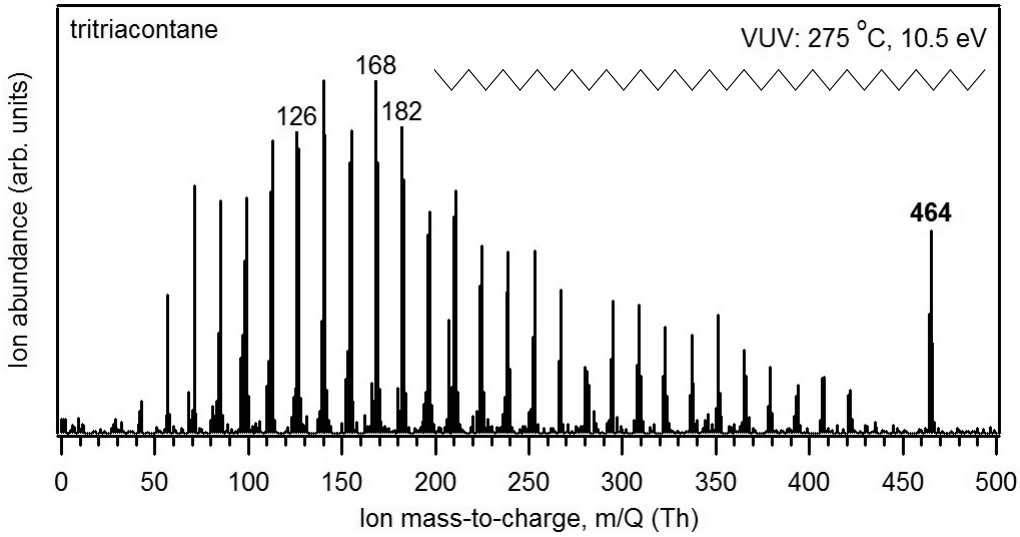

octacosane
VUV: 275 °C, 10.5 eV
85
113
140
182
394
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

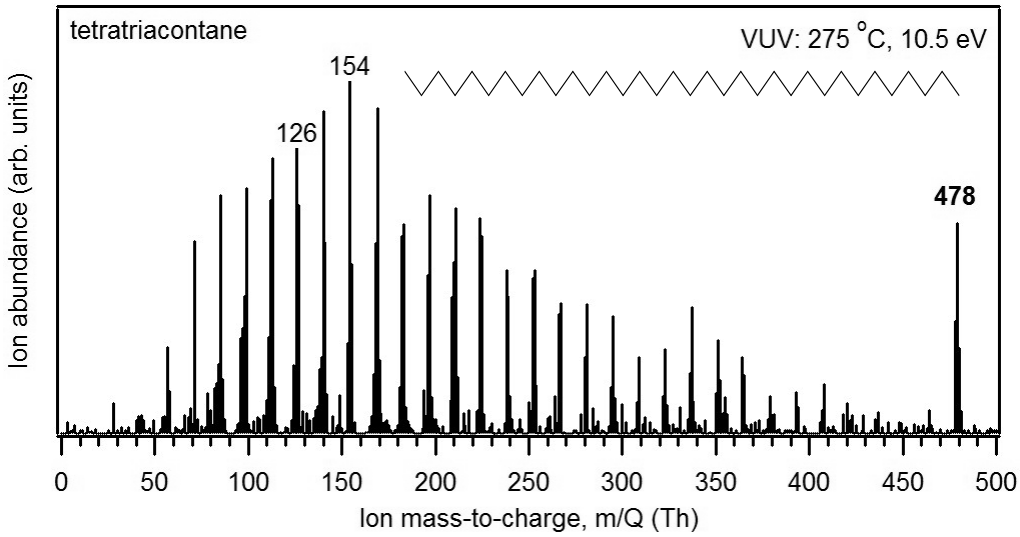

nonacosane
VUV: 275 °C, 10.5 eV
85
113
140
154
408
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

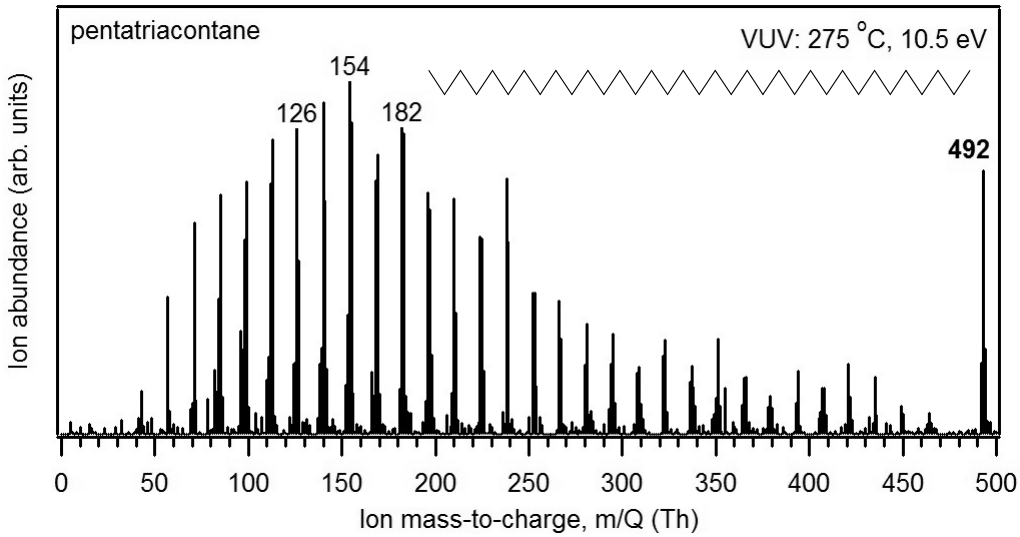

triacontane
VUV: 275 °C, 10.5 eV
99
126
140
154
422
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)


hentriacontane
VUV: 275 °C, 10.5 eV
126
154
436
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

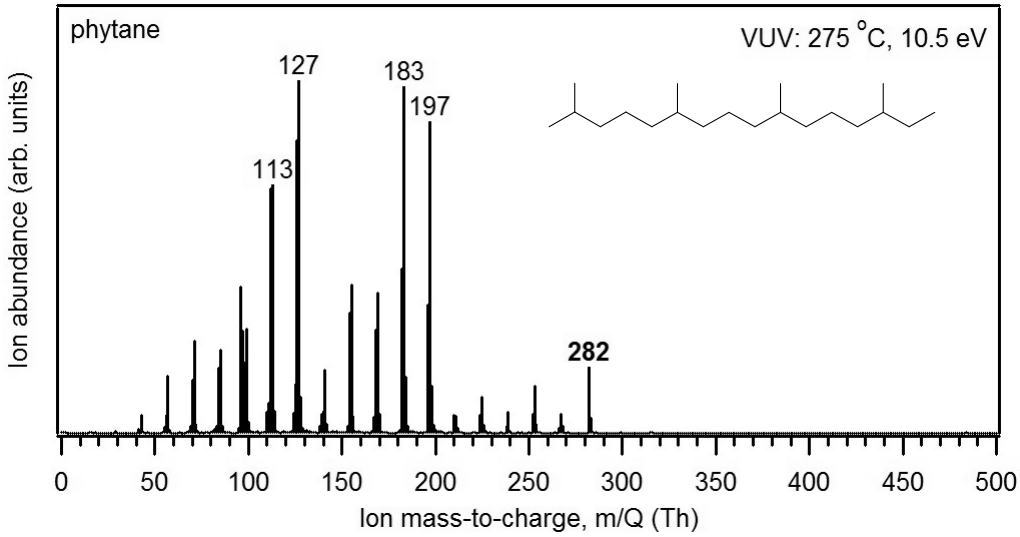

dotriacontane
VUV: 275 °C, 10.5 eV
140
168
450
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

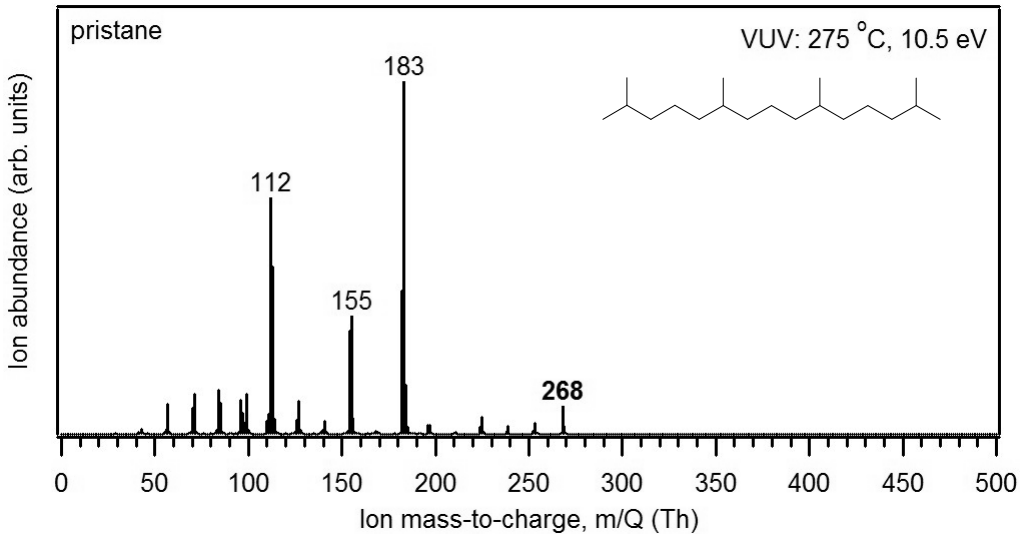

tritriacontane
VUV: 275 °C, 10.5 eV
168
126
182
464
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

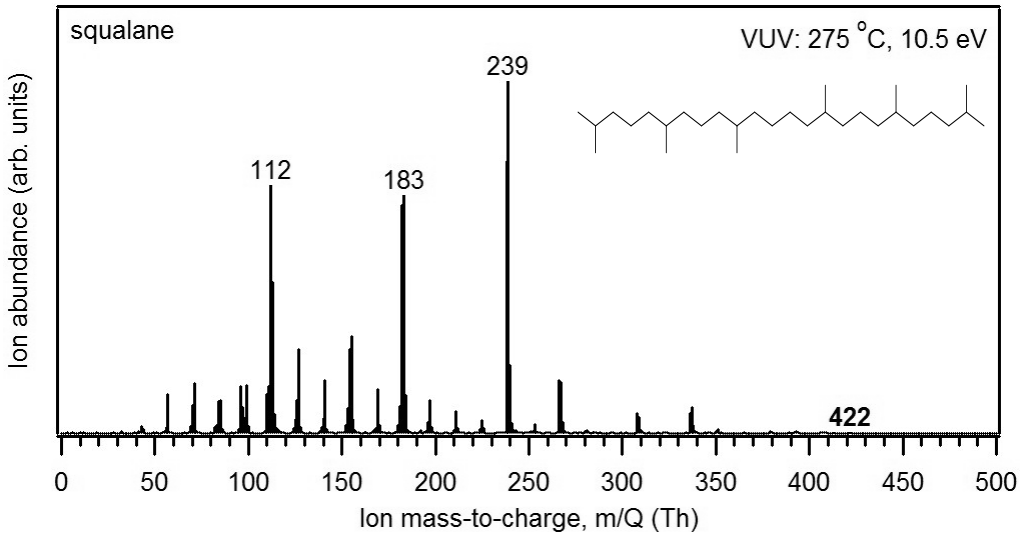

tetratriacontane
VUV: 275 °C, 10.5 eV
154
126
478
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

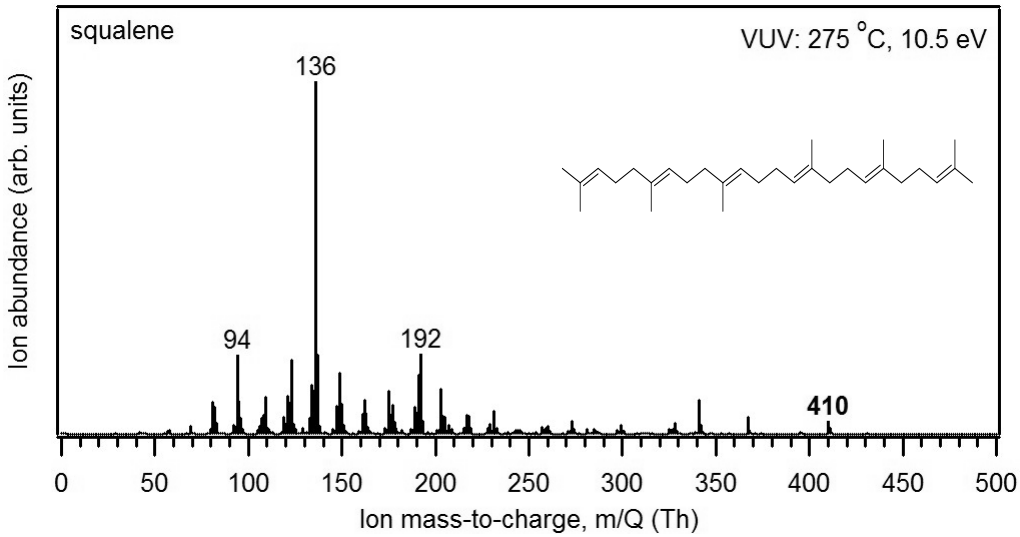

pentatriacontane
VUV: 275 °C, 10.5 eV
154
126
182
492
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

S.2.2. Branched aliphatic hydrocarbons

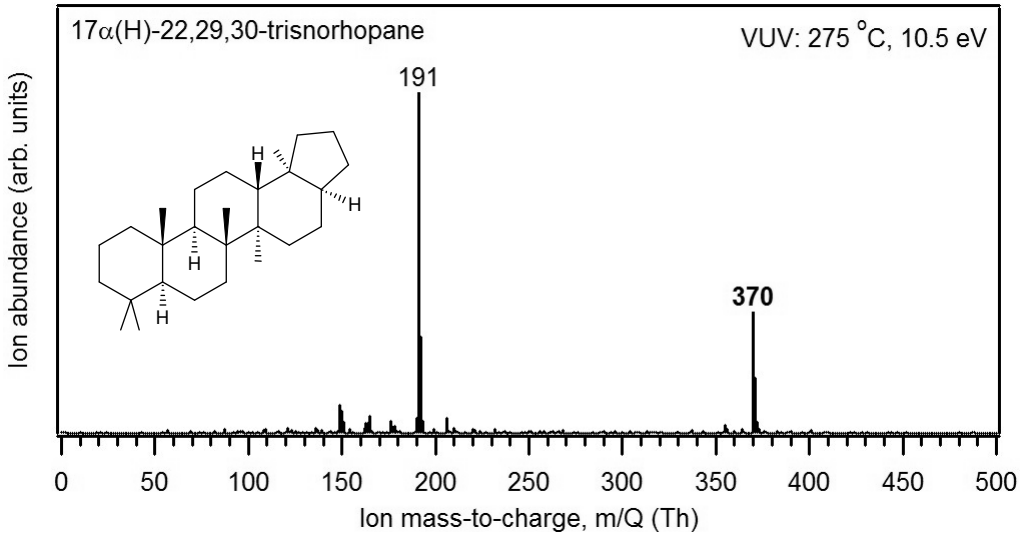


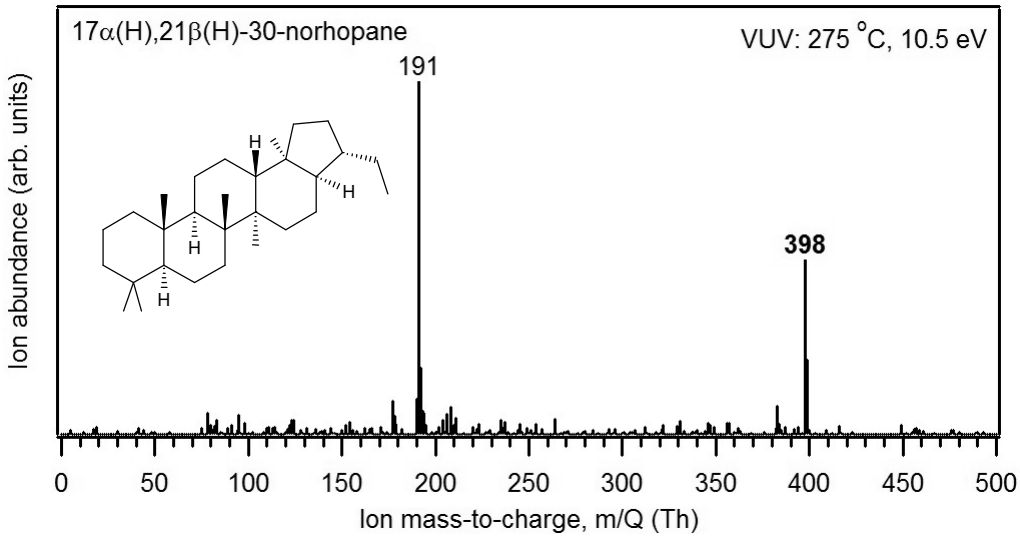


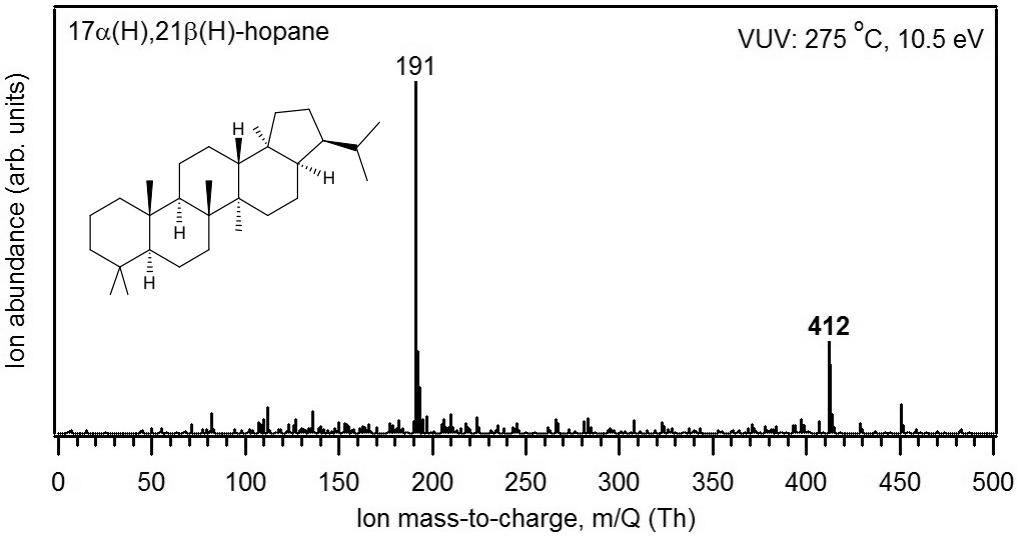

squalane
VUV: 275 °C, 10.5 eV
239
112
183
422
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

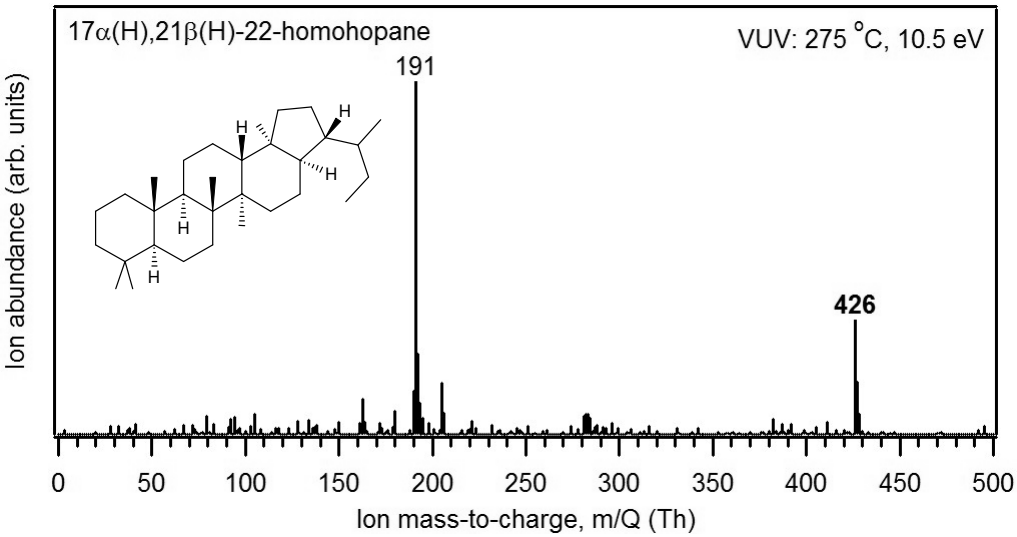

squalene
VUV: 275 °C, 10.5 eV
136
94
192
410
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

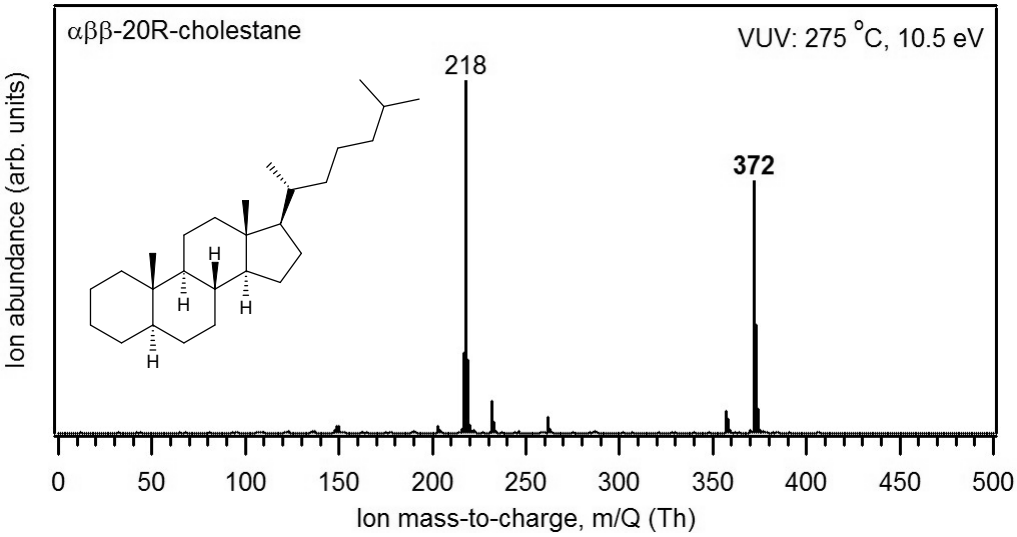
S.2.3. Hopanes and steranes

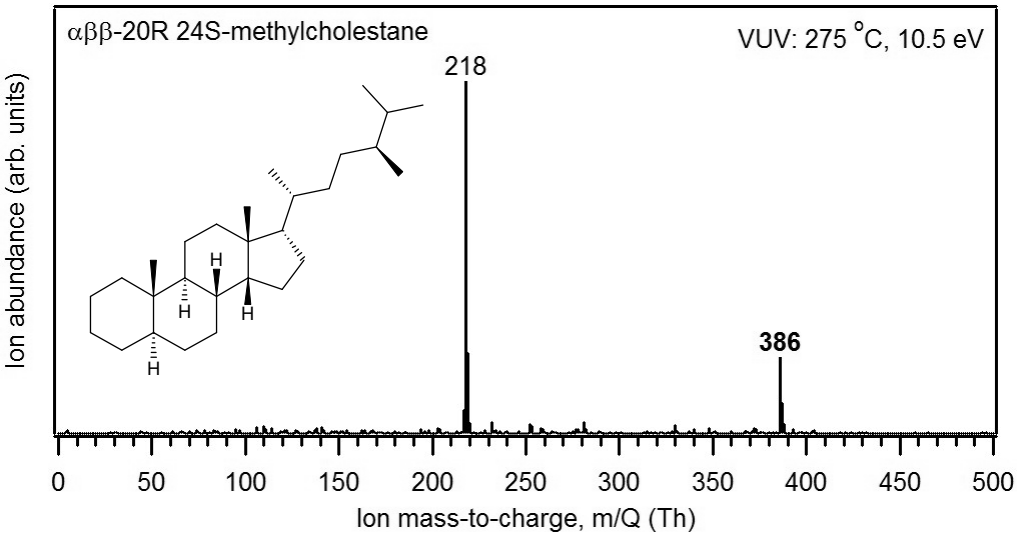


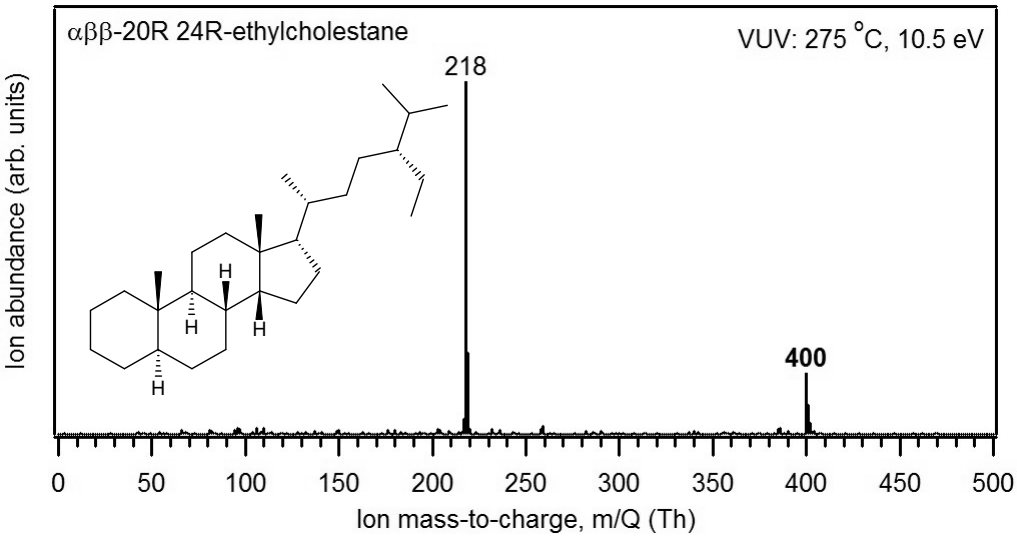



17α(H),21β(H)-hopane
VUV: 275 °C, 10.5 eV
191
412
Ion abundance (arb. units)
Ion mass-to-charge, m/Q (Th)

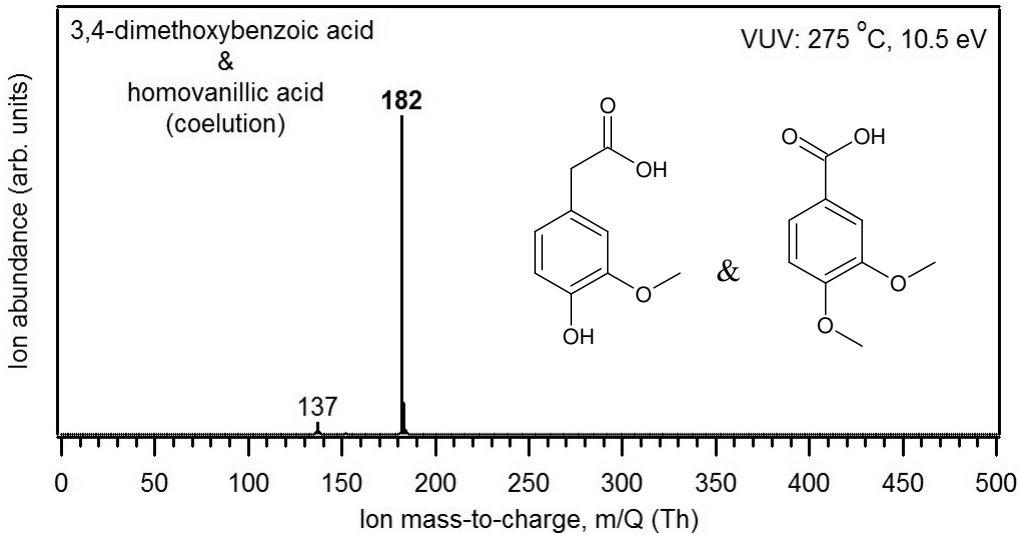

17α(H),21β(H)-22-homohopane
VUV: 275 °C, 10.5 eV
191
426
Ion abundance (arb. units)
Ion mass-to-charge, m/Q (Th)

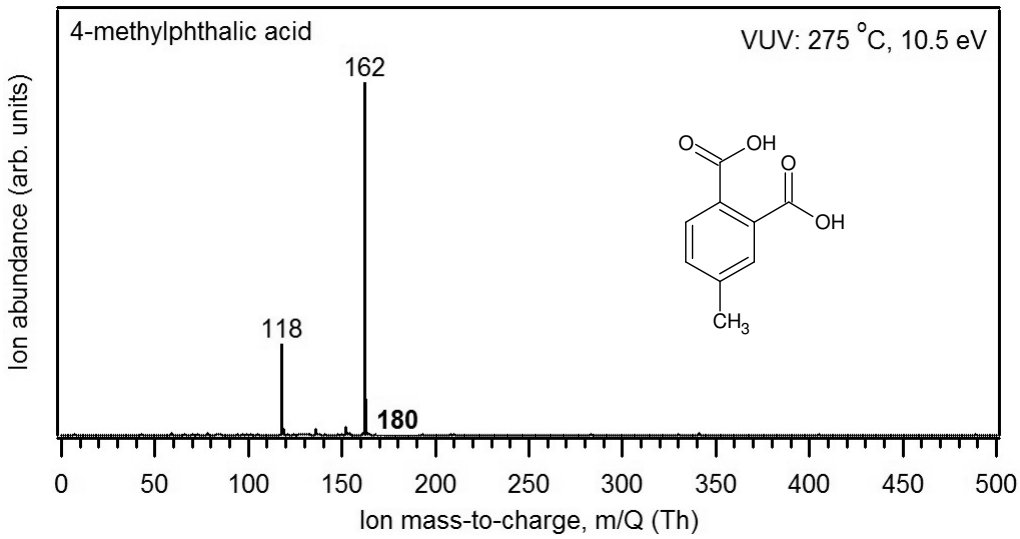

αββ-20R-cholestane
VUV: 275 °C, 10.5 eV
218
372
Ion abundance (arb. units)
Ion mass-to-charge, m/Q (Th)

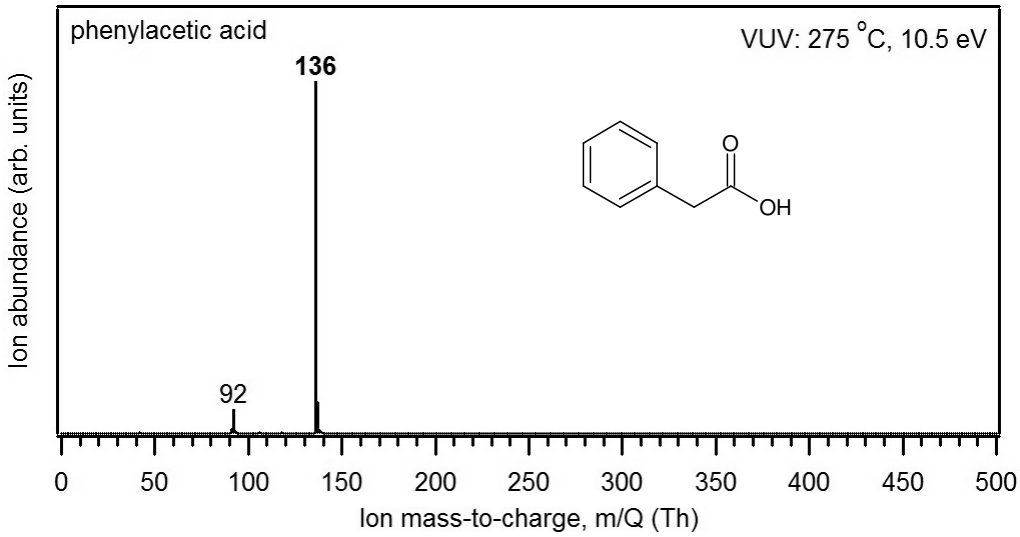

αββ-20R 24S-methylcholestane
VUV: 275 °C, 10.5 eV
218
386
H
H
H
H
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

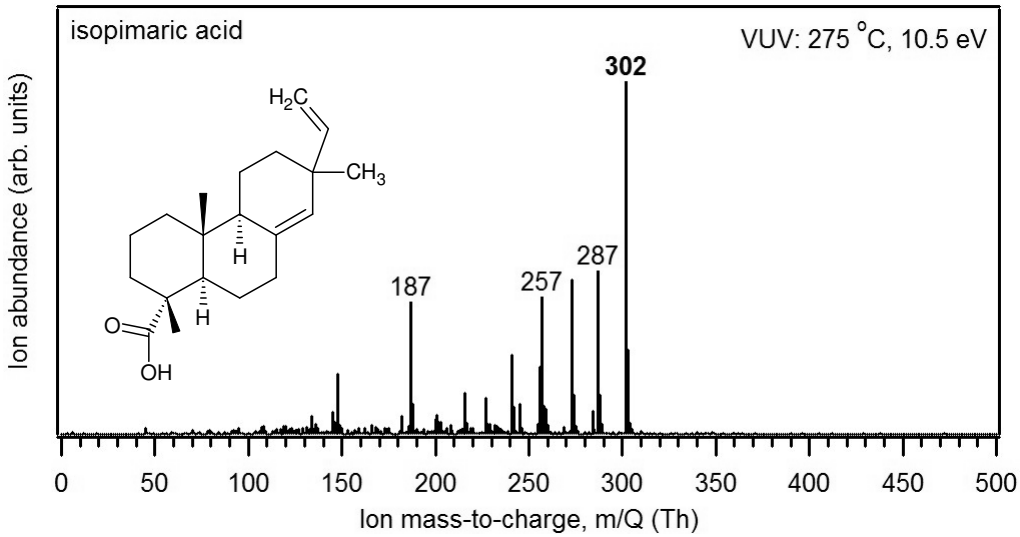

αββ-20R 24R-ethylcholestane
VUV: 275 °C, 10.5 eV
218
400
H
H
H
H
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

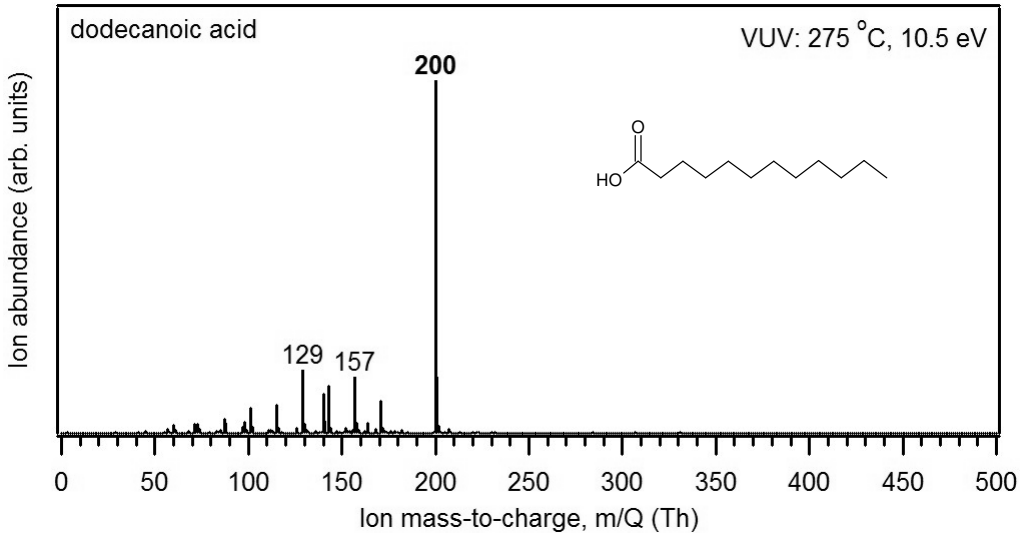
S.2.4. Acids

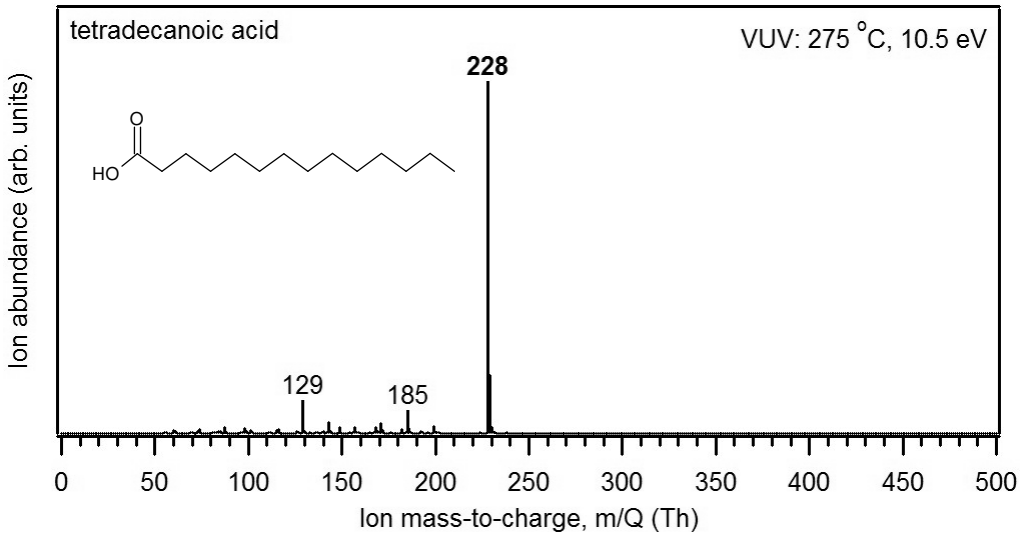

3,4-dimethoxybenzoic acid
&
homovanillic acid
(coelution)
VUV: 275 °C, 10.5 eV
182
137
&
Ion abundance (arb. units)
Ion mass-to-charge, m/Q (Th)

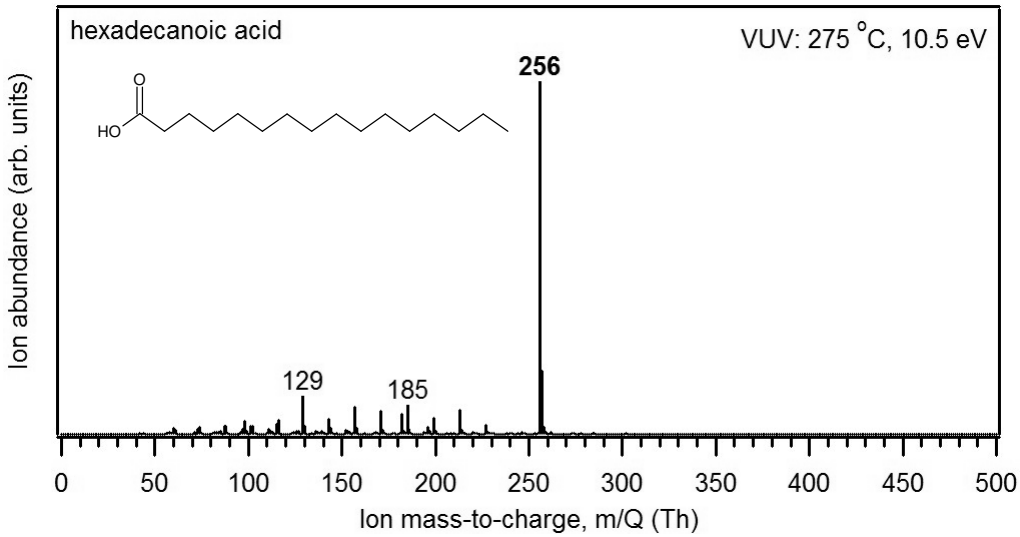

4-methylphthalic acid
VUV: 275 °C, 10.5 eV
162
118
180
Ion abundance (arb. units)
Ion mass-to-charge, m/Q (Th)

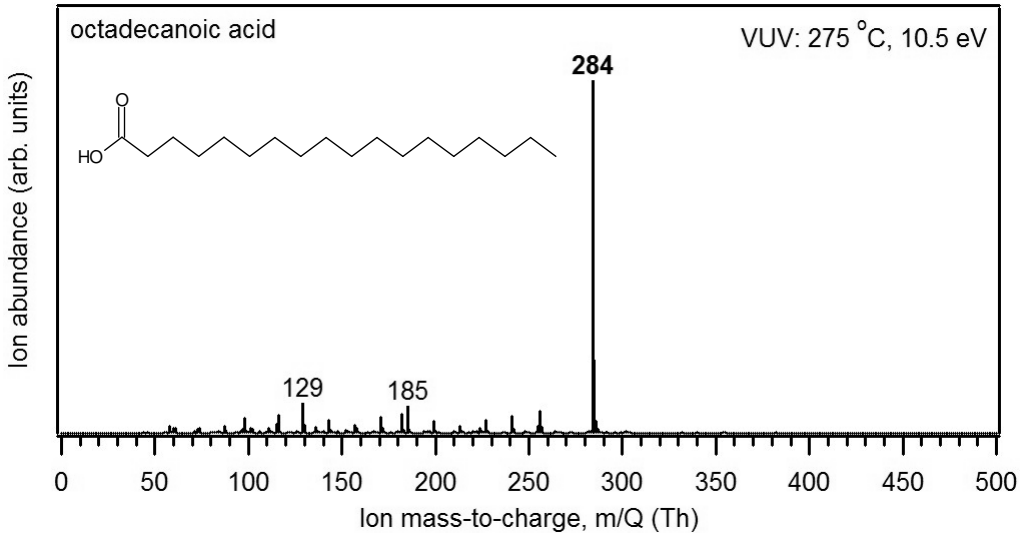

phenylacetic acid
VUV: 275 °C, 10.5 eV
136
92
O
OH
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

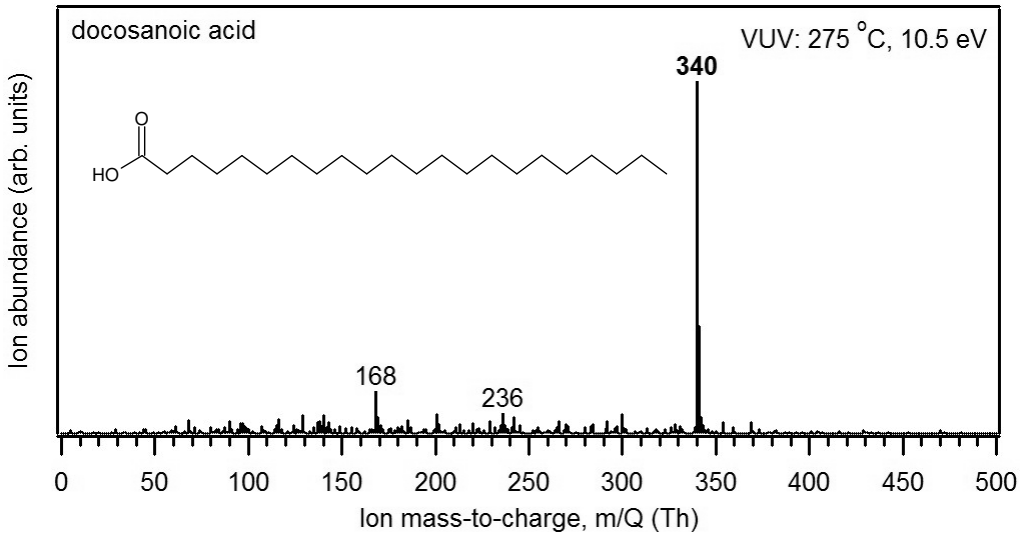

isopimaric acid
VUV: 275 °C, 10.5 eV
302
287
257
187
H2C
CH3
H
H
O
OH
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

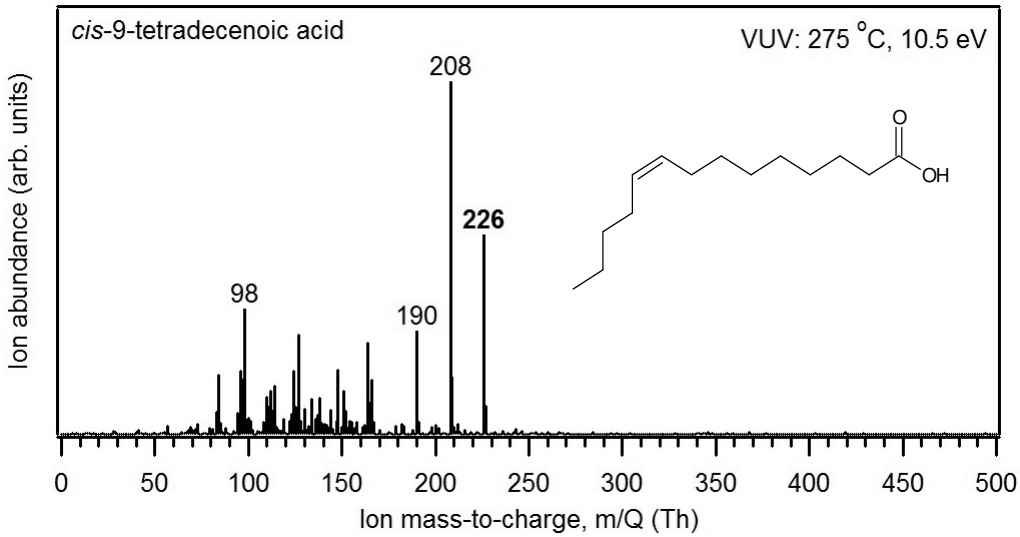

dodecanoic acid
VUV: 275 °C, 10.5 eV
200
129
157
O
HO
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

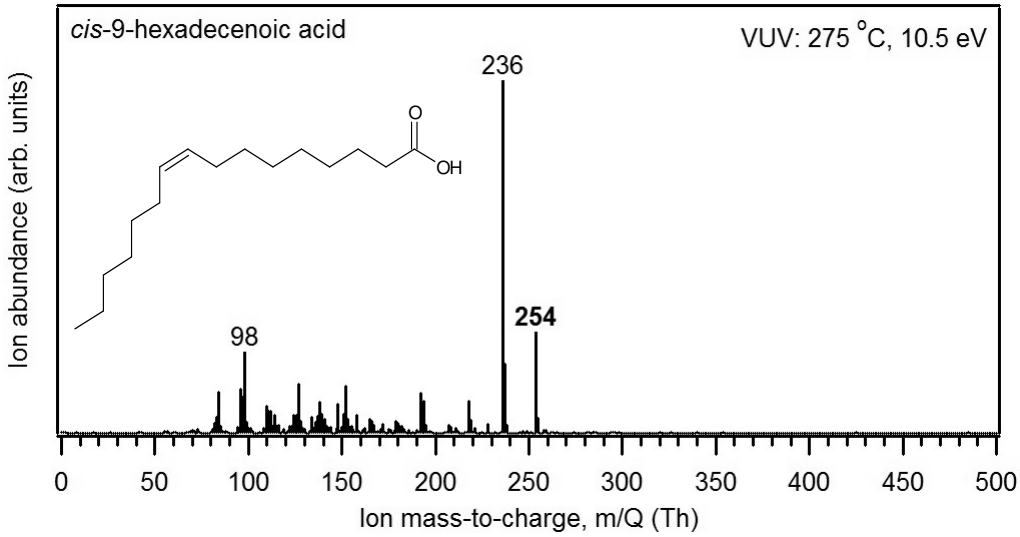

tetradecanoic acid
VUV: 275 °C, 10.5 eV
228
129
185
HO
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

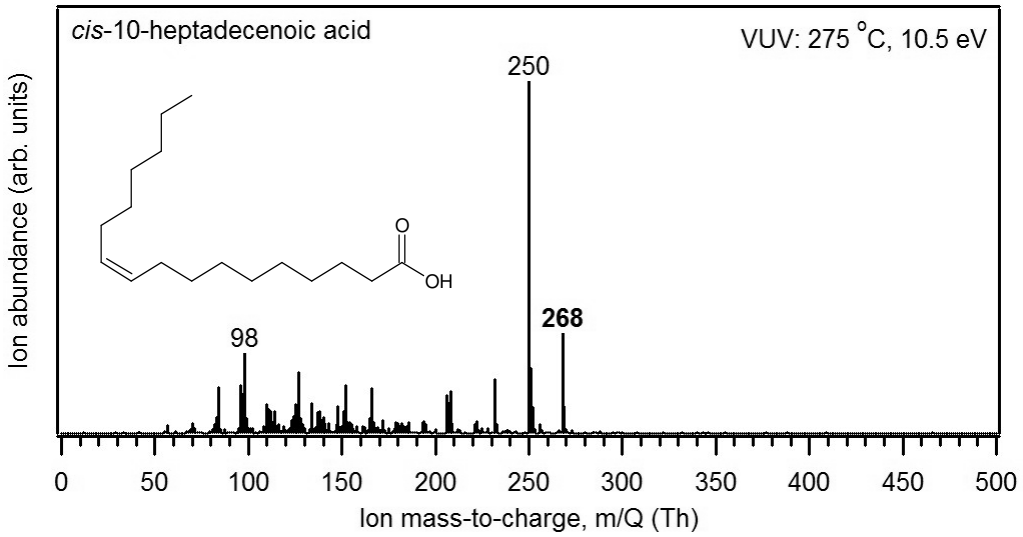

hexadecanoic acid
VUV: 275 °C, 10.5 eV
256
129
185
HO
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

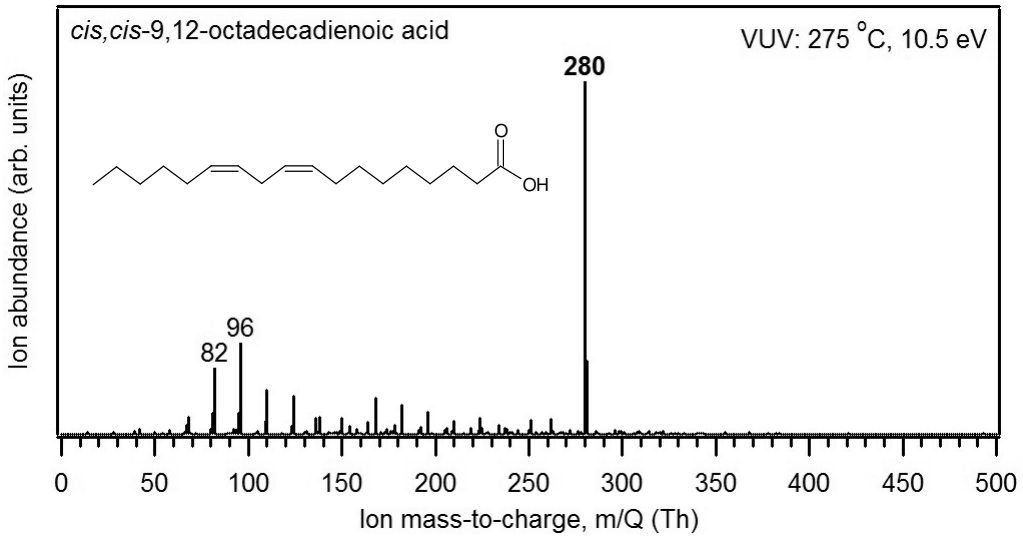

octadecanoic acid
VUV: 275 °C, 10.5 eV
284
129
185
HO
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

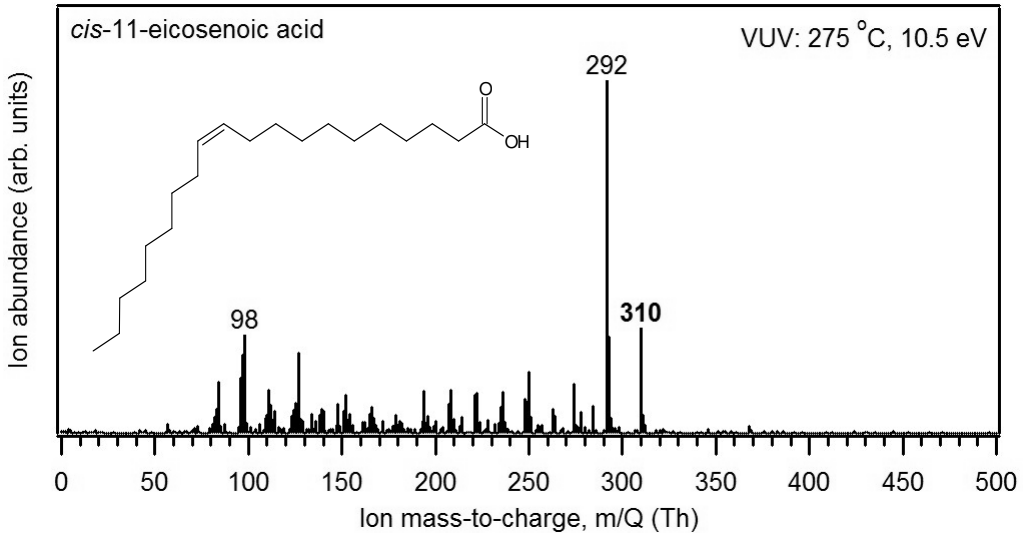

docosanoic acid
VUV: 275 °C, 10.5 eV
340
168
236
HO
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

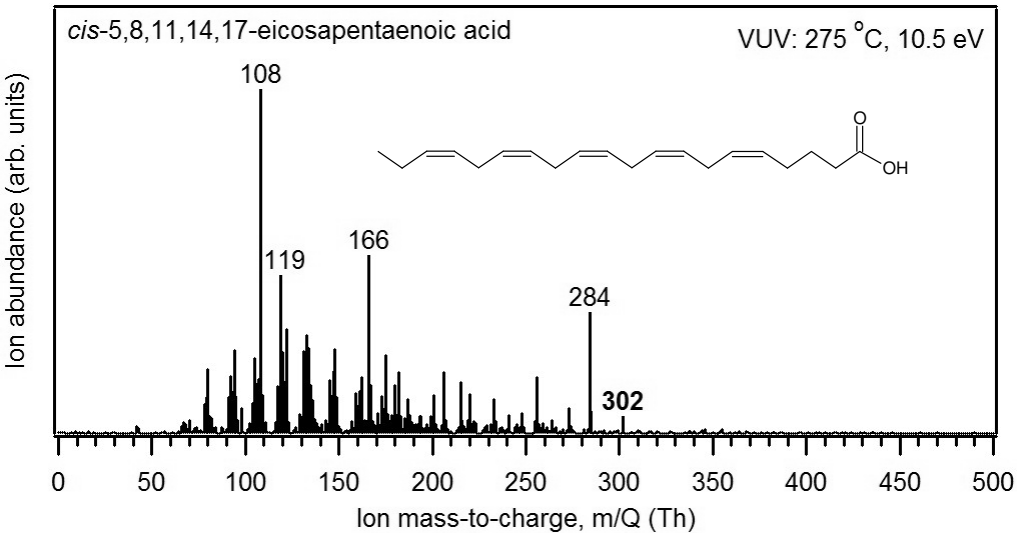

cis-9-tetradecenoic acid
VUV: 275 °C, 10.5 eV
208
226
98
190
O
OH
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)


cis-9-hexadecenoic acid
VUV: 275 °C, 10.5 eV
236
254
98
O
OH
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

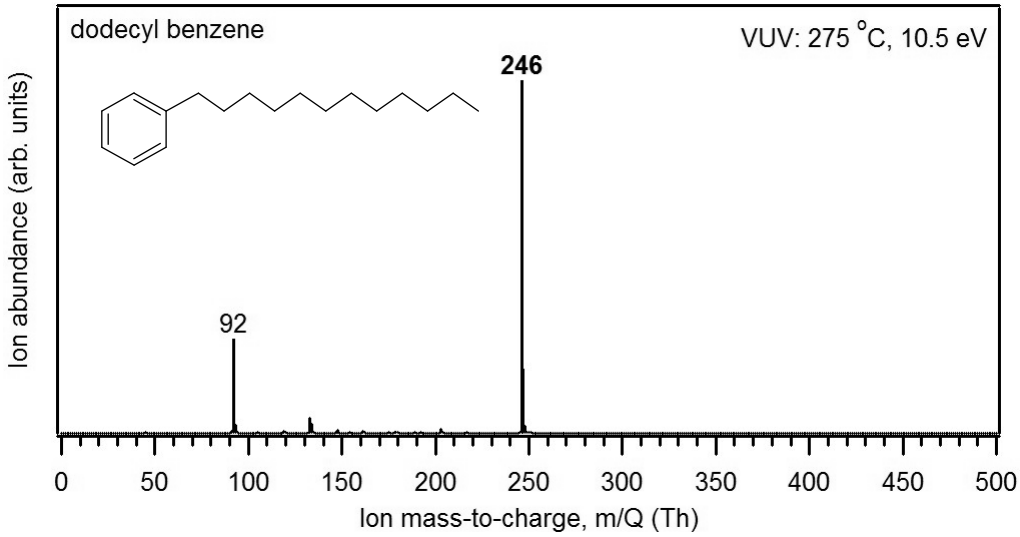

cis-10-heptadecenoic acid
VUV: 275 °C, 10.5 eV
250
268
98
O
OH
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

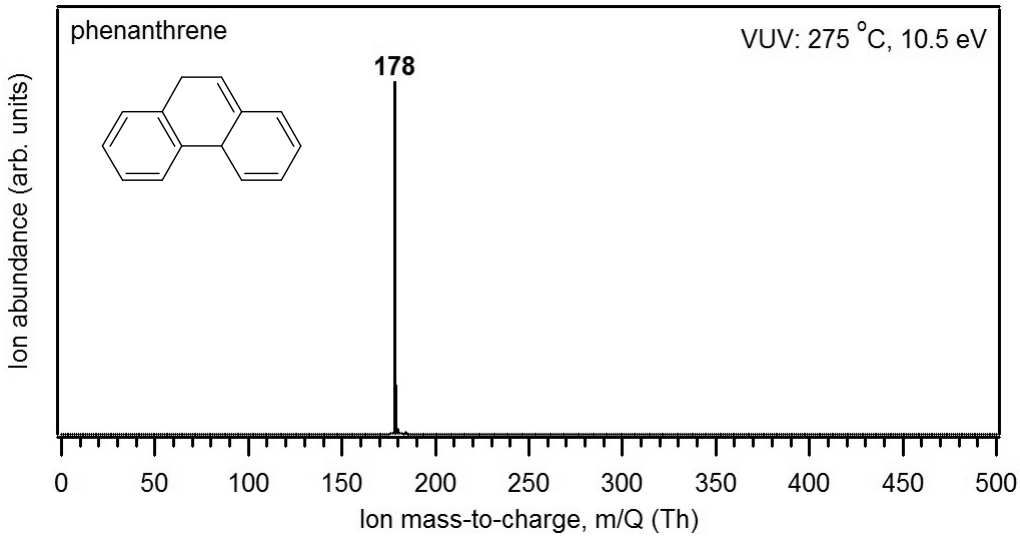

cis,cis-9,12-octadecadienoic acid
VUV: 275 °C, 10.5 eV
280
96
82
O
OH
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

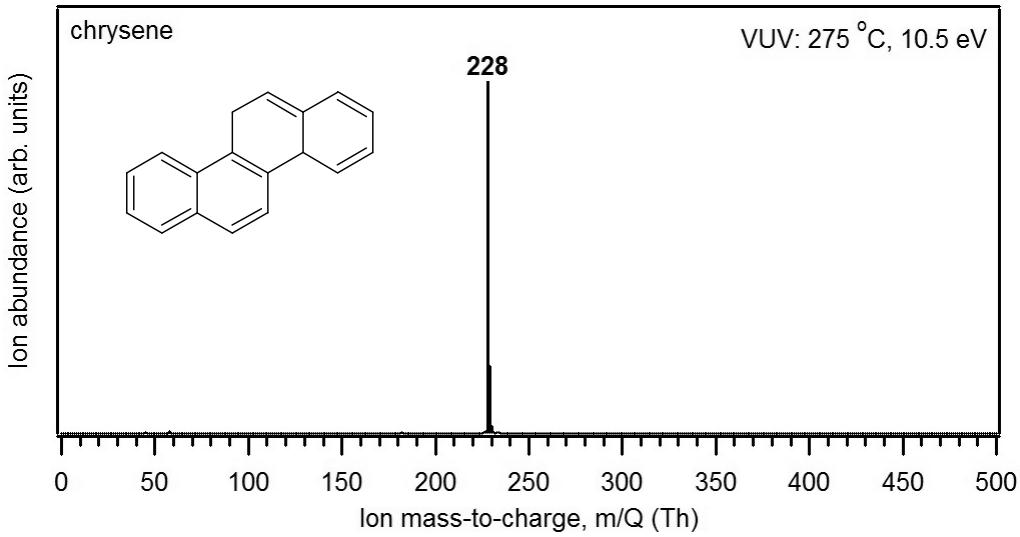

cis-11-eicosenoic acid
VUV: 275 °C, 10.5 eV
292
310
98
O
OH
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

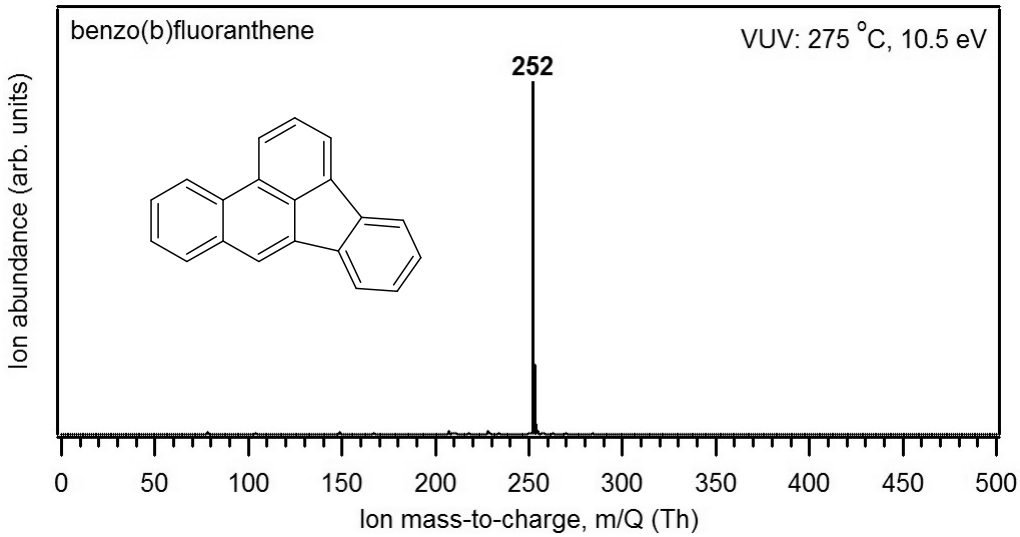

cis-5,8,11,14,17-eicosapentaenoic acid
VUV: 275 °C, 10.5 eV
108
119
166
284
302
O
OH
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

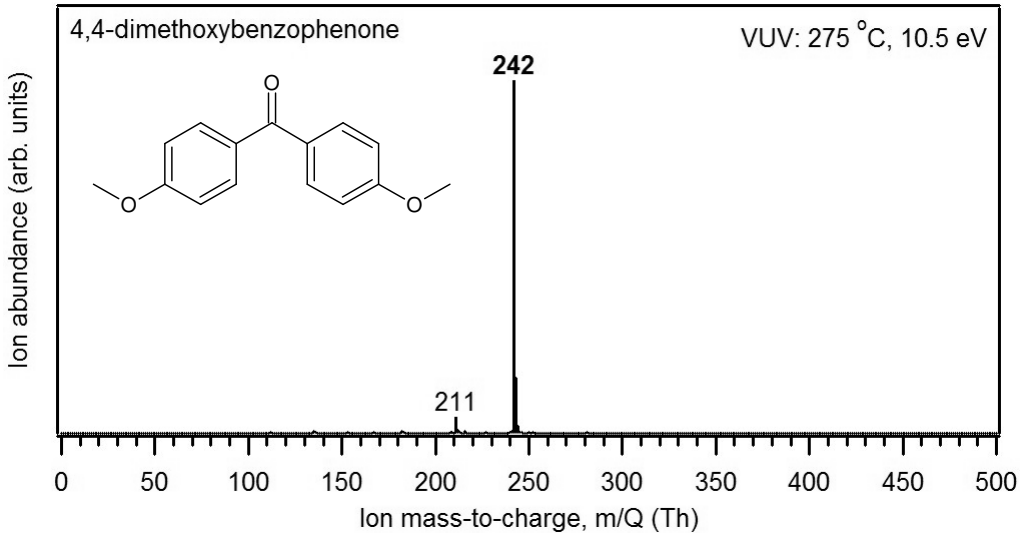
S.2.5. Aromatics and oxygenated polycyclic aromatic hydrocarbons

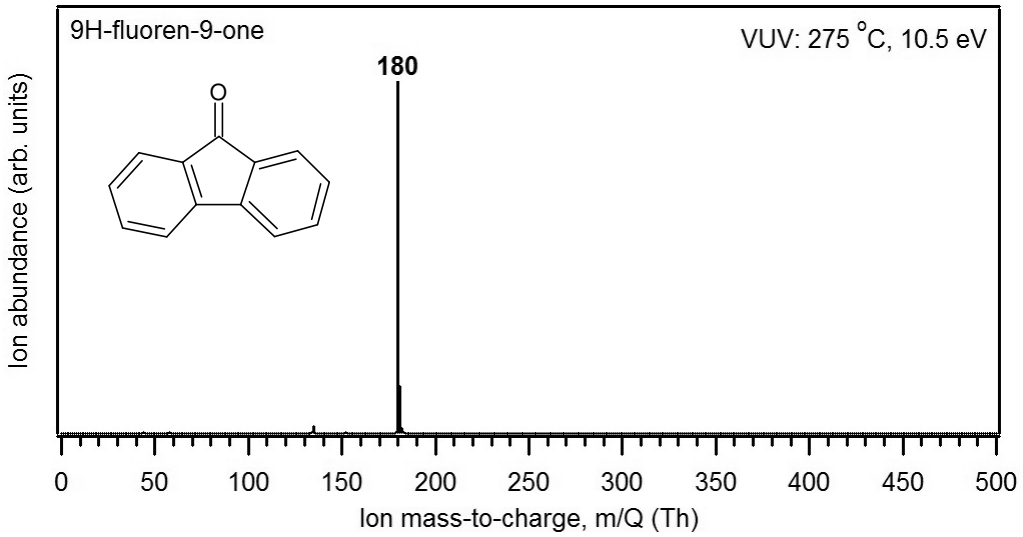


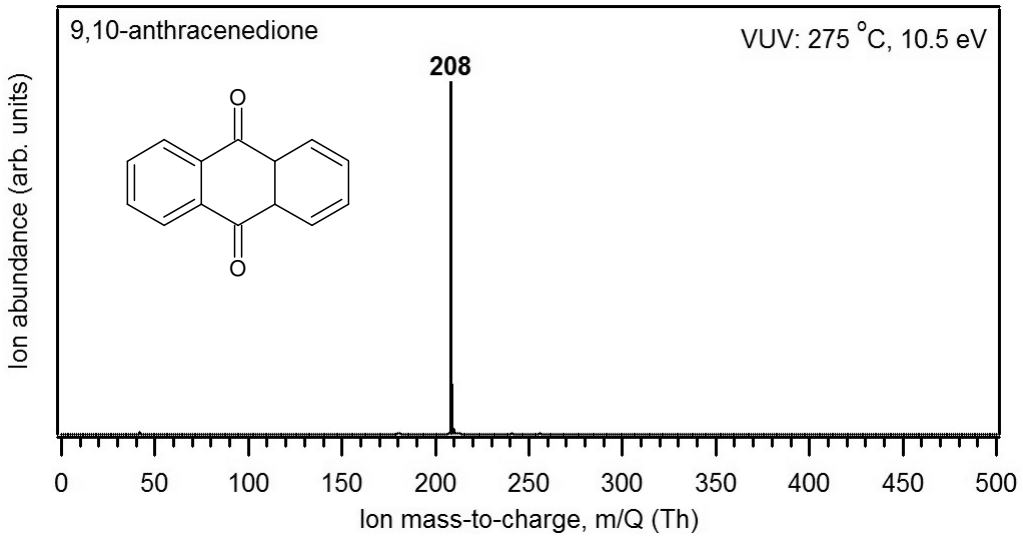


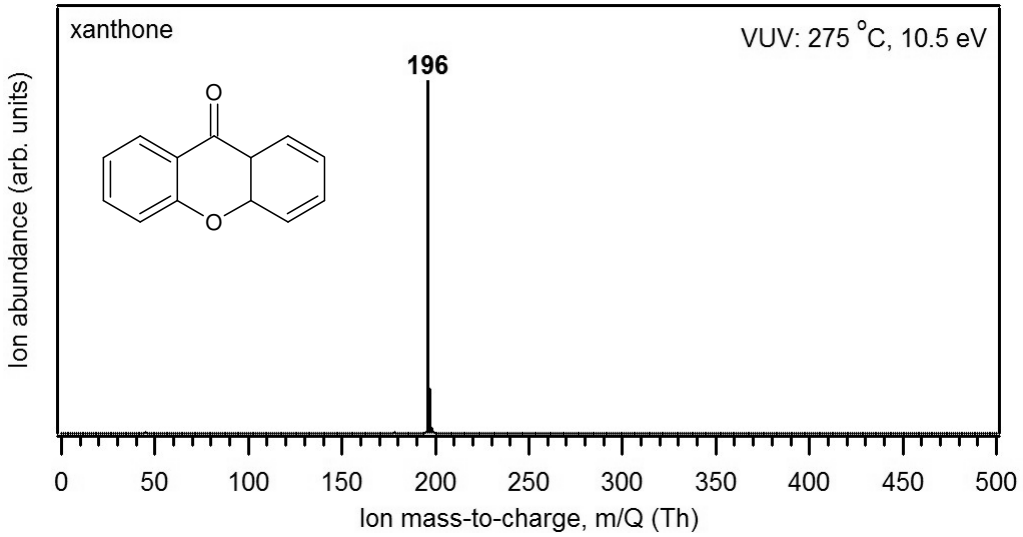

chrysene
VUV: 275 °C, 10.5 eV
228
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)


benzo(b)fluoranthene
VUV: 275 °C, 10.5 eV
252
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

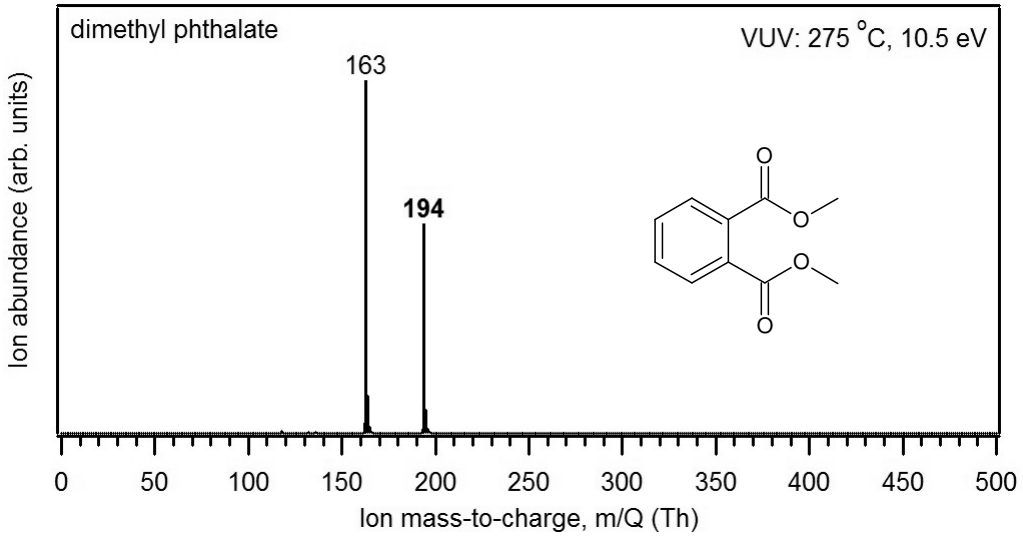

4,4-dimethoxybenzophenone
VUV: 275 °C, 10.5 eV
242
211
O
O
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

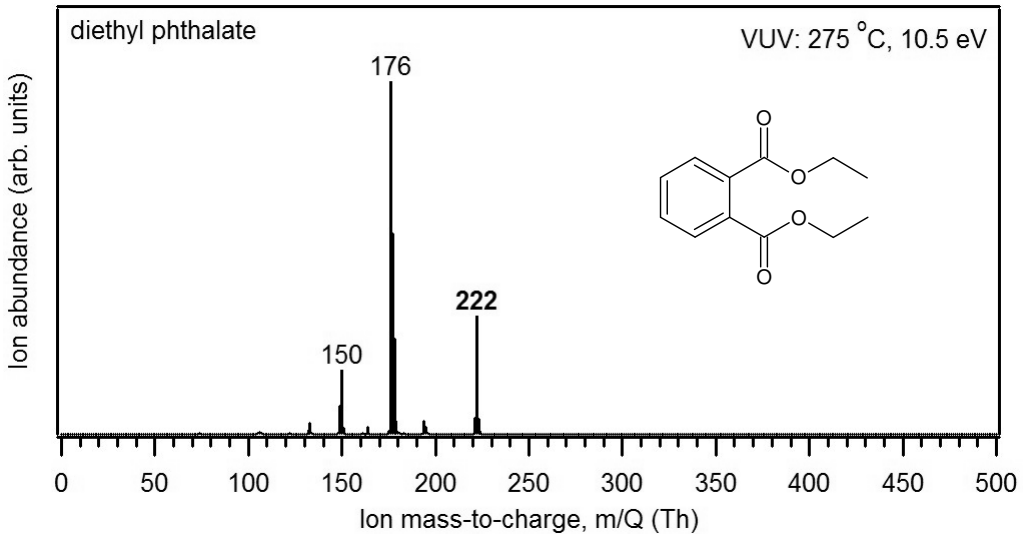

9H-fluoren-9-one
VUV: 275 °C, 10.5 eV
180
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

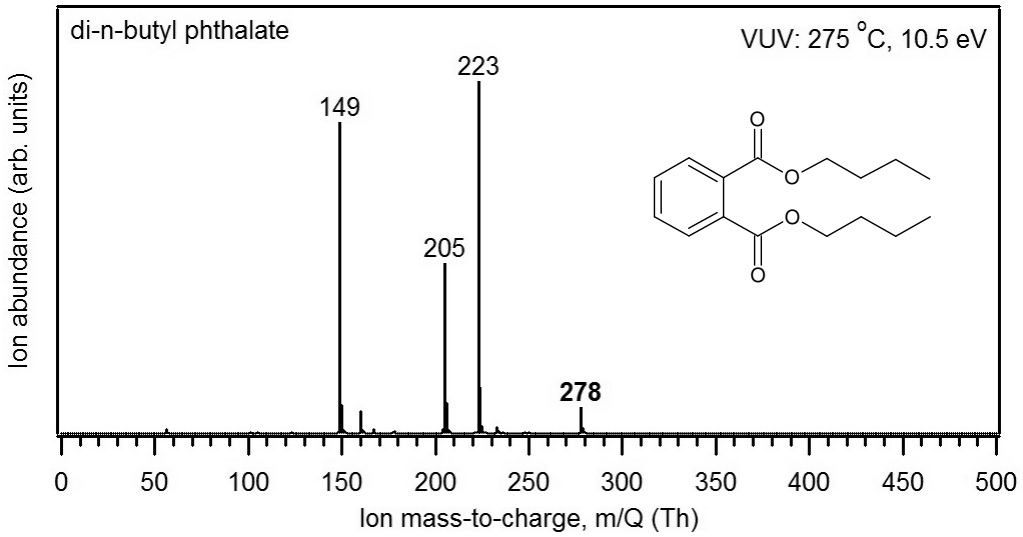

9,10-anthracenedione
VUV: 275 °C, 10.5 eV
208
O
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

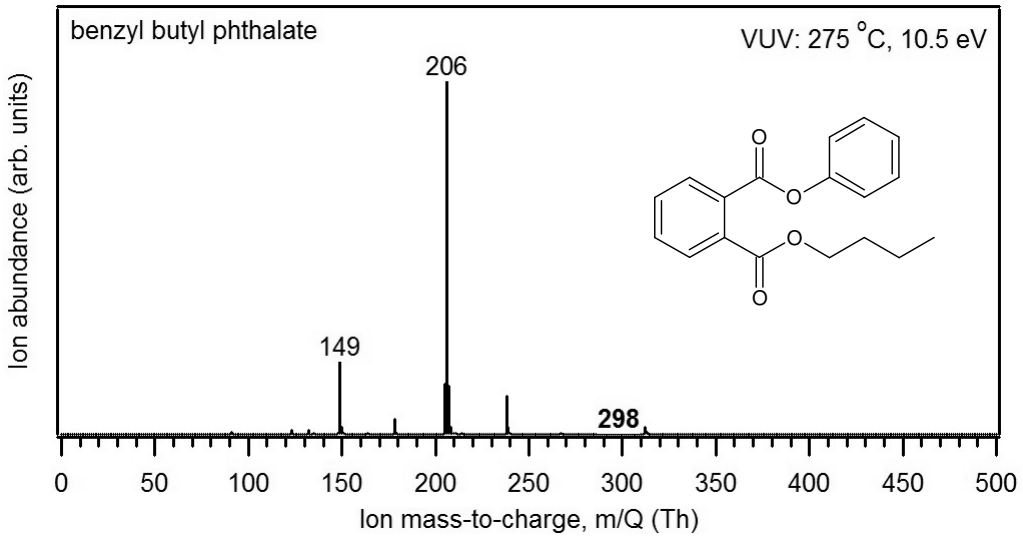

xanthone
VUV: 275 °C, 10.5 eV
196
O
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

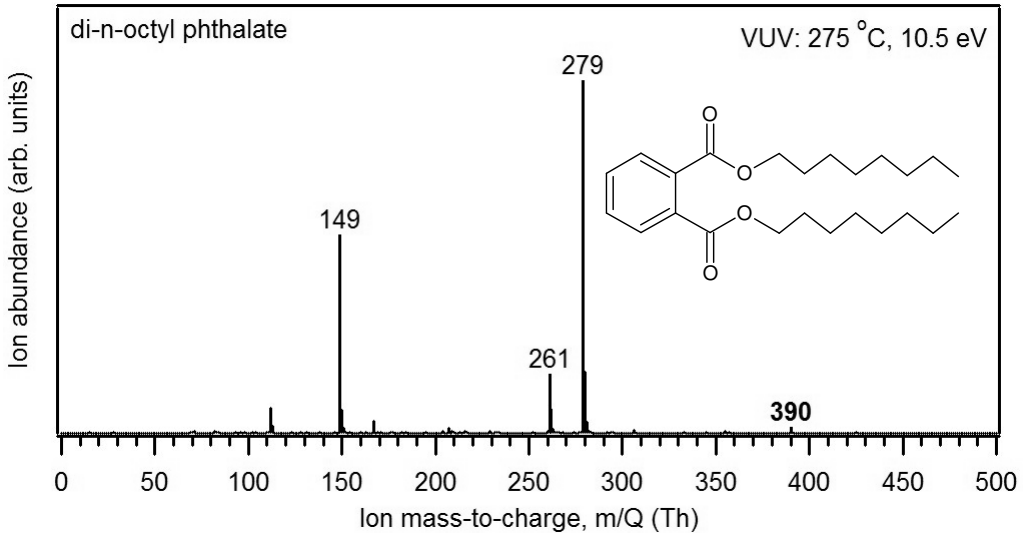
S.2.6. Phthalates and other oxygenated aromatics

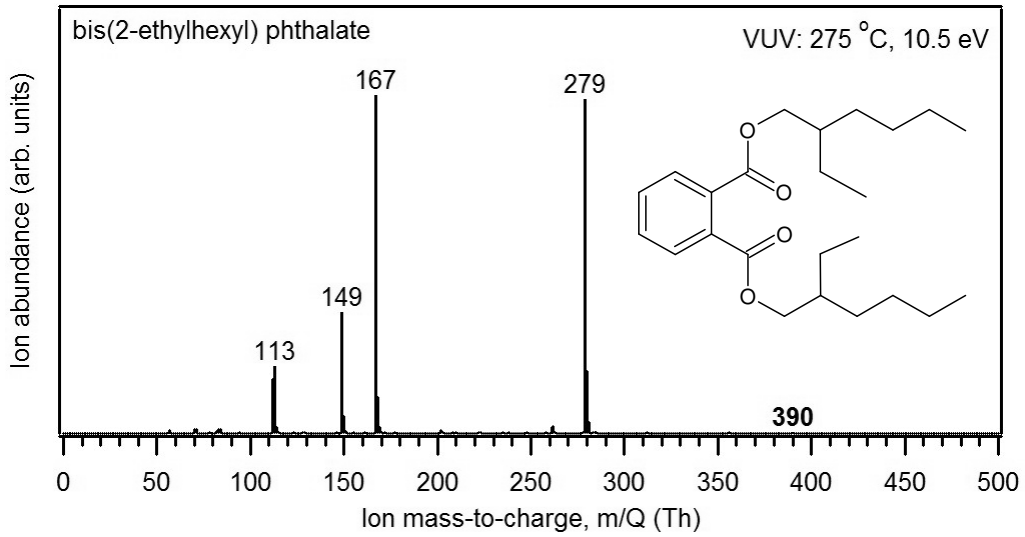


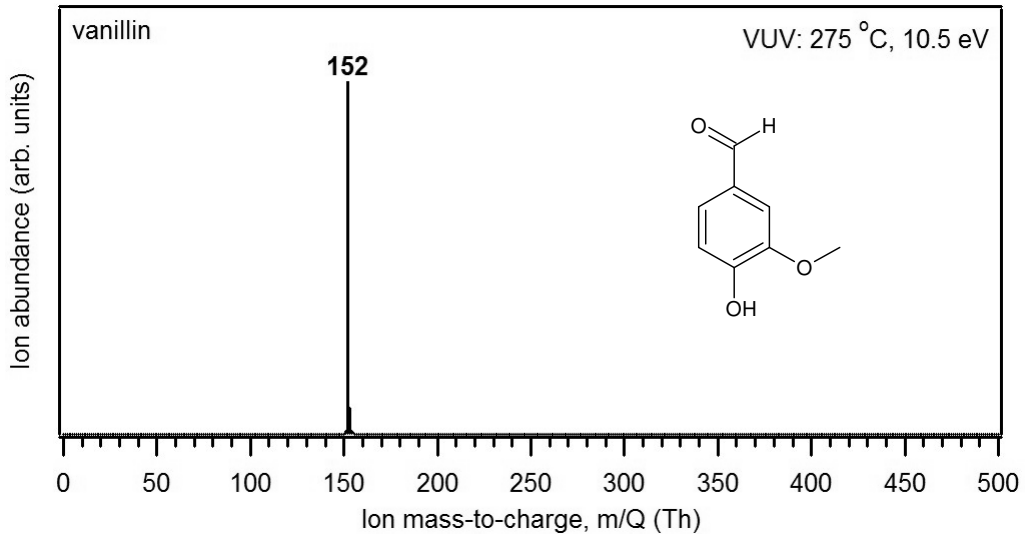


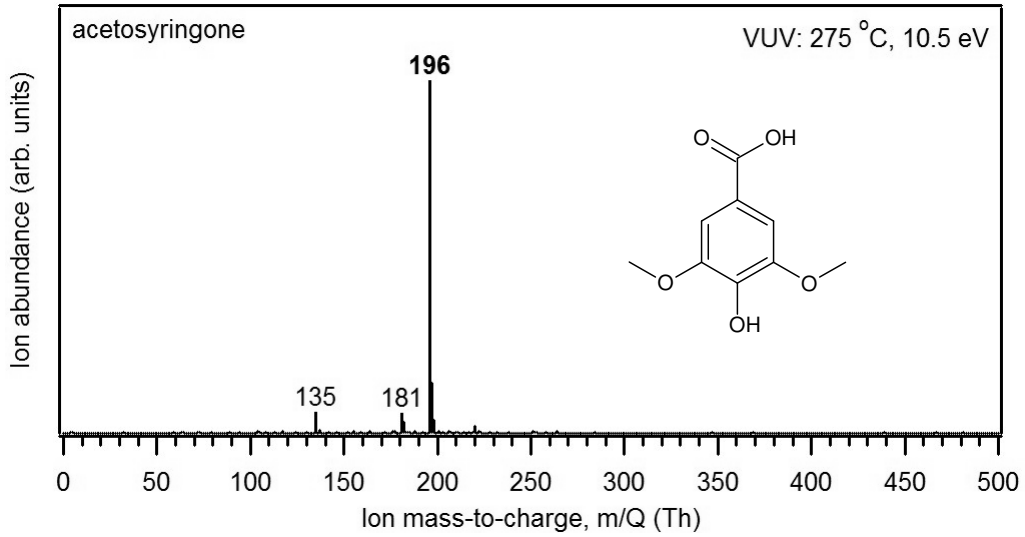

di-n-butyl phthalate
VUV: 275 °C, 10.5 eV
223
149
205
278
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)


benzyl butyl phthalate
VUV: 275 °C, 10.5 eV
206
149
298
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

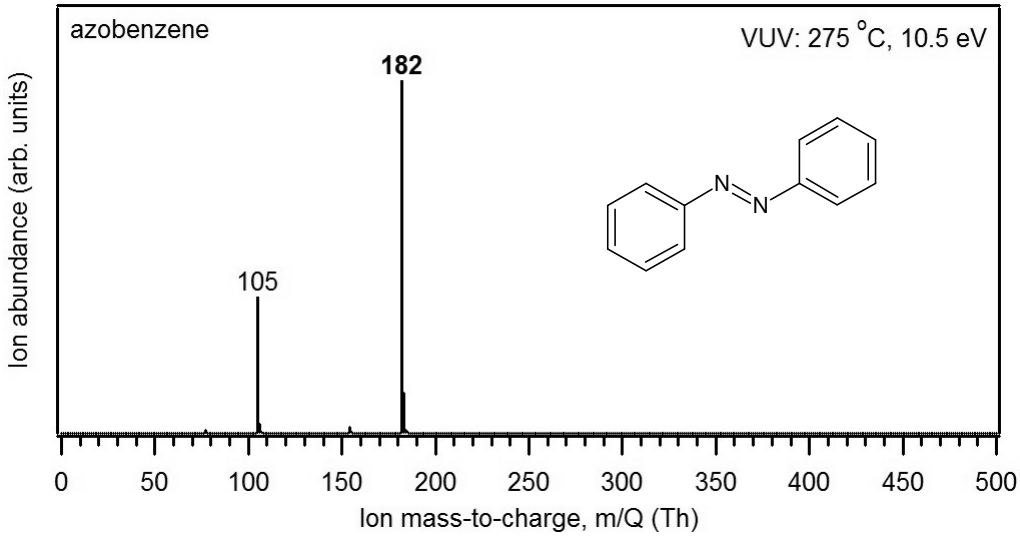

di-n-octyl phthalate
VUV: 275 °C, 10.5 eV
279
149
261
390
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

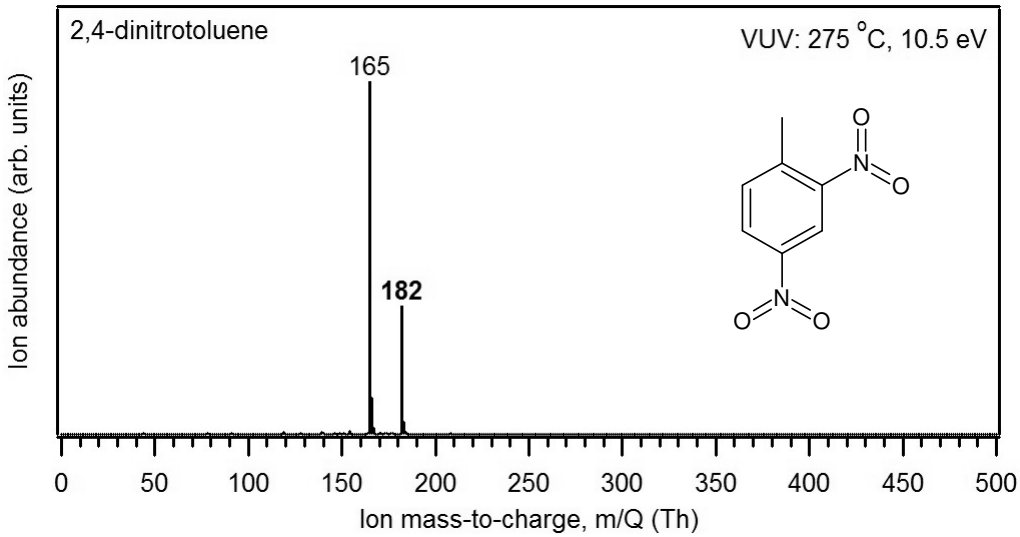

bis(2-ethylhexyl) phthalate
VUV: 275 °C, 10.5 eV
167
279
149
113
390
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

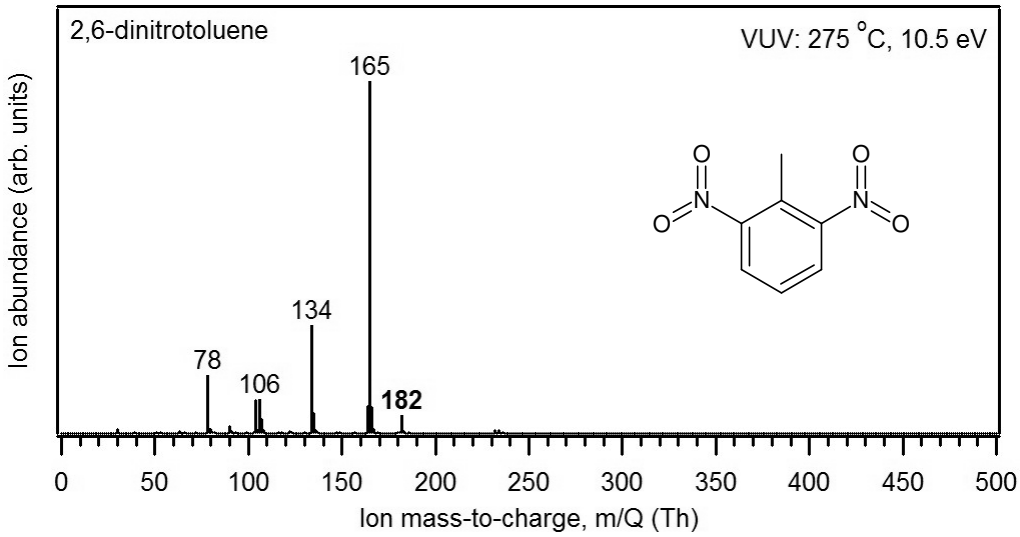

vanillin
VUV: 275 °C, 10.5 eV
152
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

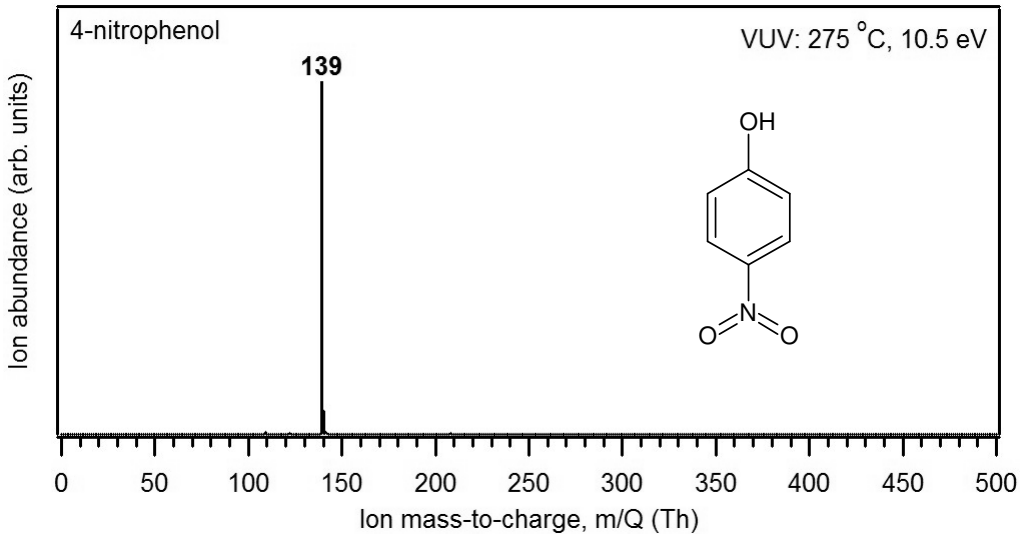

acetosyringone
VUV: 275 °C, 10.5 eV
196
135
181
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

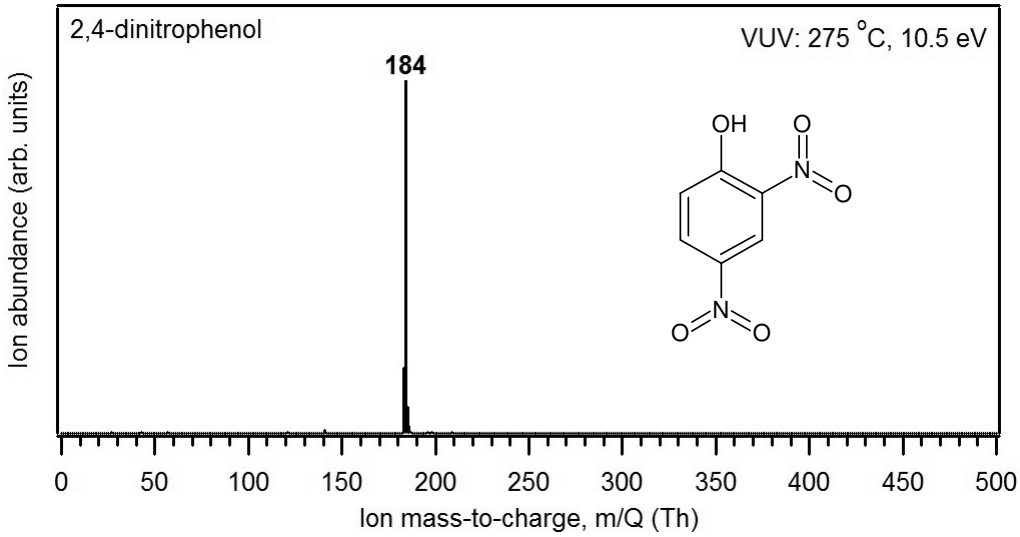
S.2.7. Nitrogenated aromatics

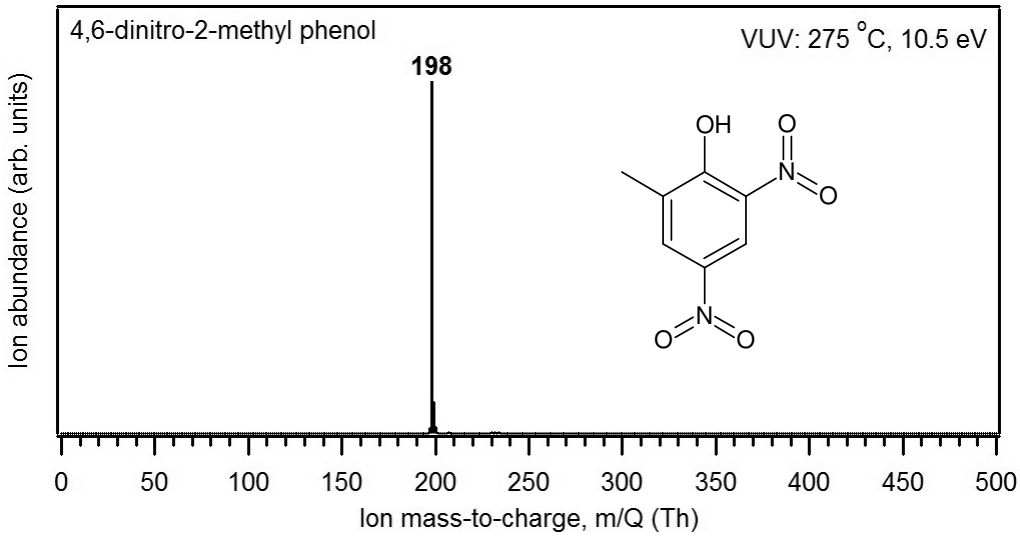




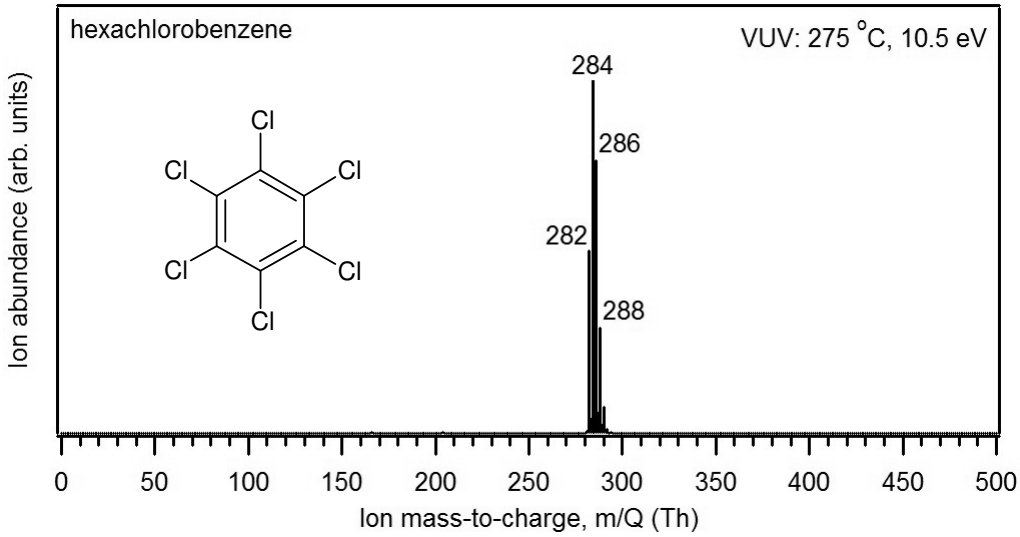

2,6-dinitrotoluene
VUV: 275 °C, 10.5 eV
165
134
78
106
182
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

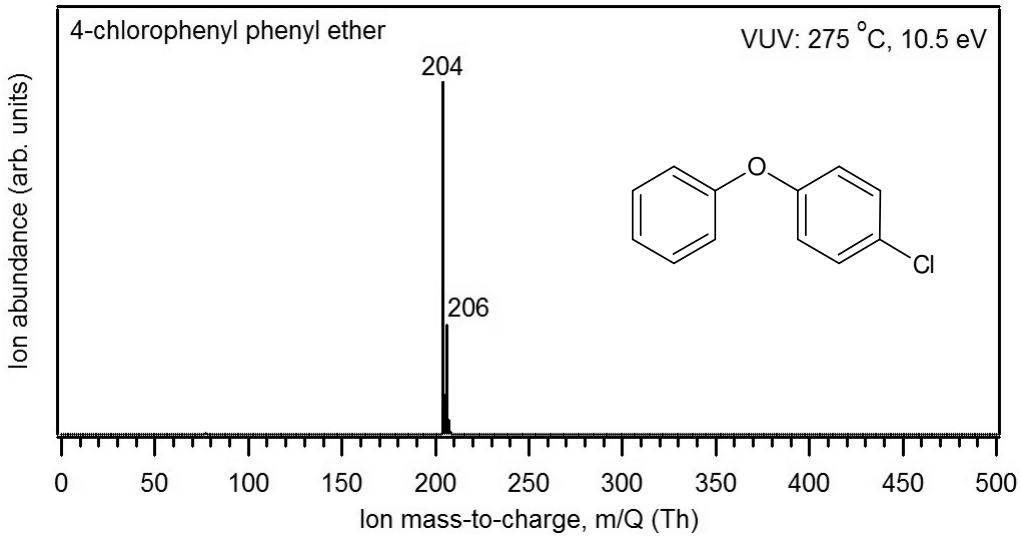

4-nitrophenol
VUV: 275 °C, 10.5 eV
139
OH
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

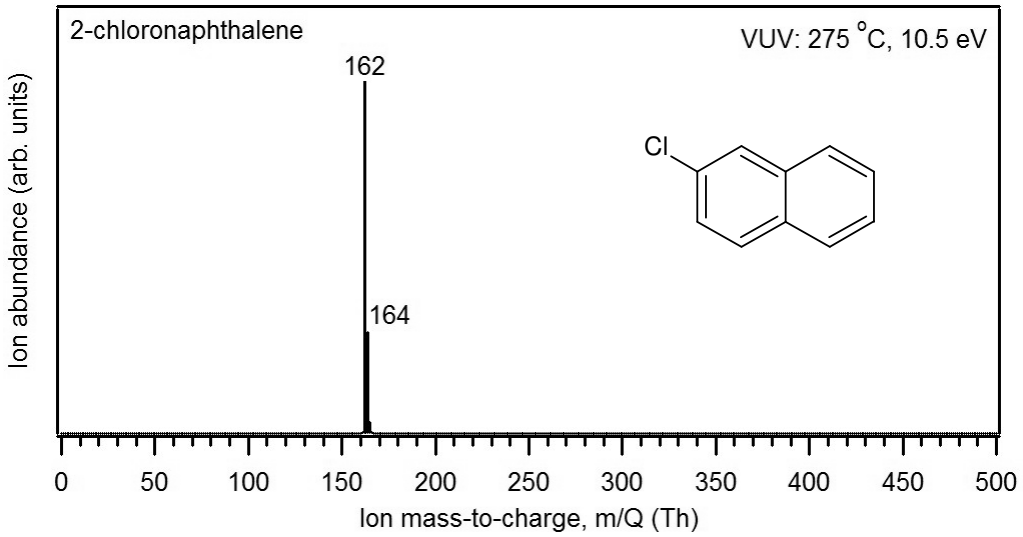

2,4-dinitrophenol
VUV: 275 °C, 10.5 eV
184
OH
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

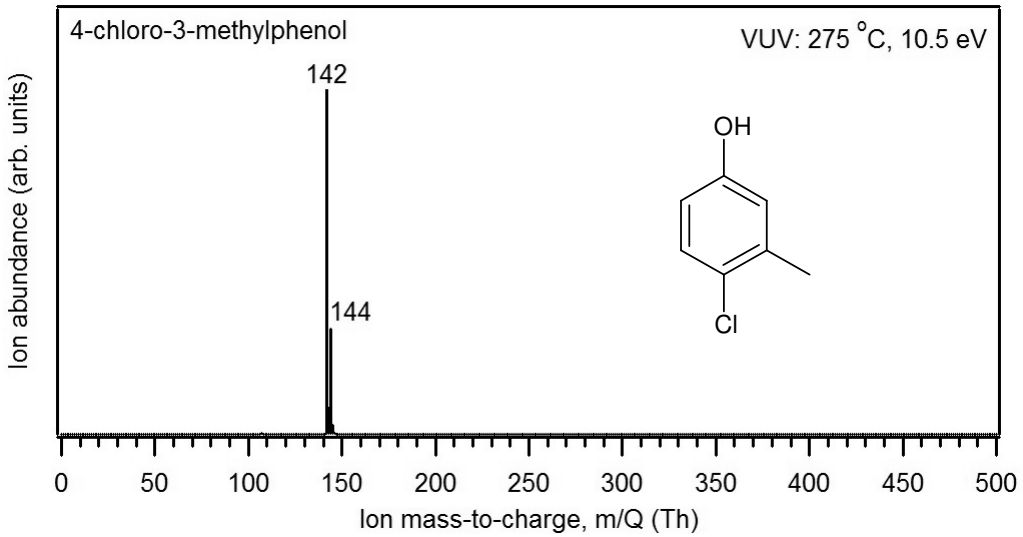

4,6-dinitro-2-methyl phenol
VUV: 275 °C, 10.5 eV
198
OH
O
N
O
N
O
O
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

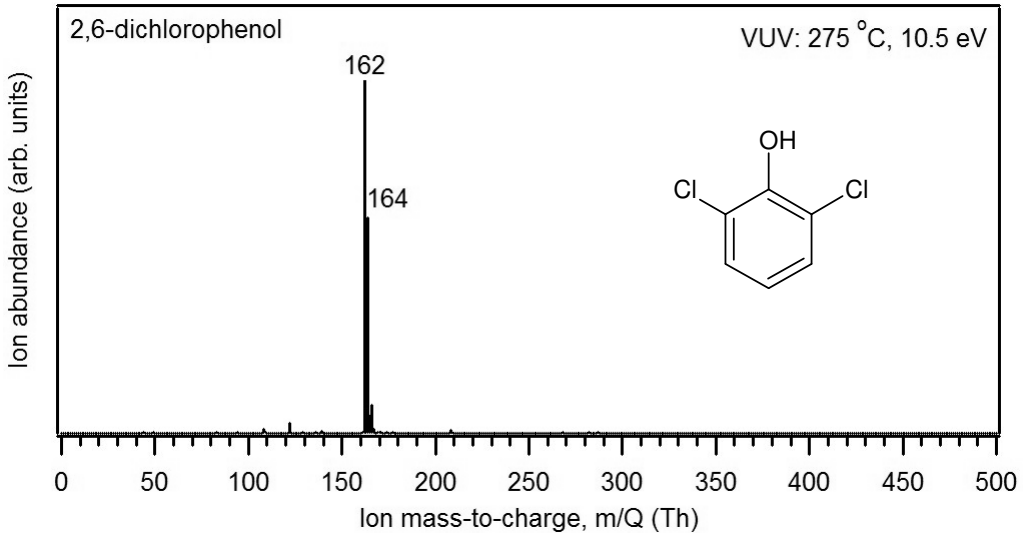
S.2.8. Chlorinated aromatics

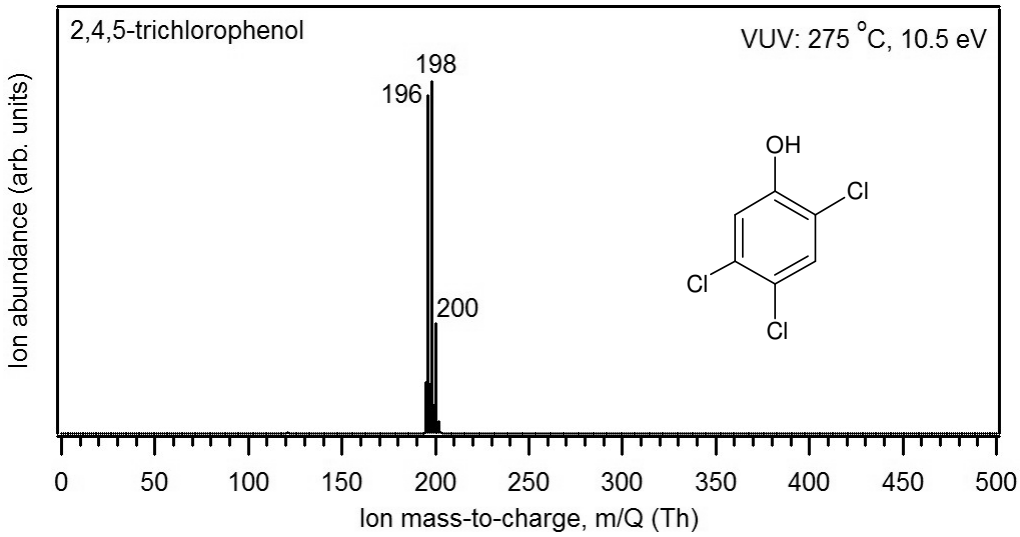


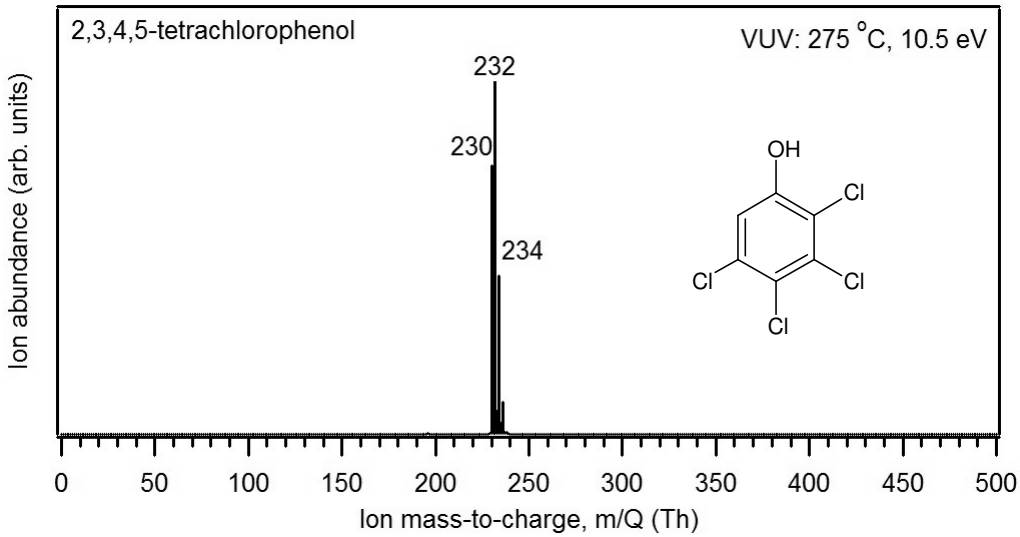


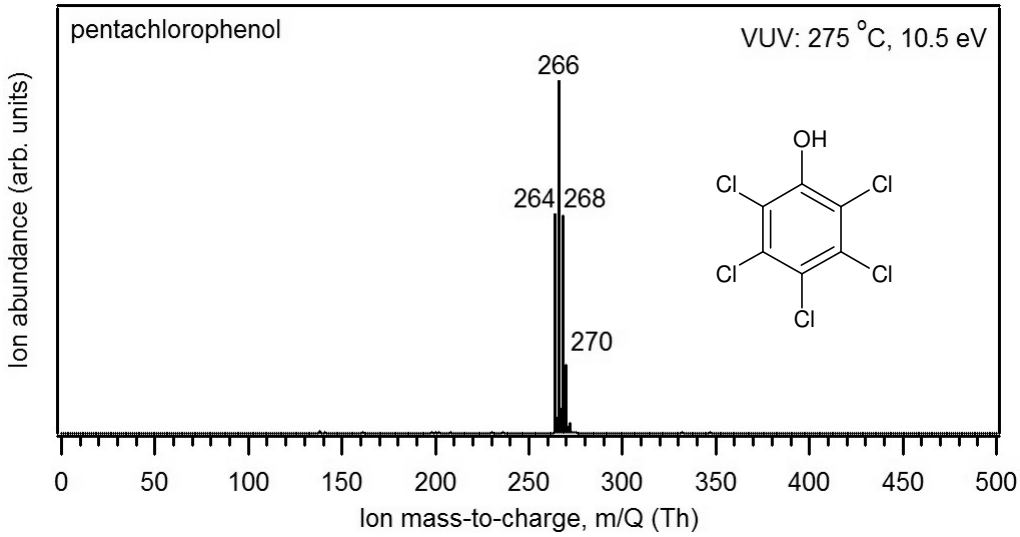

2-chloronaphthalene
VUV: 275 °C, 10.5 eV
162
164
Cl
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)


4-chloro-3-methylphenol
VUV: 275 °C, 10.5 eV
142
144
OH
Cl
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

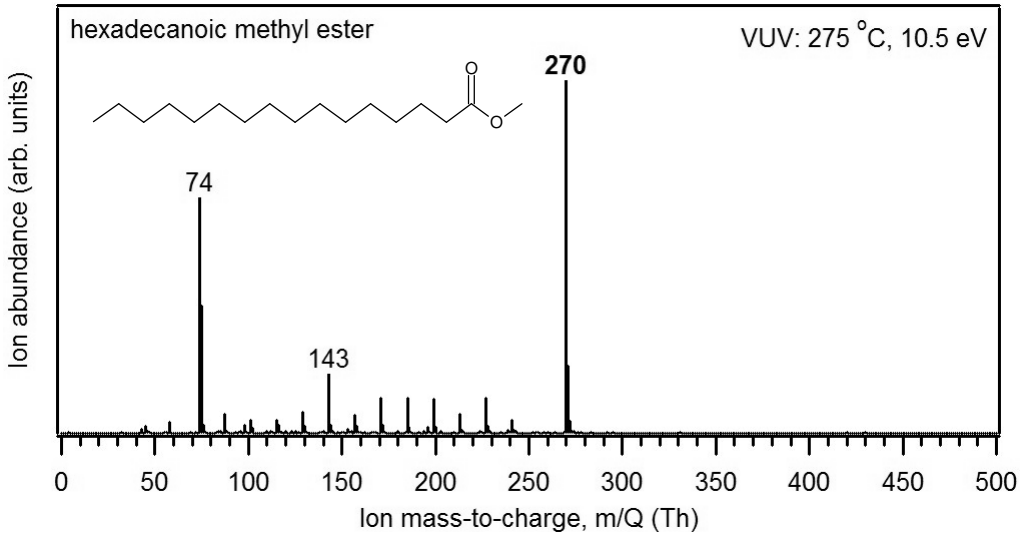

2,6-dichlorophenol
VUV: 275 °C, 10.5 eV
162
164
OH
Cl
Cl
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

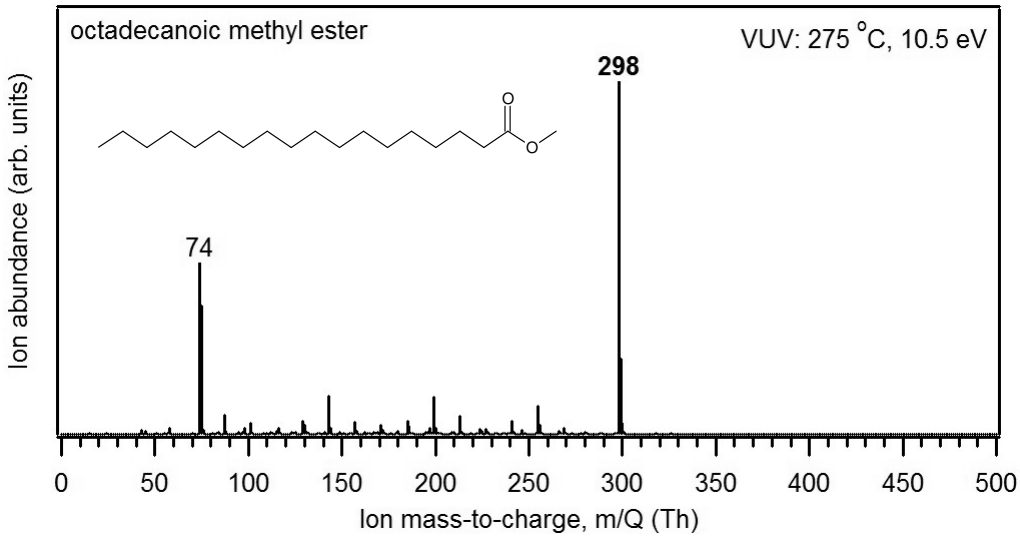

2,4,5-trichlorophenol
VUV: 275 °C, 10.5 eV
198
196
200
OH
Cl
Cl
Cl
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

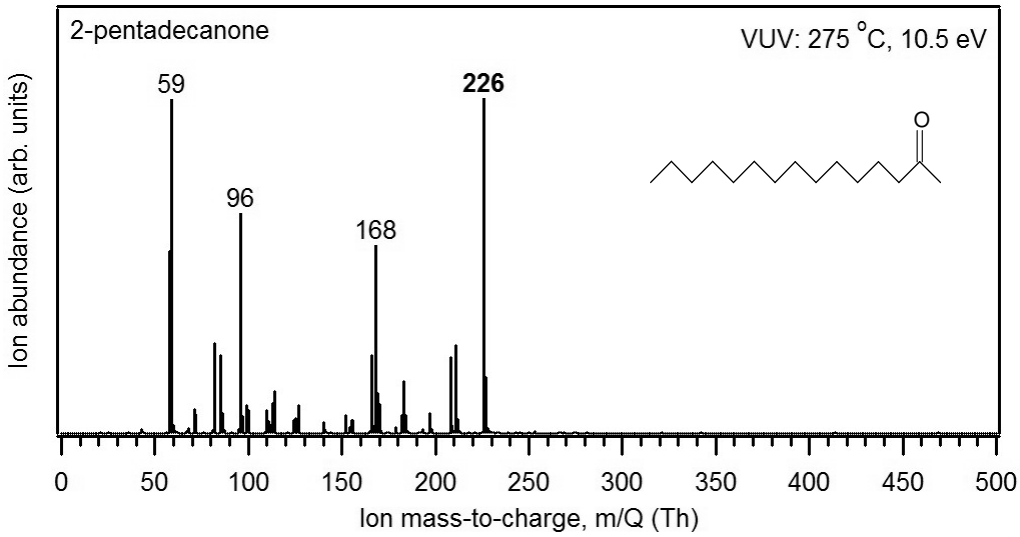

2,3,4,5-tetrachlorophenol
VUV: 275 °C, 10.5 eV
232
230
234
OH
Cl
Cl
Cl
Cl
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

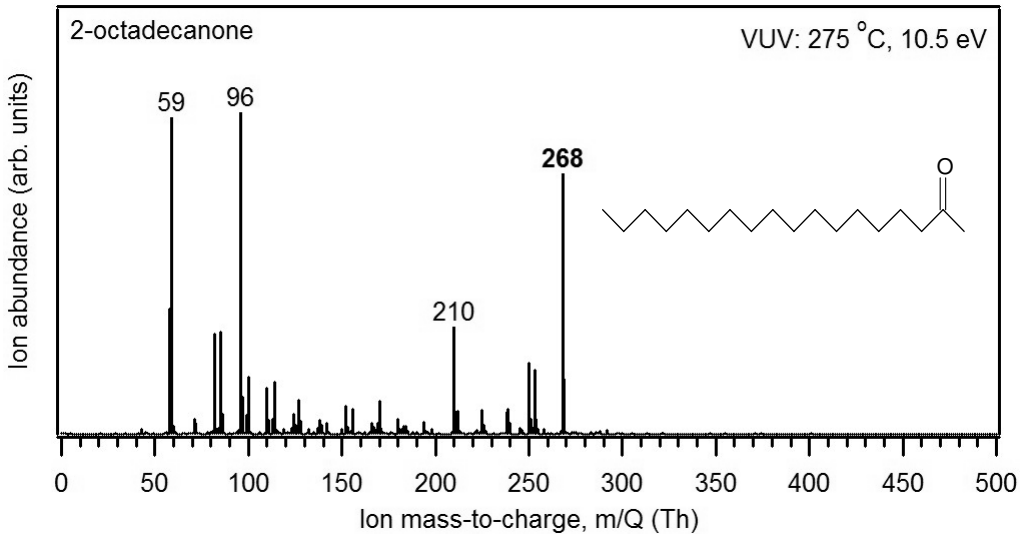

pentachlorophenol
VUV: 275 °C, 10.5 eV
266
264
268
270
OH
Cl
Cl
Cl
Cl
Cl
Ion abundance (arb. units)
0
50
100
150
200
250
300
350
400
450
500
Ion mass-to-charge, m/Q (Th)

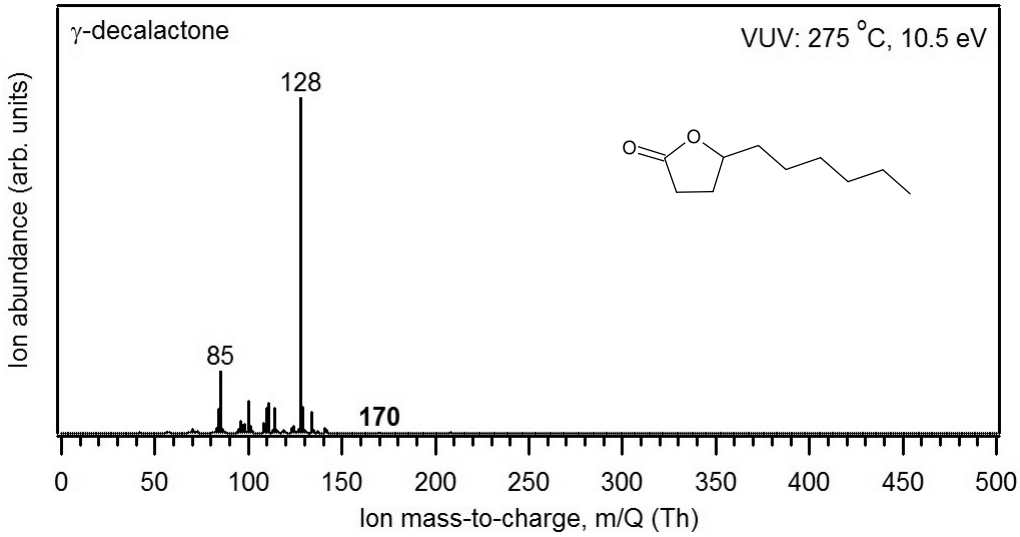
S.2.9. Oxygenated aliphatic compounds (ketones, esters, aldehydes)

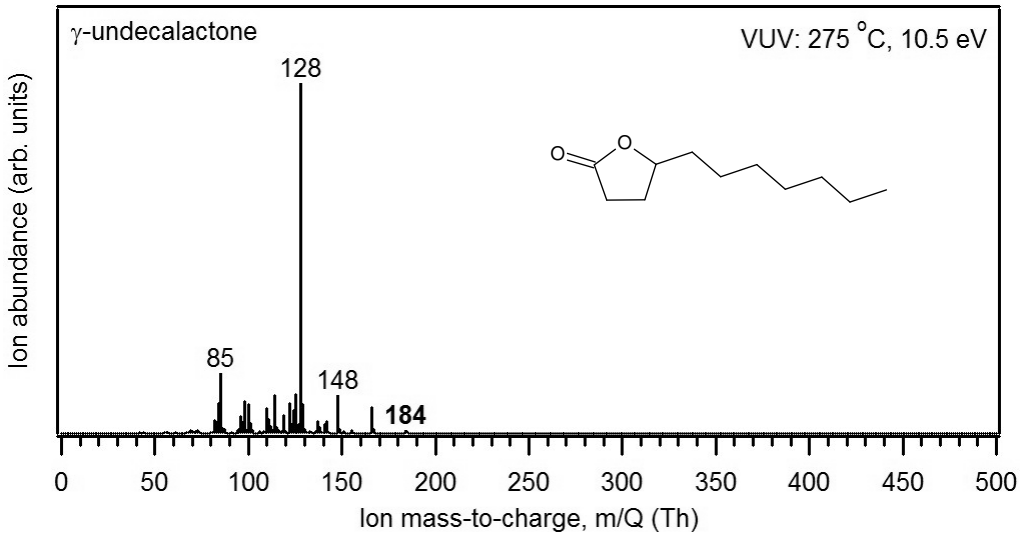


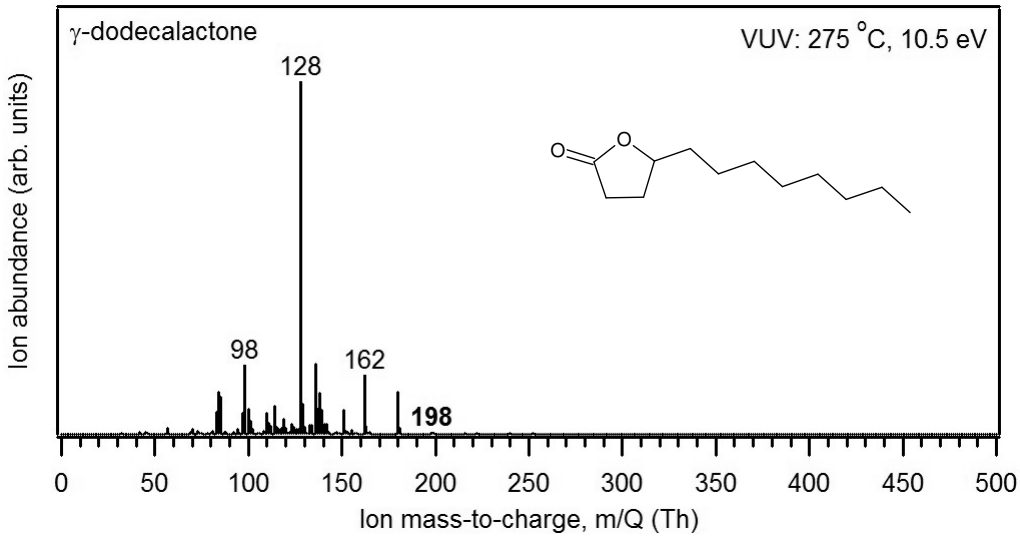


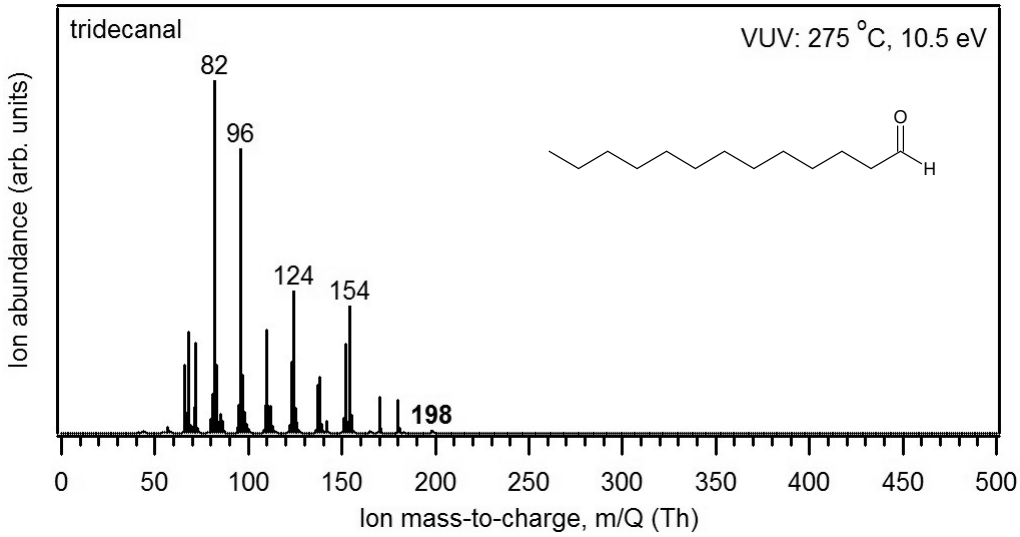

2-pentadecanone
VUV: 275 °C, 10.5 eV
59
96
168
226
O
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)


2-octadecanone
VUV: 275 °C, 10.5 eV
59
96
210
268
O
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)


γ-decalactone
VUV: 275 °C, 10.5 eV
85
128
170
O
O
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)


γ-undecalactone
VUV: 275 °C, 10.5 eV
128
85
148
184
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)


γ-dodecalactone
VUV: 275 °C, 10.5 eV
128
98
162
198
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)


tridecanal
VUV: 275 °C, 10.5 eV
82
96
124
154
198
Ion abundance (arb. units)
0 50 100 150 200 250 300 350 400 450 500
Ion mass-to-charge, m/Q (Th)

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