JEOL

Solutions for Innovation

Scientific / Metrology Instruments
Mass Spectrometry Guidebook

JEOL GC-MS Soft Ionization Mass Spectra Collection

A comparison of electron ionization and soft ionization methods for GC-MS applications
Chemical Ionization (CI)
Photoionization (PI)
Field Ionization (FI)

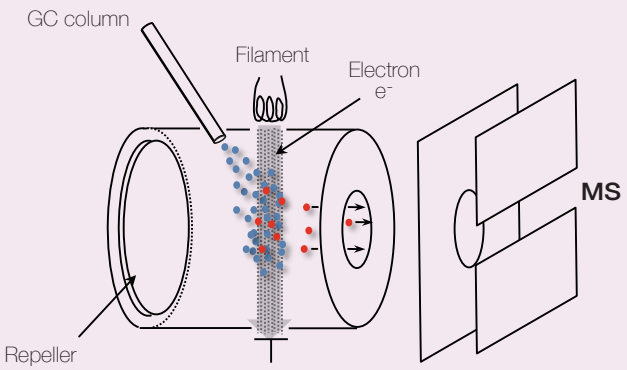
JEOL Ltd.

Ionization methods available for JEOL GC-MS

Electron Ionization (EI)

This is the ionization method most widely used for GC-MS. A thermal filament emits high-energy electrons that collide with gas-phase molecules to produce ions. The gas-phase requirement for ionization makes EI readily compatible with gas chromatography (GC) sample introduction. Ion/electron collisions can produce many fragment ions (“hard ionization”). Because the relative intensity of each ion observed (spectral pattern) has high reproducibility, components can be identified by comparing the acquired spectrum against EI mass spectrum library databases. More than 300,000 compounds from multiple databases are available with measured EI spectra, supporting various GC-MS applications.

Electron ionization (EI)



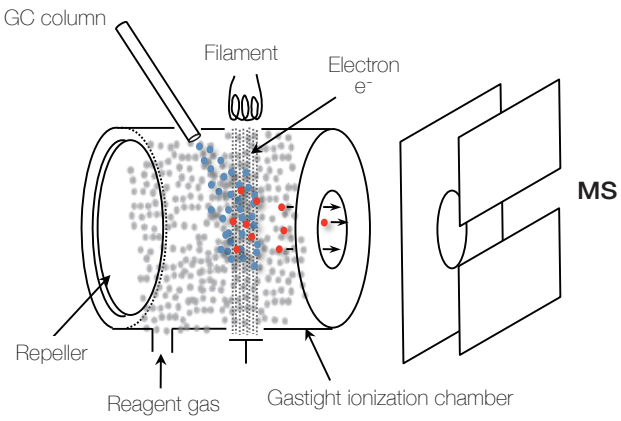
$M + e^- \longrightarrow M^{+\cdot} + 2e^-$

$M^{+\cdot} \longrightarrow m^+ + n^\cdot$

Chemical Ionization (CI)

This is a common soft ionization method used for GC-MS. A reagent gas is introduced into a highly gastight ionization chamber (approx. 10^{-2} Pa), and the reagent gas (B) is ionized by thermal electrons. Reagent gas ions undergo ion-molecule reactions with sample molecules (M) to produce protonated molecules, adducts, and fragments. Compared to EI, CI produces fewer fragments ("soft ionization") and provides information about the sample elemental composition. Methane, isobutane, and ammonia are commonly used as reagent gases. Methane and isobutane typically produce protonated molecules $[M + H]^+$, while ammonia produces ammonium adducts $[M + NH_4]^+$.

Chemical ionization (CI)



Proton adduct (most predominant reaction)

$M+[B+H]^+ \longrightarrow [M+H]^+ + B$

Reagent gas adduct

$M+[B+H]^+ \longrightarrow [M+B+H]^+$

Hydride ion abstraction

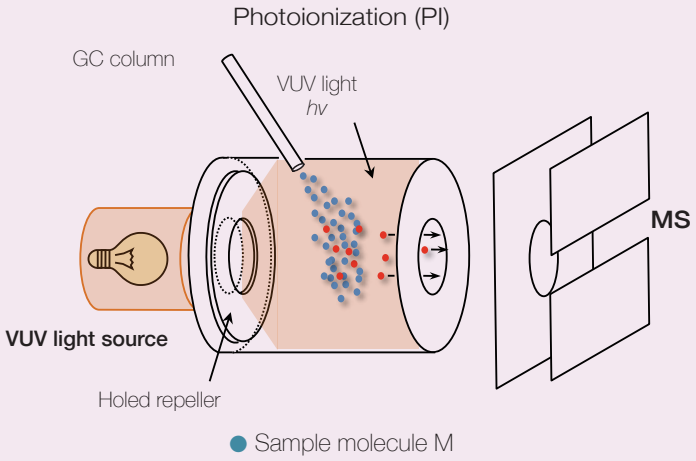
$M+[B+H]^+ \longrightarrow [M-H]^+ + [B+2H]$

Charge exchange

$M+B^{+\cdot} \longrightarrow M^{+\cdot} + B$

Photoionization (PI)

Photoionization uses vacuum ultraviolet (VUV) light with a photon energy at 8 to 10 eV to irradiate and ionize sample molecules. Because the photon energy is just above the ionization energy for typical organic compounds (8 to 11 eV), PI is a soft ionization method resulting in minimal fragmentation. Compounds that absorb ultraviolet light, such as aromatic compounds, tend to have higher sensitivity compared to other compounds.
Photoionization is a soft ionization method for GC-MS that does not require a reagent gas. It is easy to use and is effective in determining the elemental composition of an unknown compound.



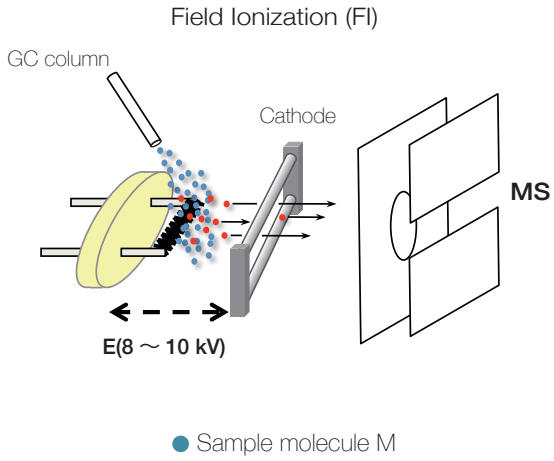
$$M + h\nu \longrightarrow M^{+\cdot} + e^{-}$$

PI source flange for
JMS-Q1600GC

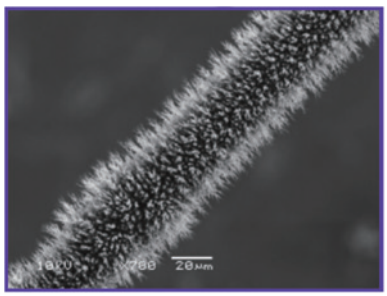
PI source flange for
JMS-T2000GC

Field Ionization (FI)

In field ionization, a high electrical potential (8 to 10 kV) is applied between a wire emitter coated with dendritic carbon microneedles and a counter electrode (cathode). Electron tunneling produces molecular ions when sample molecules are exposed to the high electric field at the sharp tip of each microneedle. The internal energy imparted into sample molecules during the ionization process is 1 eV or less, which is considerably smaller than that of the EI, CI, and PI methods, and results in minimal fragmentation. Although FI primarily produces molecular ions, protonated molecules are also possible for highly polar compounds. In practice, FI is used with GC-MS to ionize gaseous sample molecules as they elute from the GC column.
Field ionization is available for JEOL AccuTOF™ GC series GC-TOFMS systems.



$$M \xrightarrow{\text{High electric field}} M^{+\cdot} + e^{-}$$



Scanning electron micrograph of a
carbon emitter

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JEOL's GC-MS

GC-QMS
JMS-Q1600GC UltraQuad™ SQ-Zeta

GC-TQMS
JMS-TQ4000GC UltraQuad™ TQ

GC-TOFMS
JMS-T2000GC AccuTOF™ GC-Alpha

	GC-QMS	GC-TQMS	GC-TOFMS
EI	●	●	●
CI	●	●	●
PI	●	●	●
FI			●

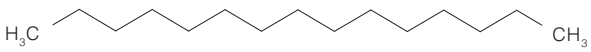
HARD

SOFT

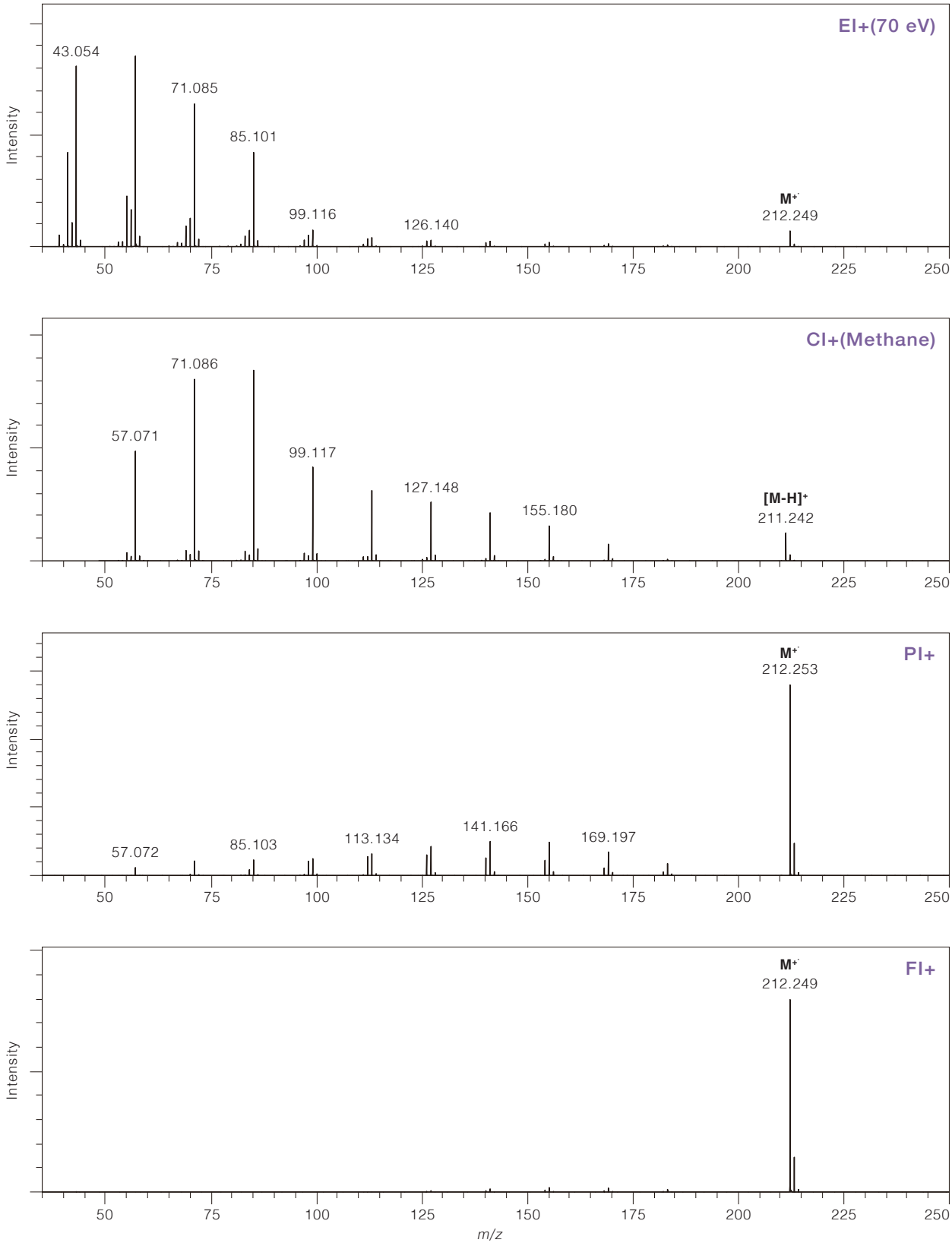
n-Alkanes

Pentadecane

CAS No.629-62-9



$C_{15}H_{32}$=212



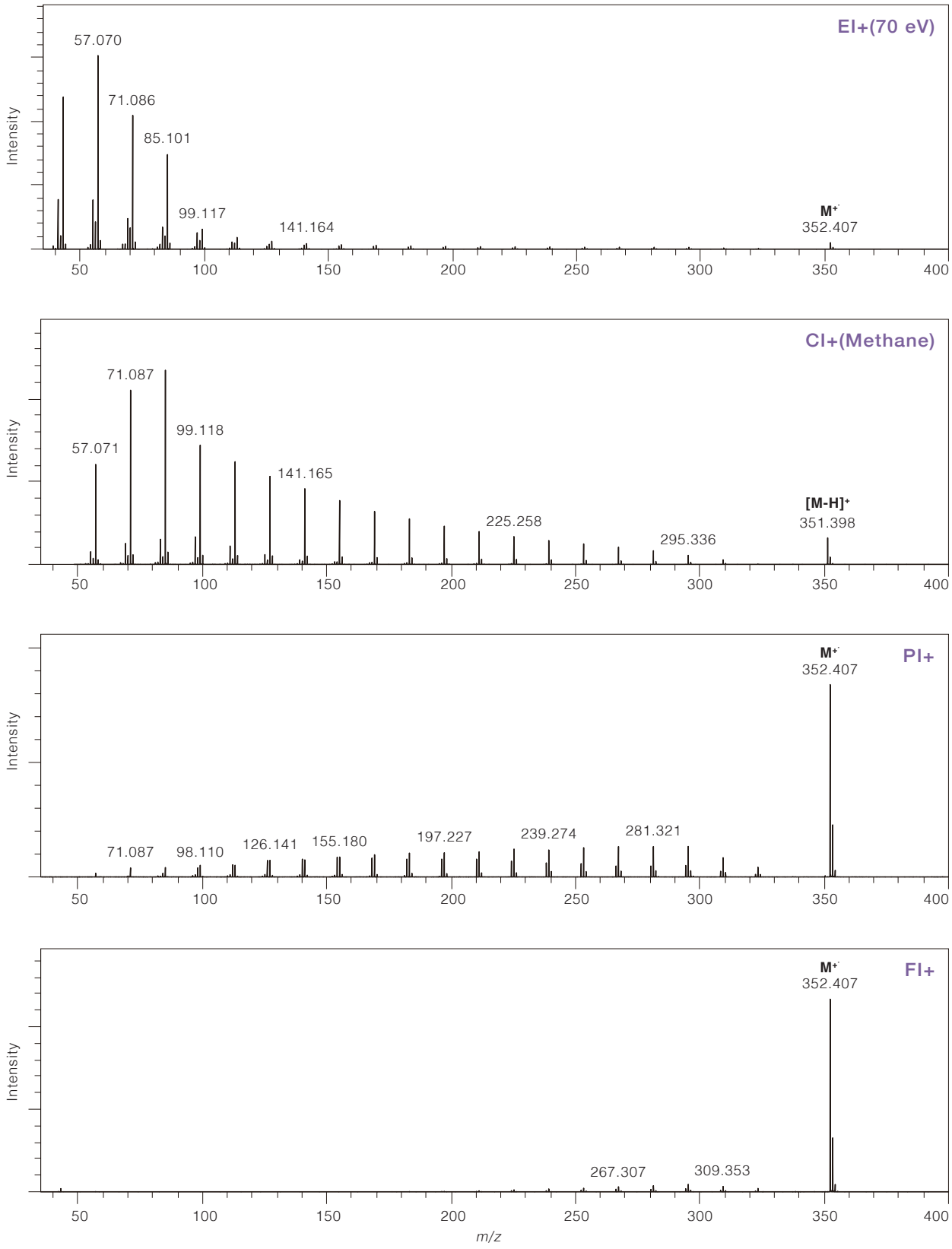
n-Alkanes

Pentacosane

CAS No.629-99-2

$CH_3(CH_2)_{23}CH_3$

$C_{25}H_{62}$=352



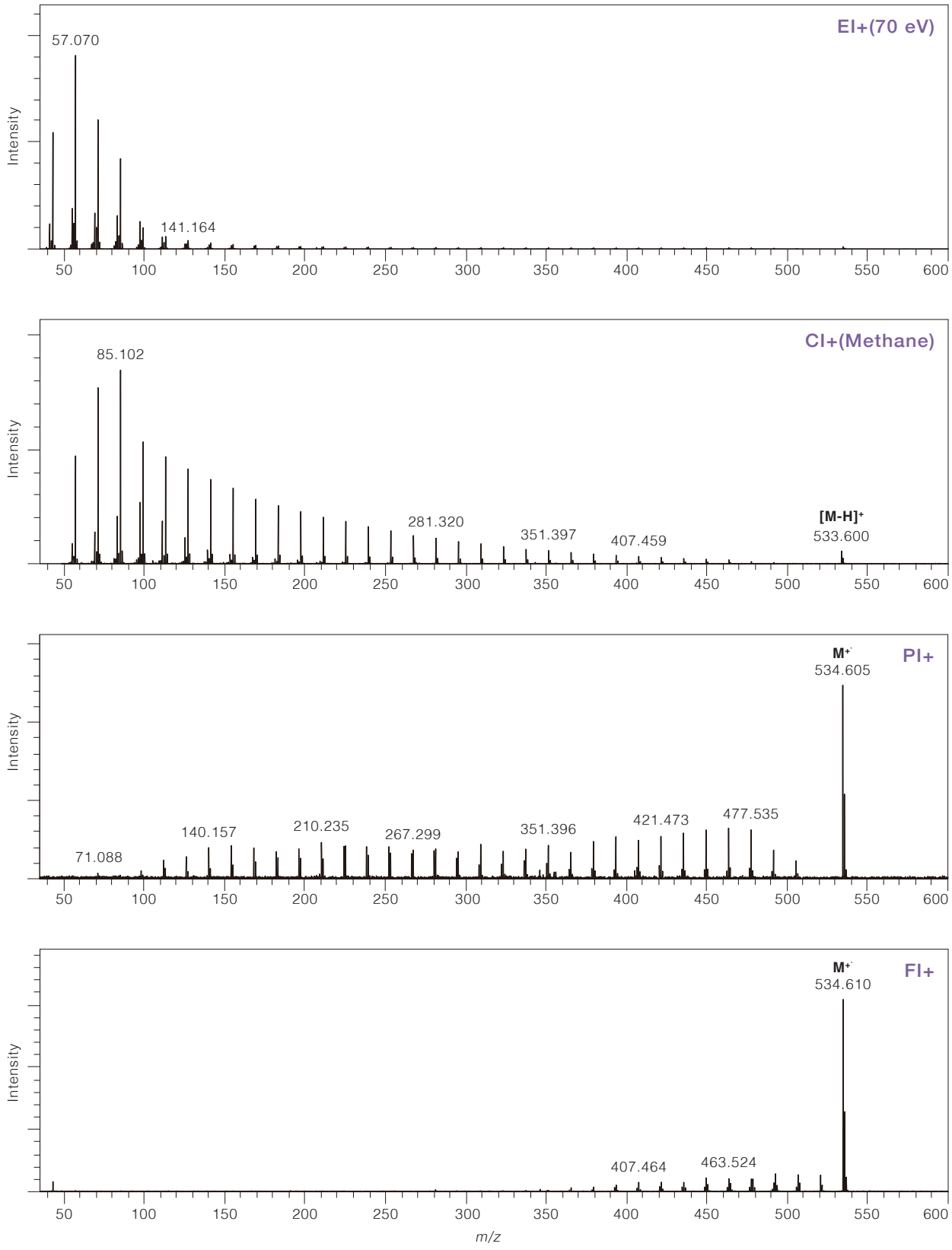
n-Alkanes

Octatriacontane

CAS No.7194-85-6

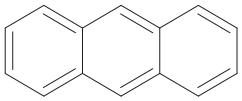
$CH_3(CH_2)_{36}CH_3$

$C_{38}H_{78}$=534

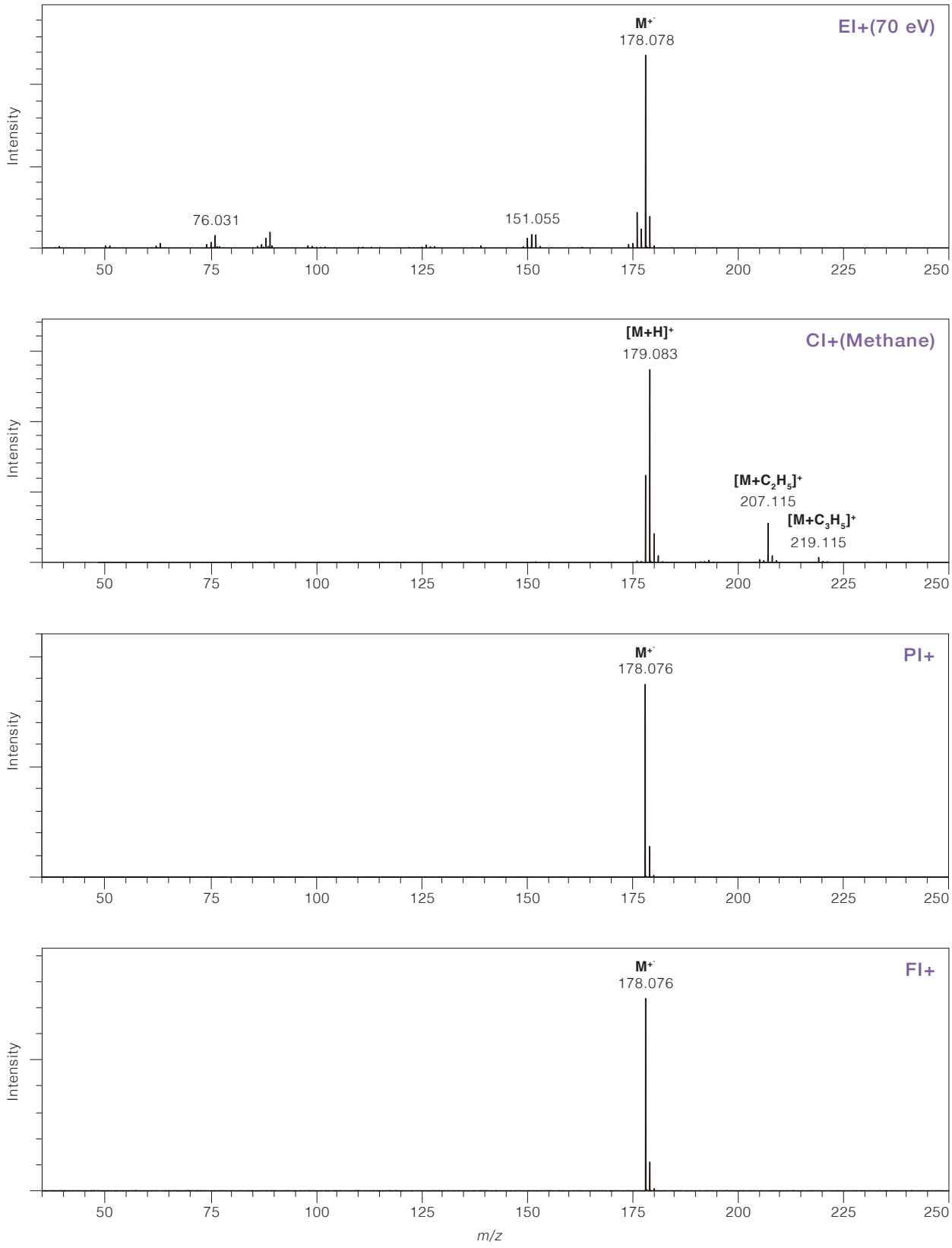


Anthracene

CAS No.120-12-7



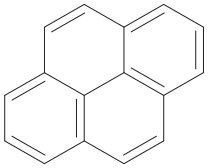
$C_{14}H_{10}$=178



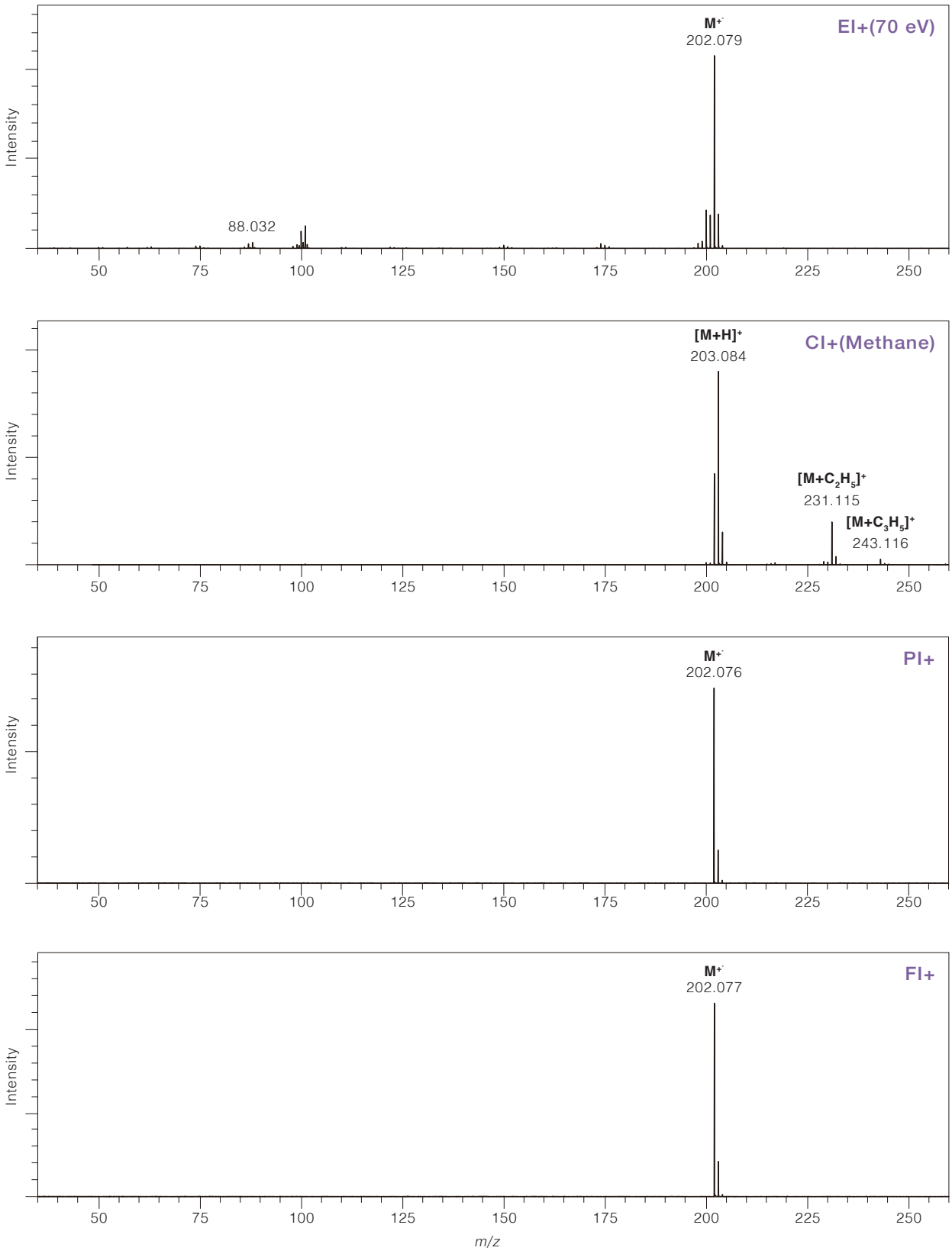
PAHs

Pyrene

CAS No.129-00-0



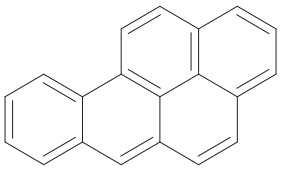
$C_{16}H_{10}$=202



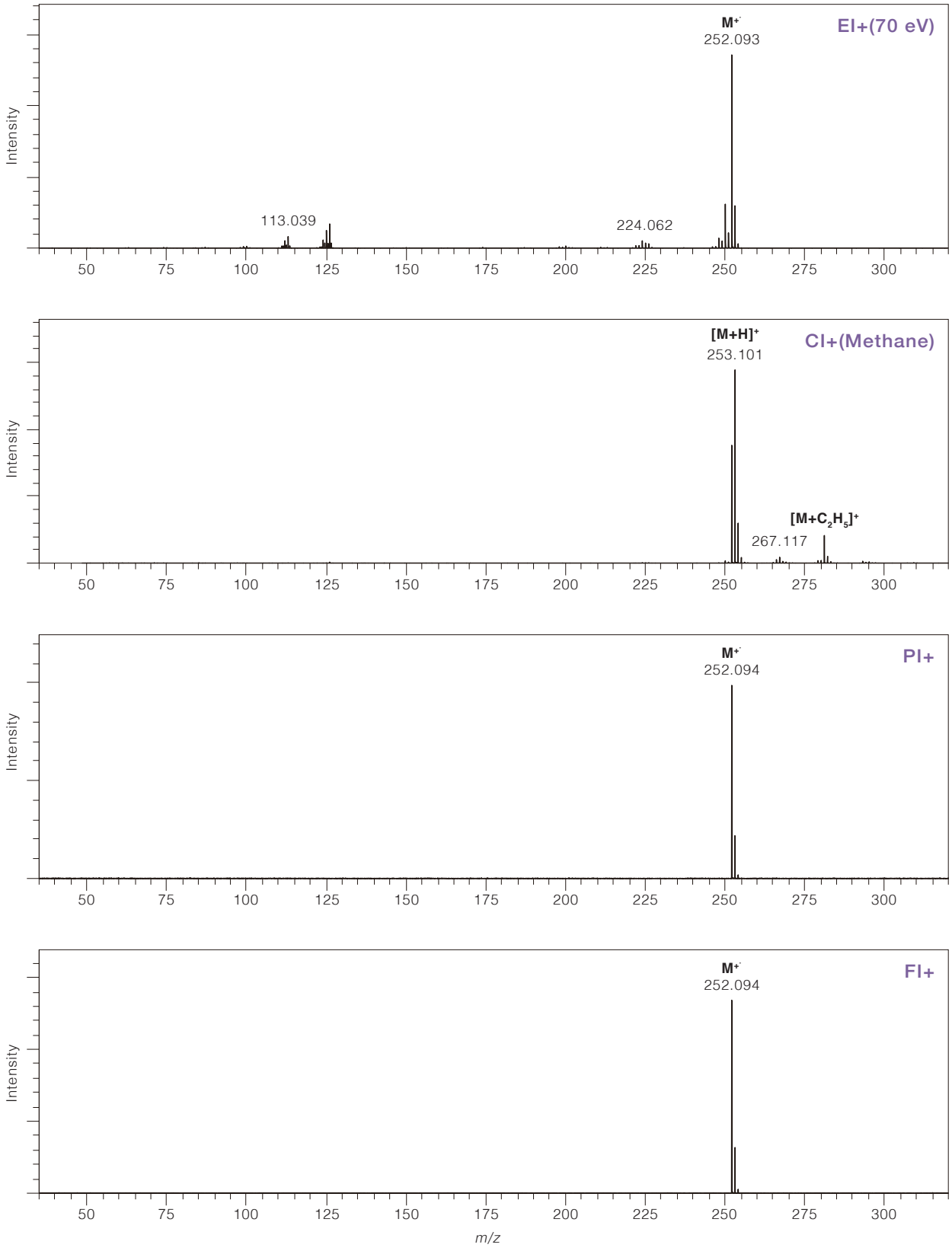
PAHs

Benzo[a]pyrene

CAS No.50-32-8



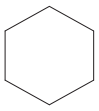
$C_{20}H_{12}$=252



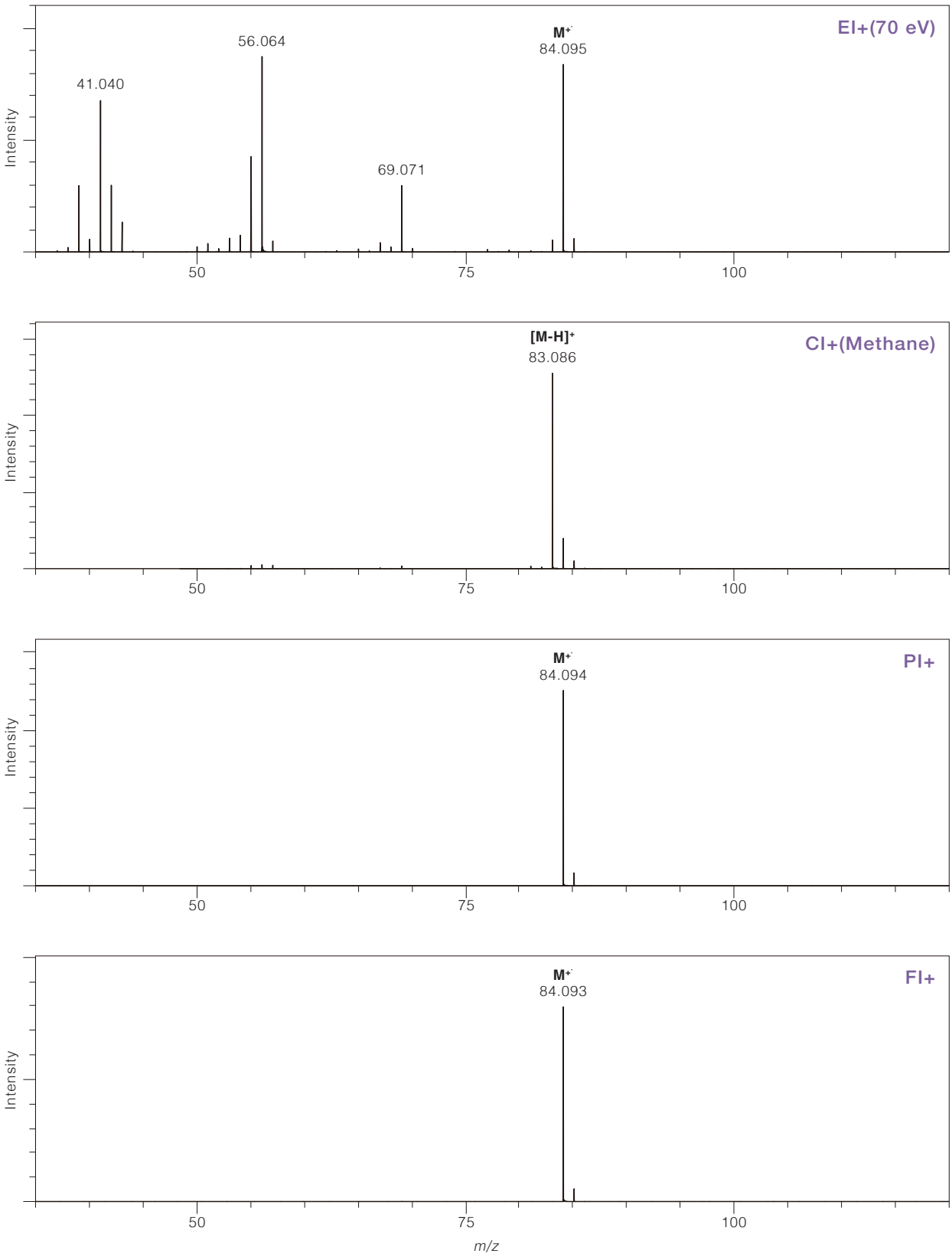
Cycloalkanes

Cyclohexane

CAS No.110-82-7



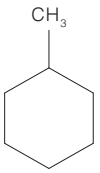
C_6H_{12}=84



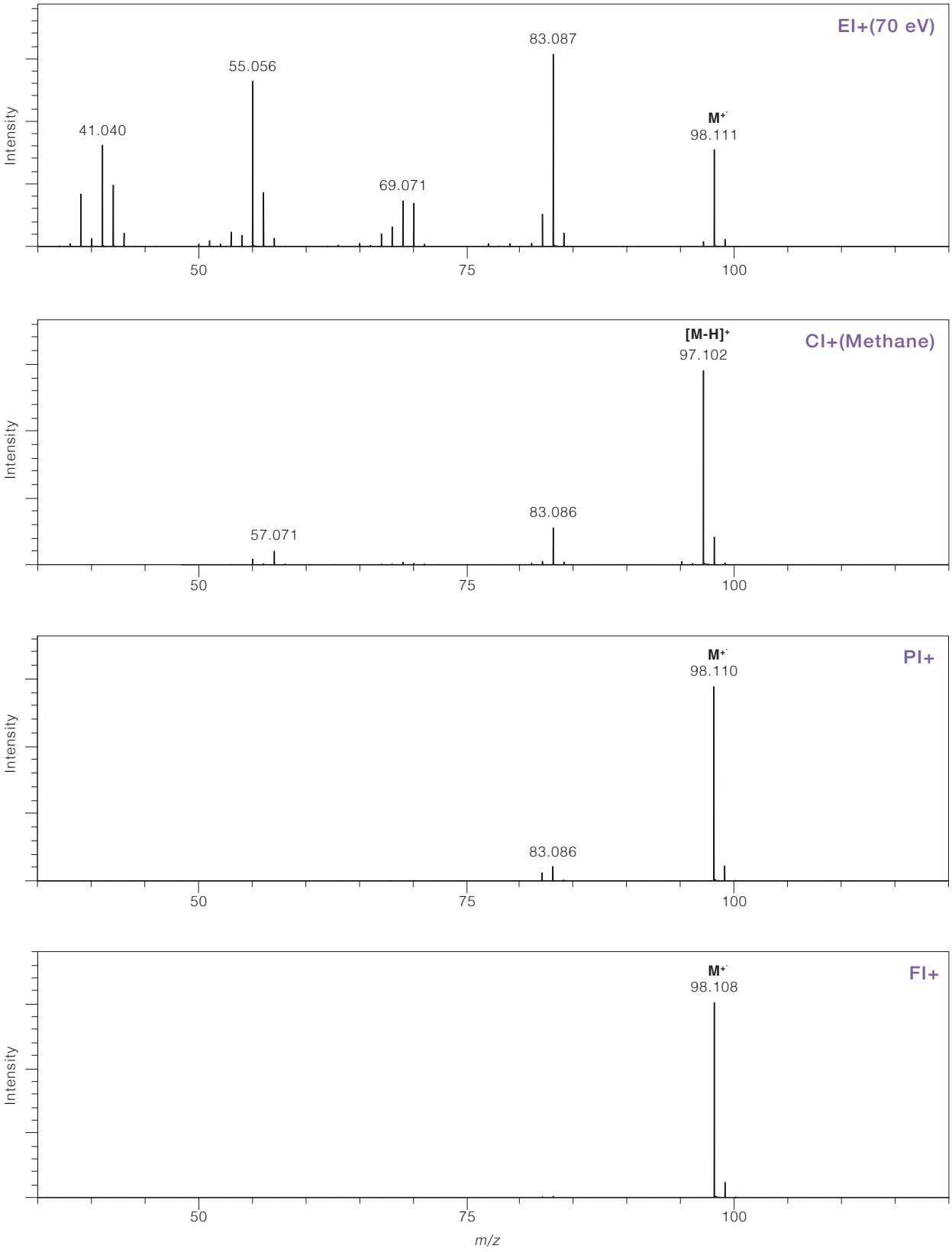
Cycloalkanes

Methylcyclohexane

CAS No.108-87-2



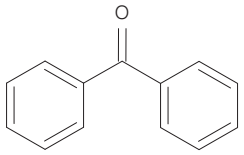
C_7H_{14}=98



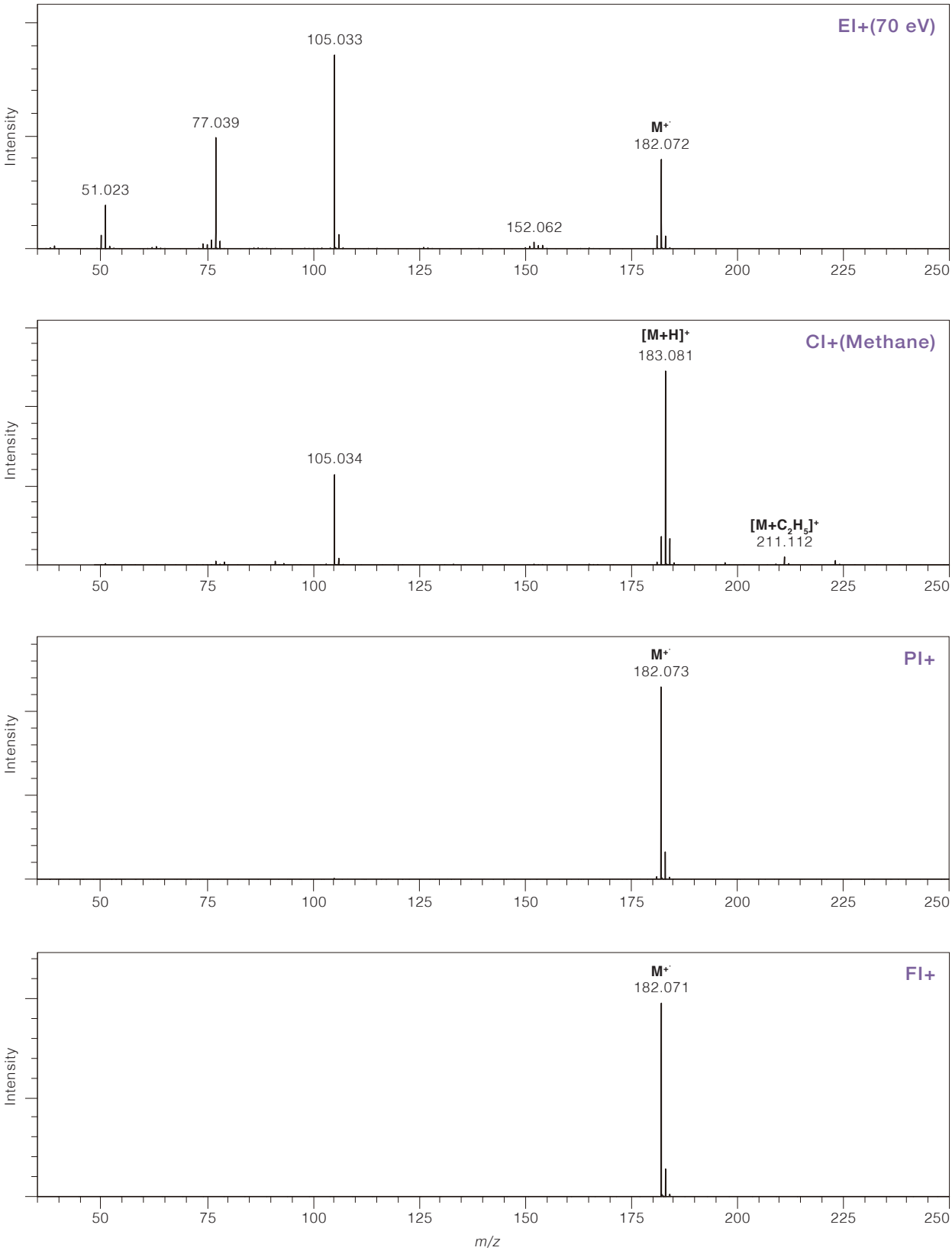
Ketones

Benzophenone

CAS No.119-61-9



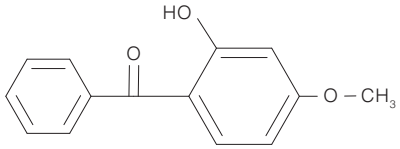
$C_{13}H_{10}O$=182



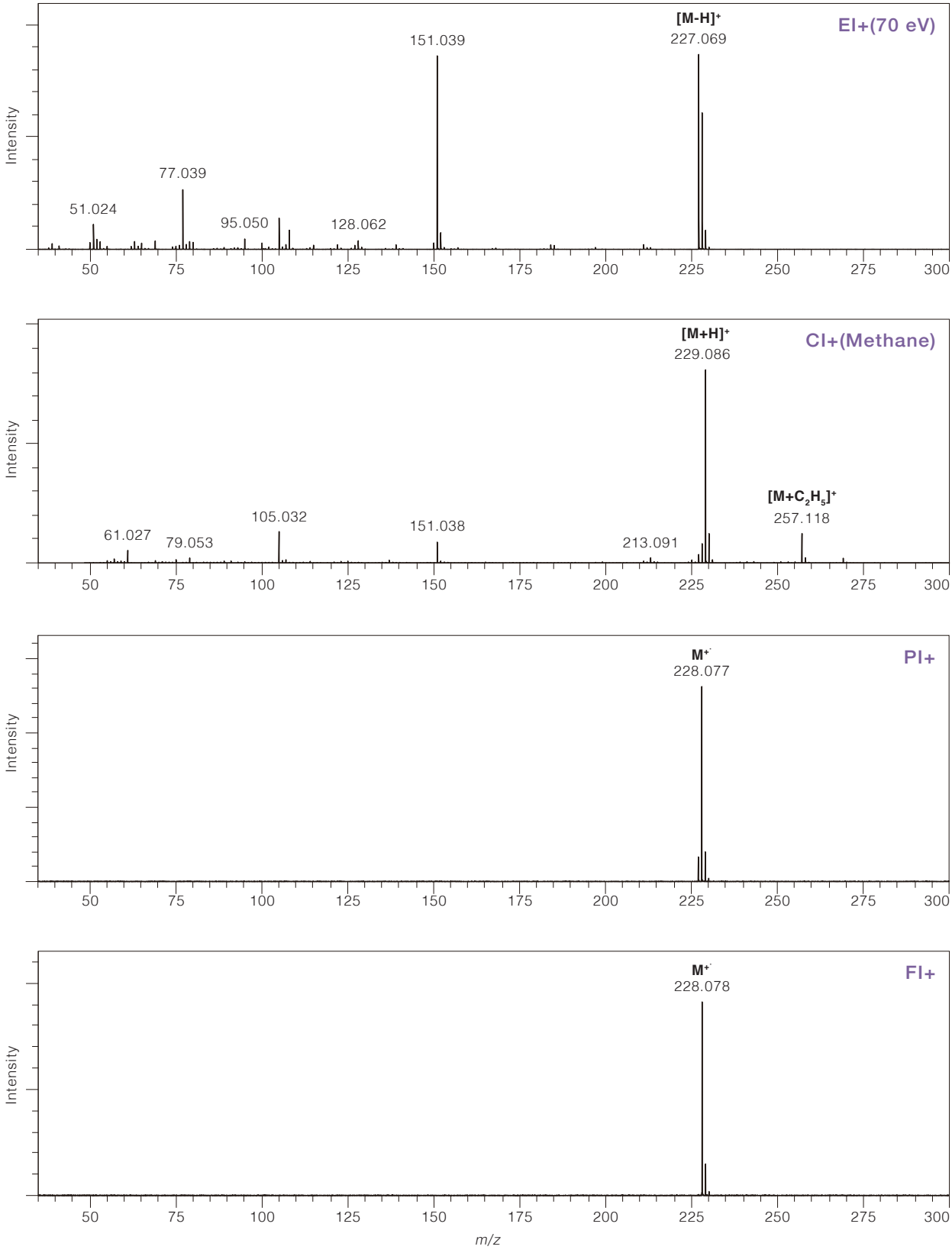
Ketones

2-Hydroxy-4-methoxybenzophenone

CAS No.131-57-7



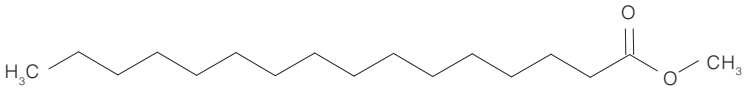
$C_{14}H_{12}O_3$=228



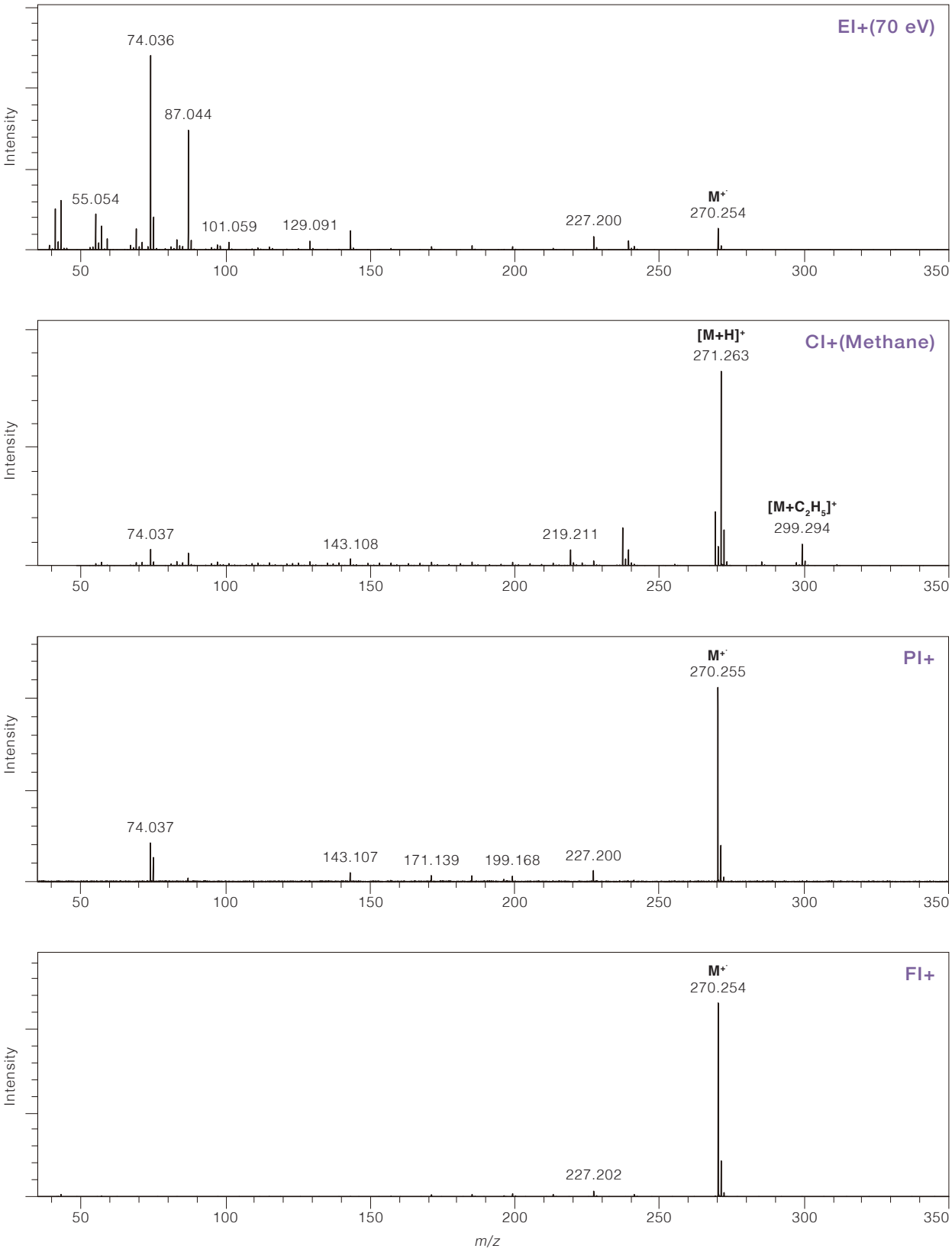
Fatty acid esters

Methyl palmitate

CAS No.112-39-0



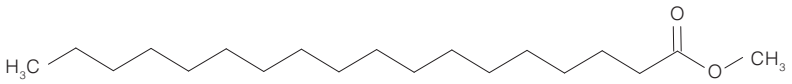
$C_{17}H_{34}O_2$=270



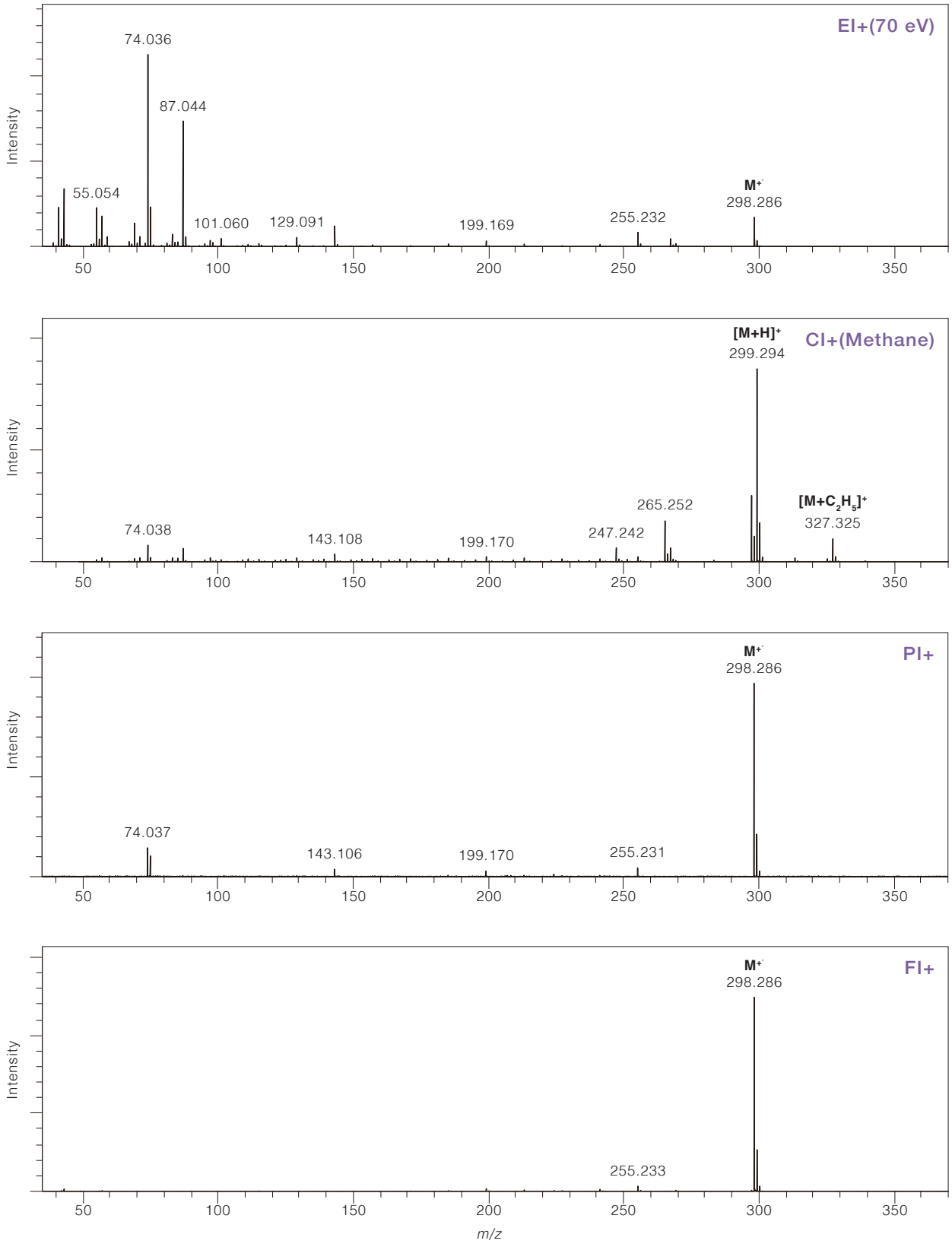
Fatty acid esters

Methyl stearate

CAS No.112-61-8



$C_{19}H_{38}O_2$=298

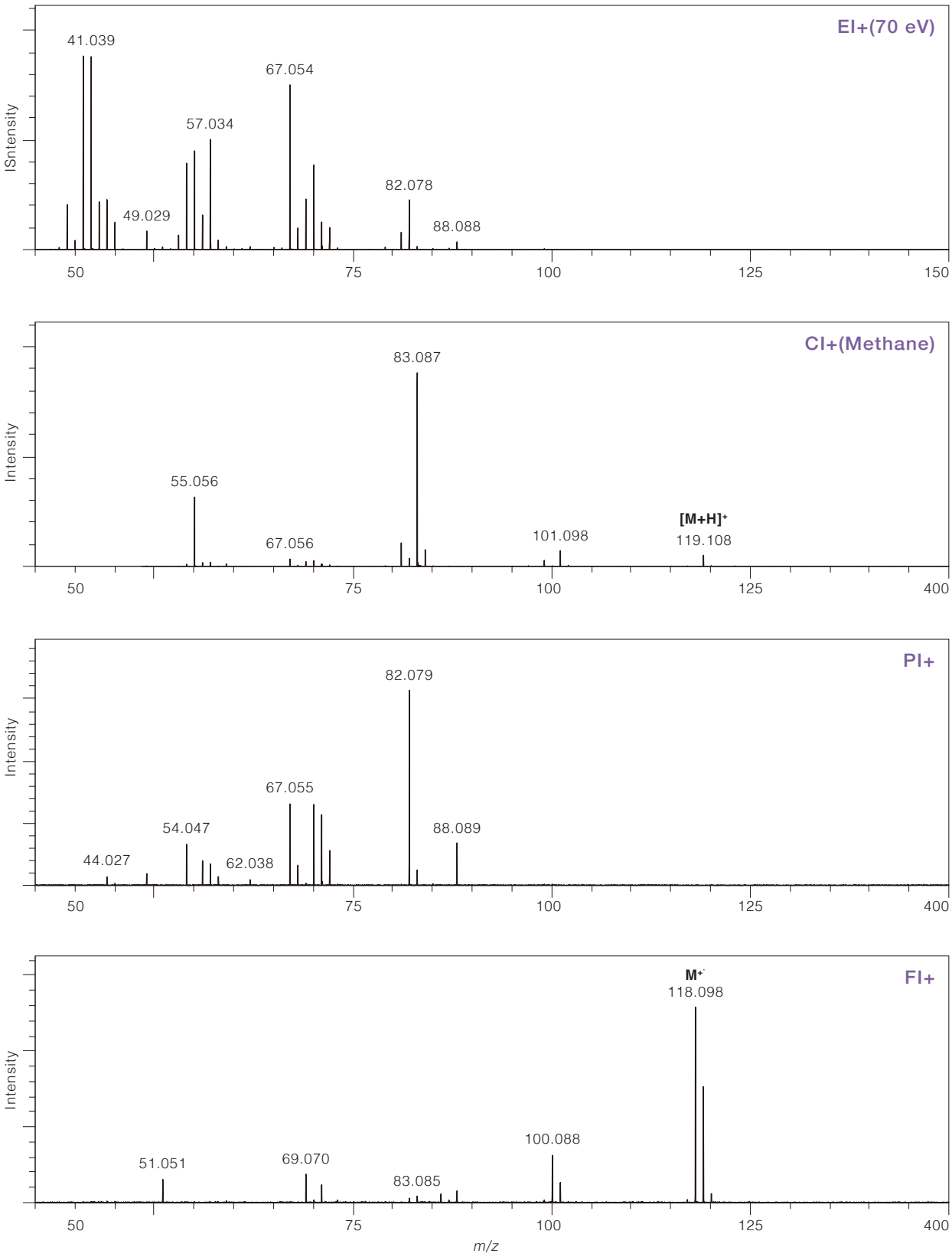


Alcohols

1,6-Hexanediol

CAS No.629-11-8

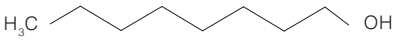
$C_6H_{14}O_2$=118



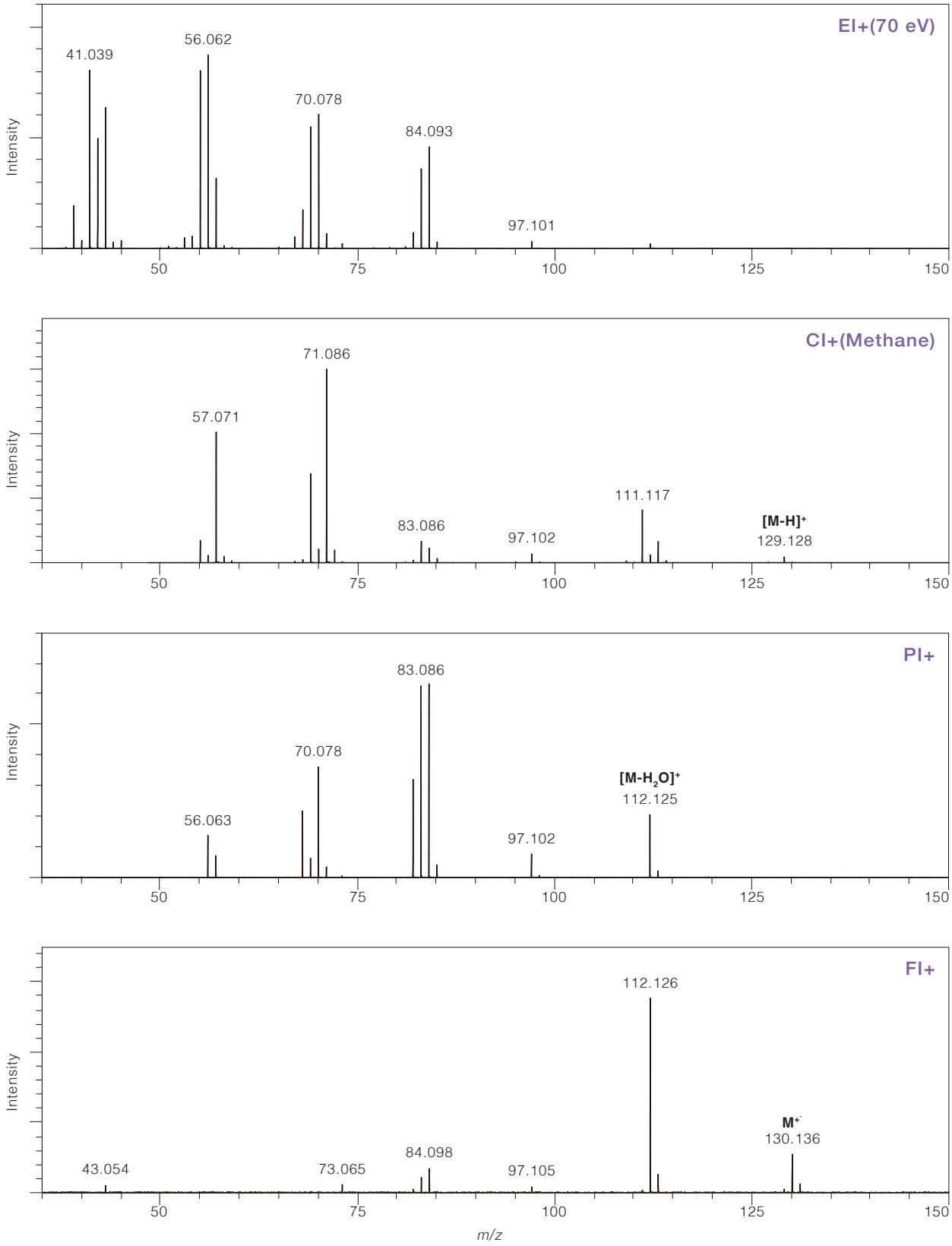
Alcohols

1-Octanol

CAS No.111-87-5



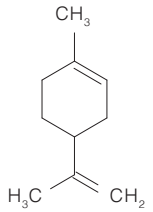
$C_8H_{18}O$=130



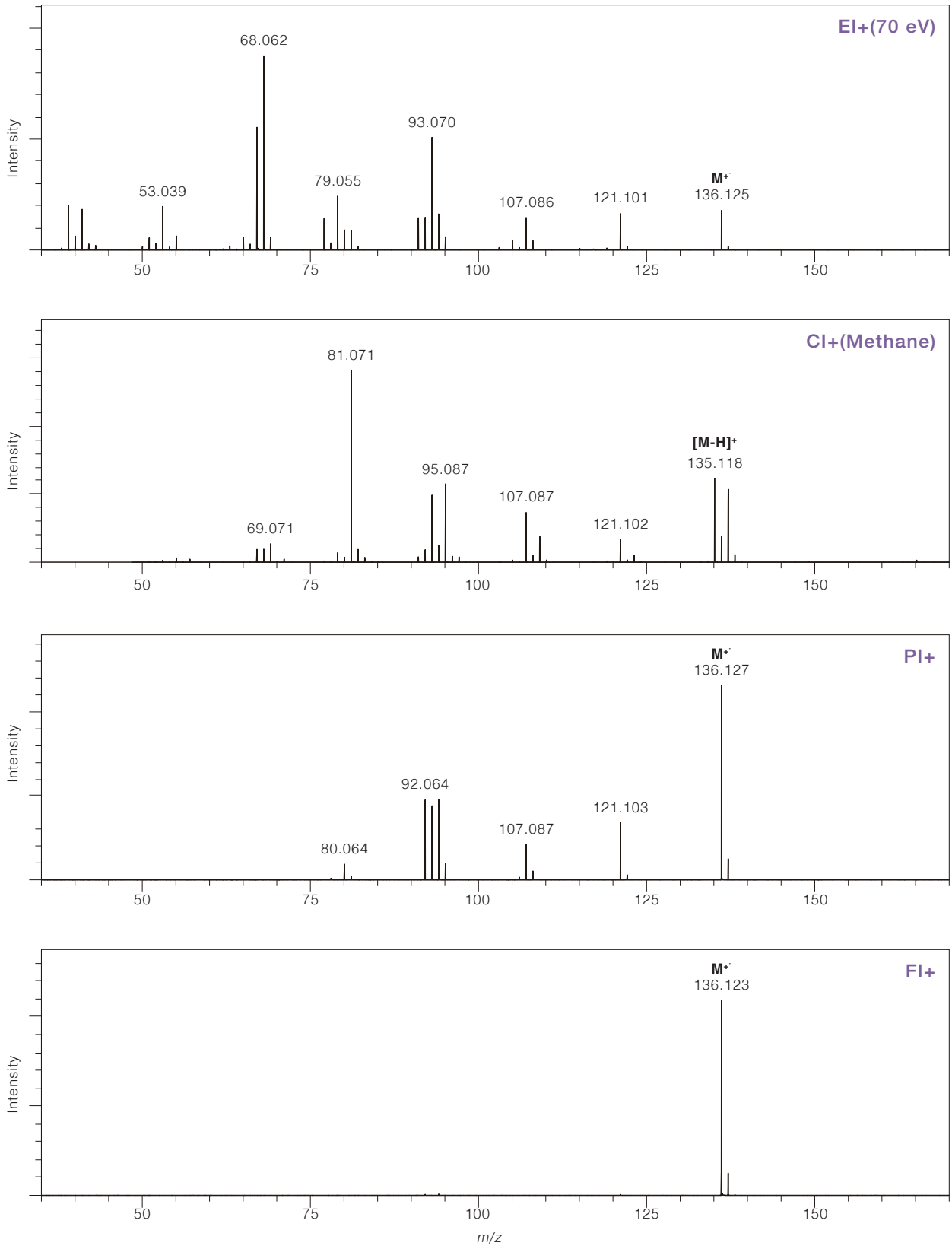
Terpenes

Limonene

CAS No.138-86-3

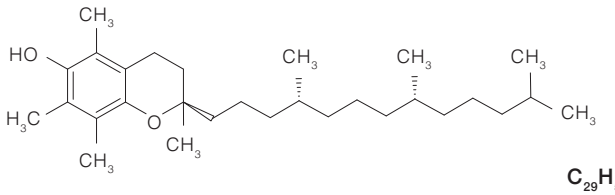


$C_{10}H_{16}$=136

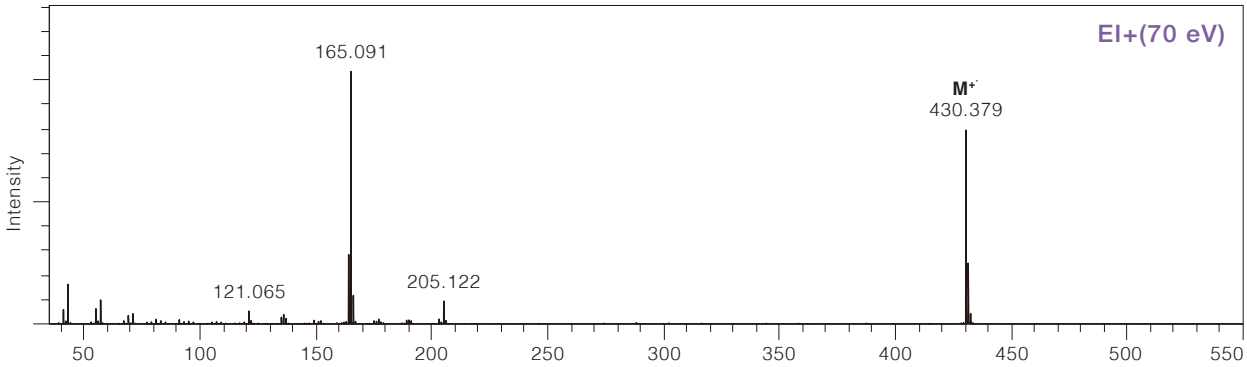


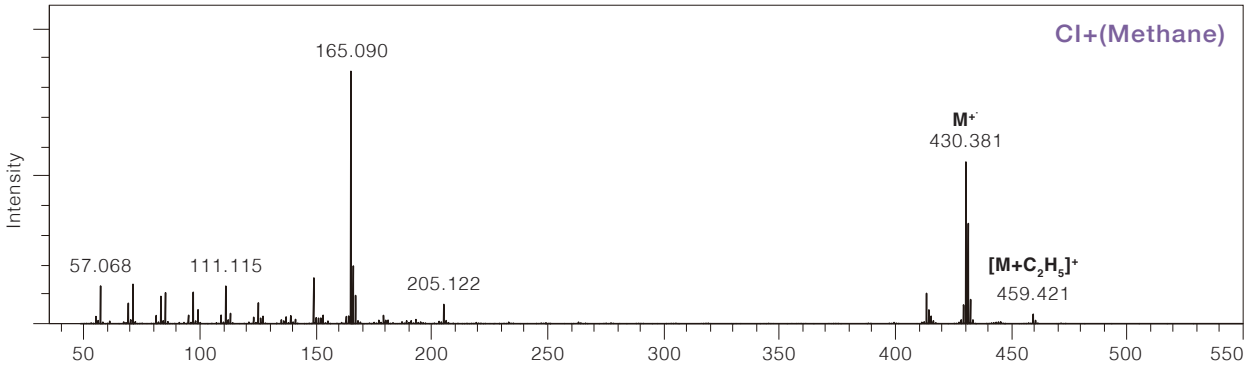
DL-α-Tocopherol [Vitamin E]

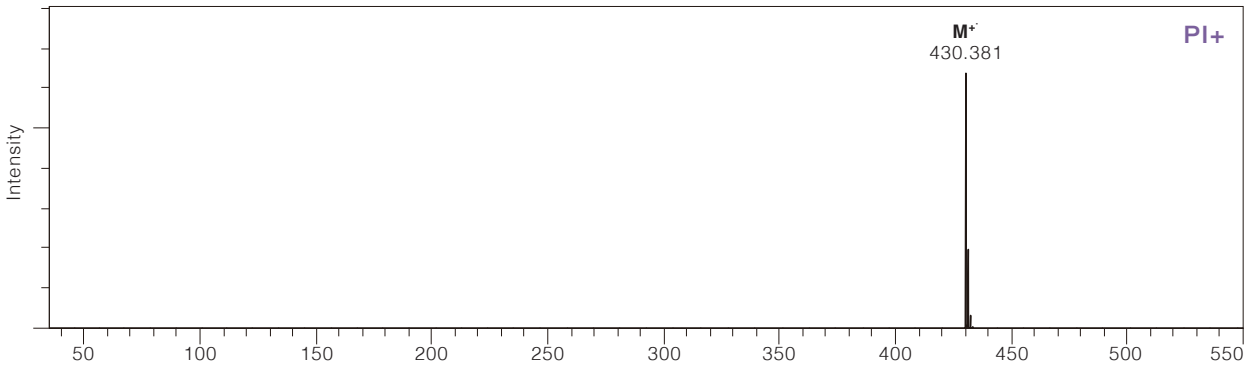
CAS No.10191-41-0

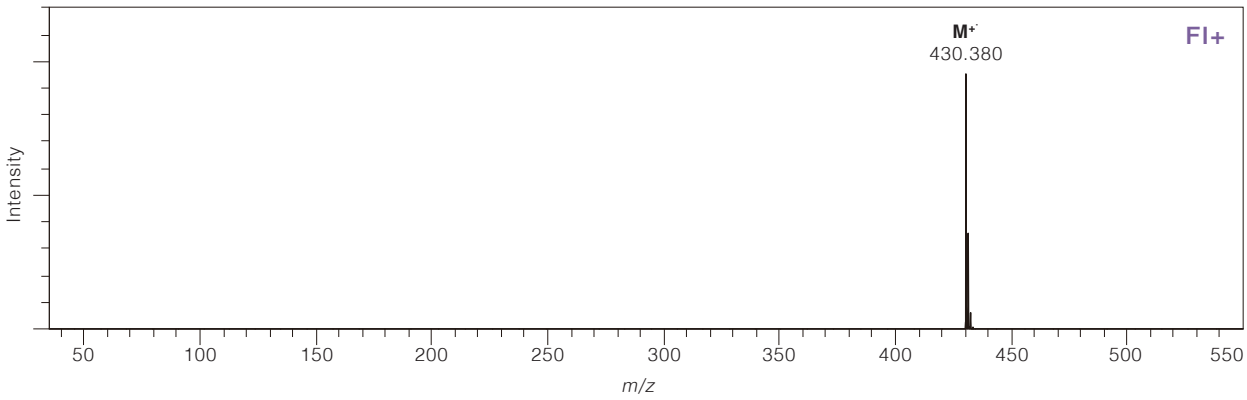


$C_{29}H_{50}O$=430





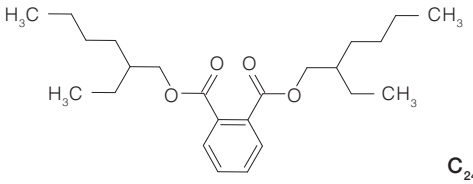




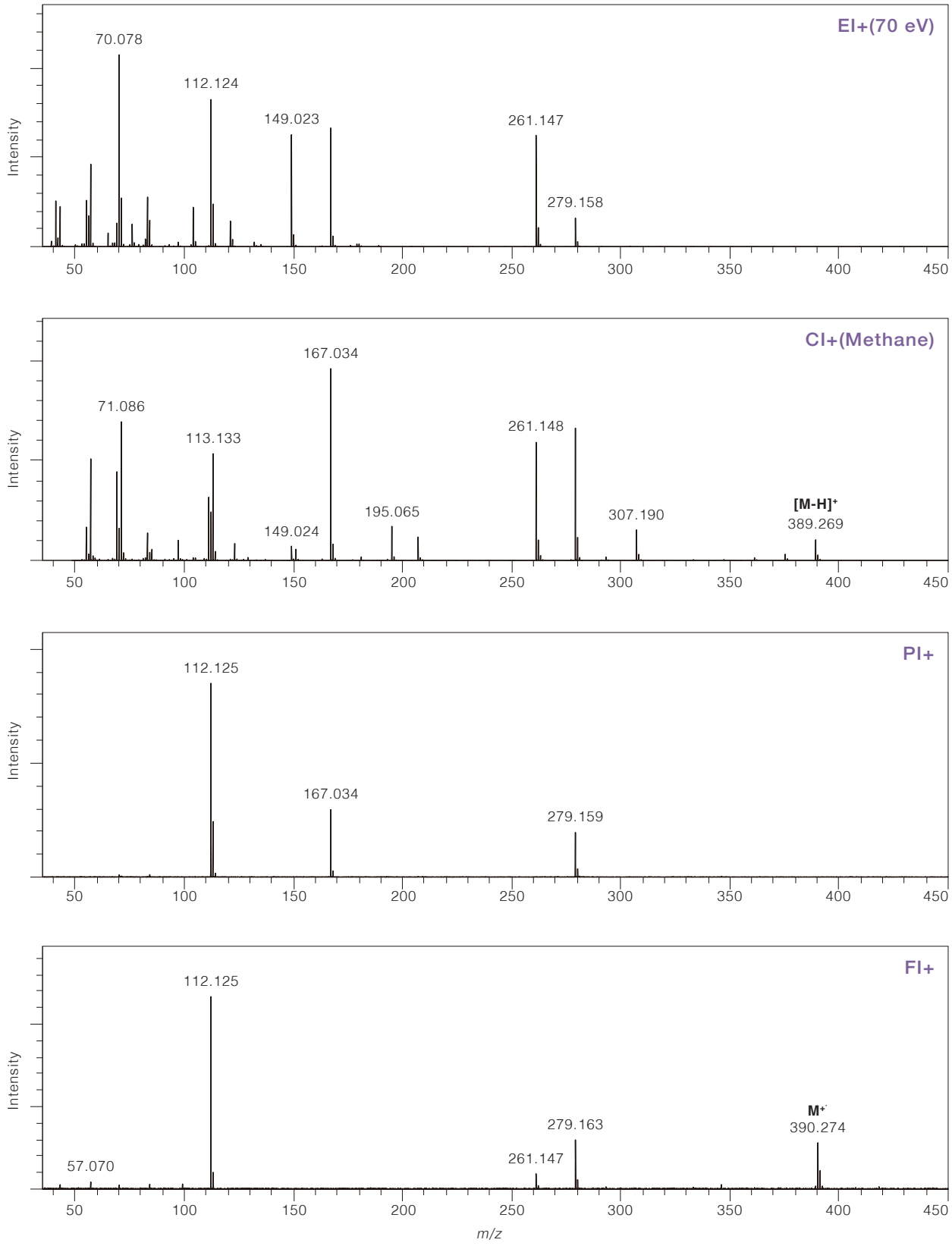
Phthalic acid esters

Bis(2-ethylhexyl)phthalate)
[DEHP]

CAS No.117-81-7



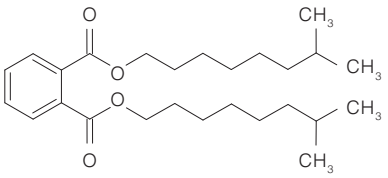
$C_{24}H_{38}O_4$=390



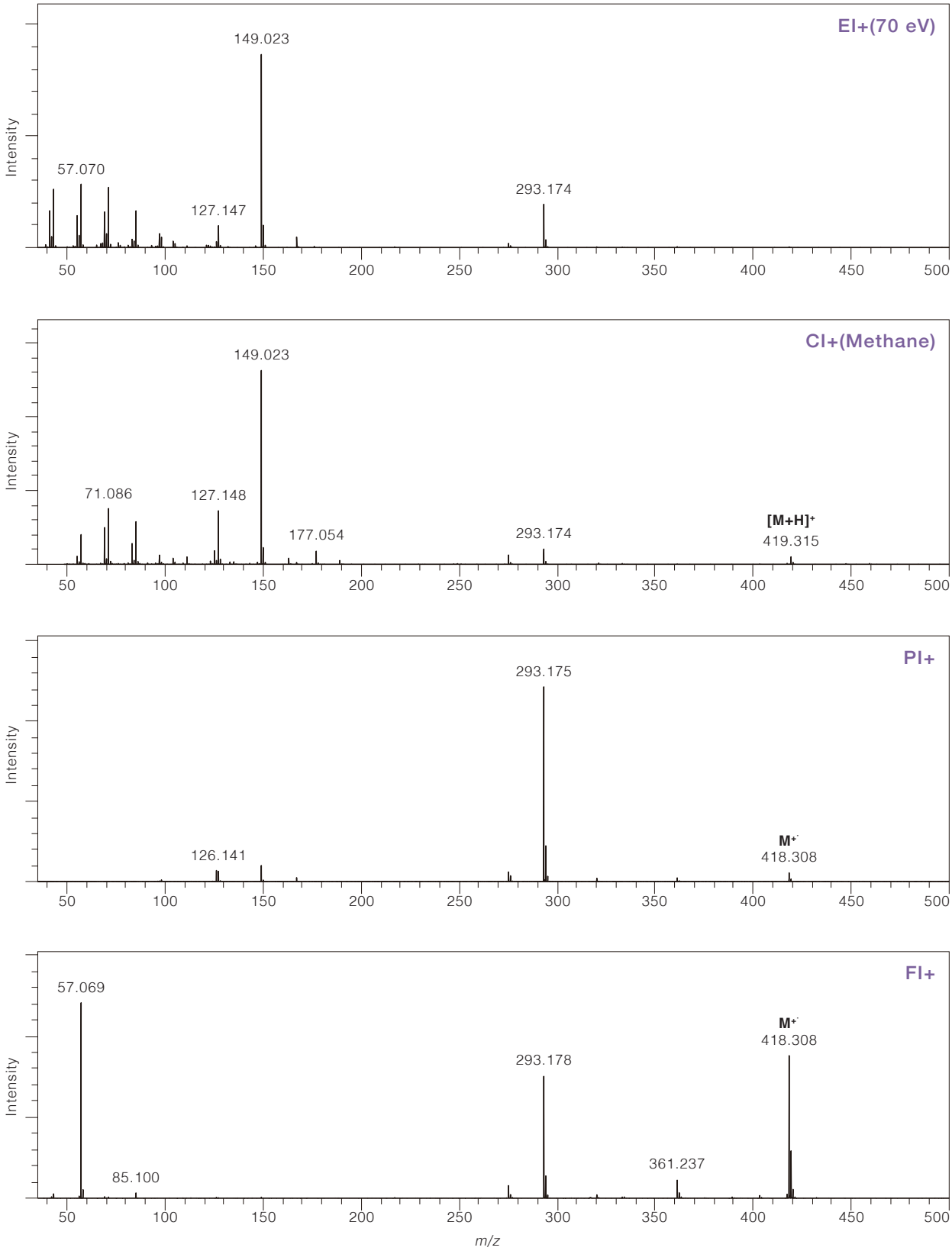
Phthalic acid esters

Diisononyl Phthalate [DINP]

CAS No.28553-12-0



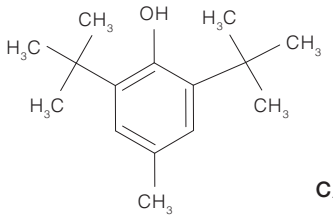
$C_{26}H_{42}O_4$=418



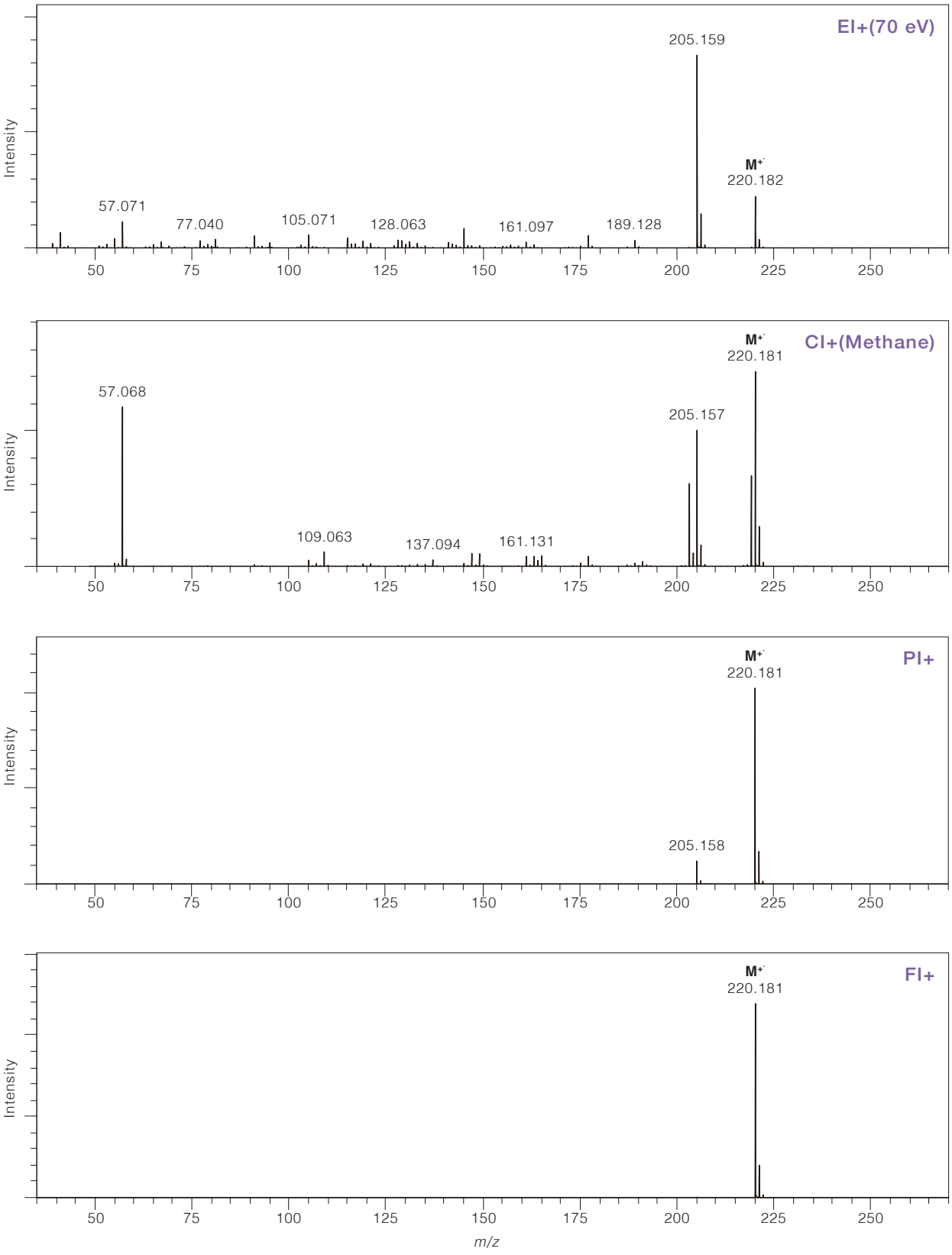
Phenols

2,6-Di-tert-butyl-p-cresol [BHT]

CAS No.128-37-0

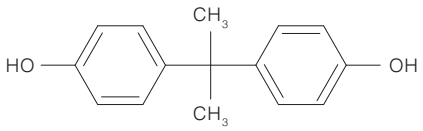


$C_{15}H_{24}O$=220

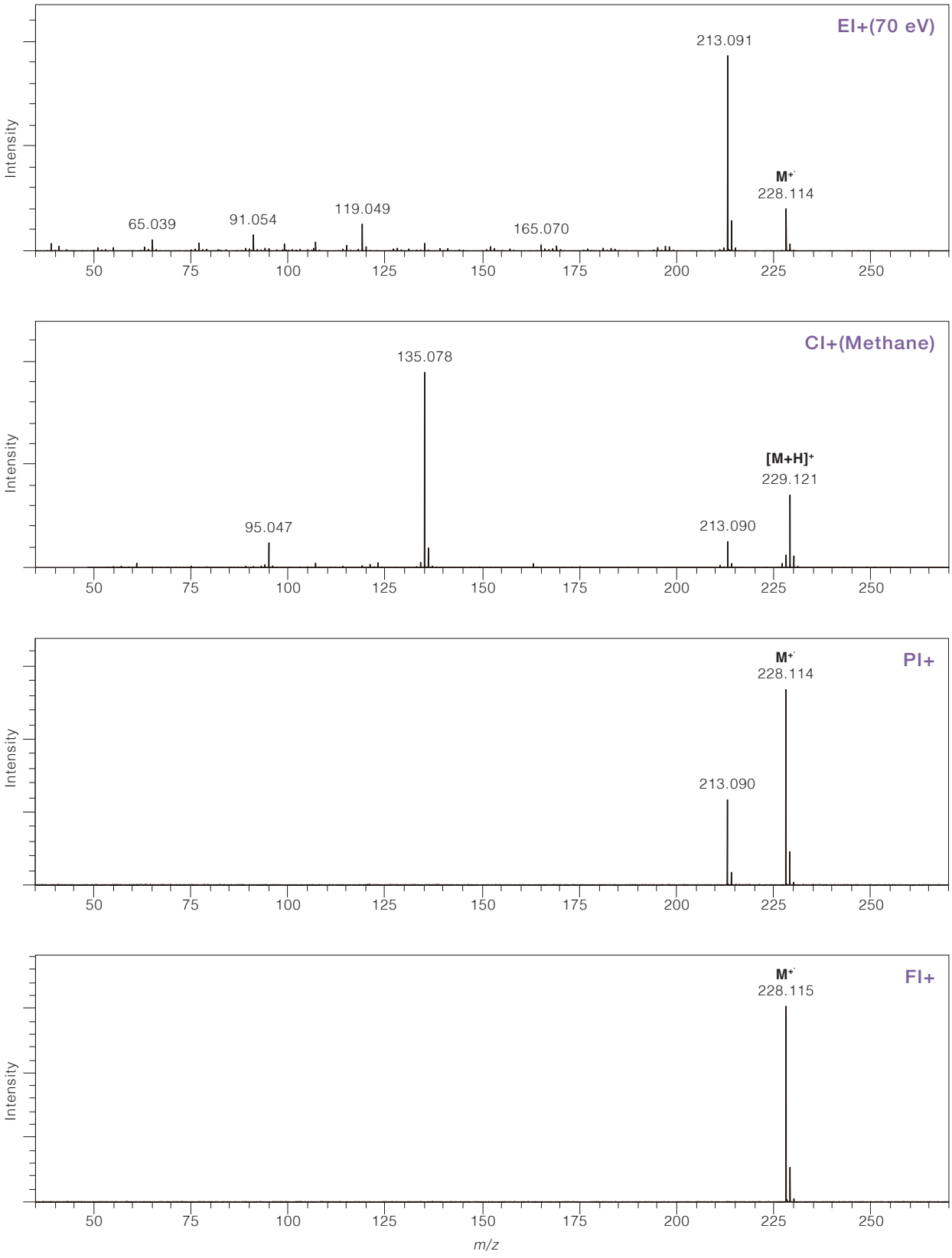


2,2-Bis(4-hydroxyphenyl)propane [Bisphenol A]

CAS No.80-05-7



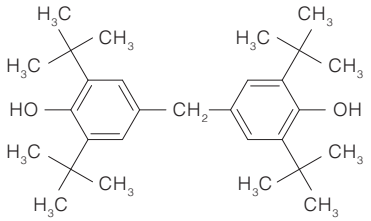
$C_{15}H_{16}O_2$=228



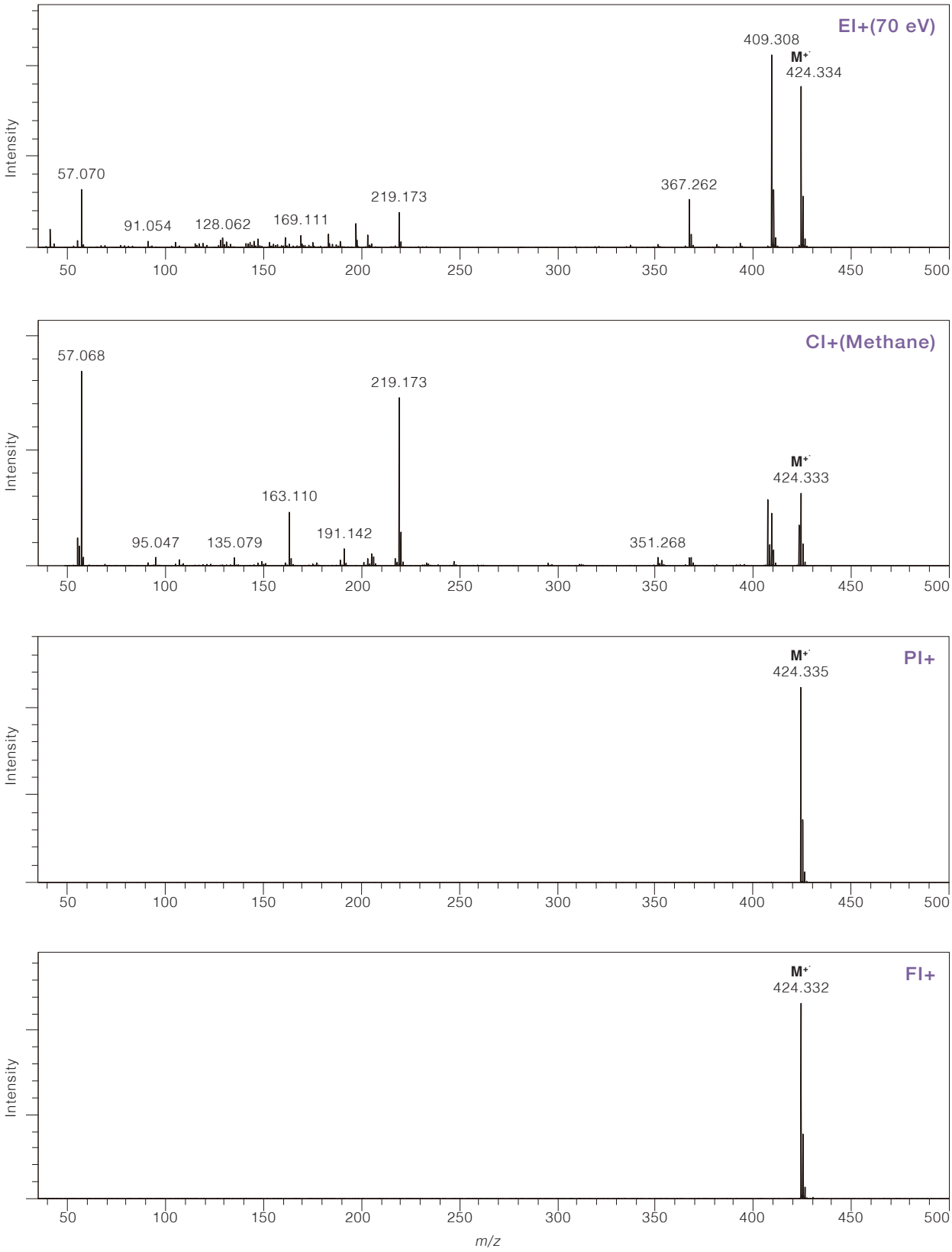
Phenols

4,4'-Methylenebis (2,6-di-tert-butylphenol) [Ethanox 702]

CAS No.118-82-1

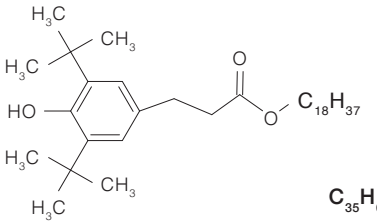


$C_{29}H_{44}O_2$=424

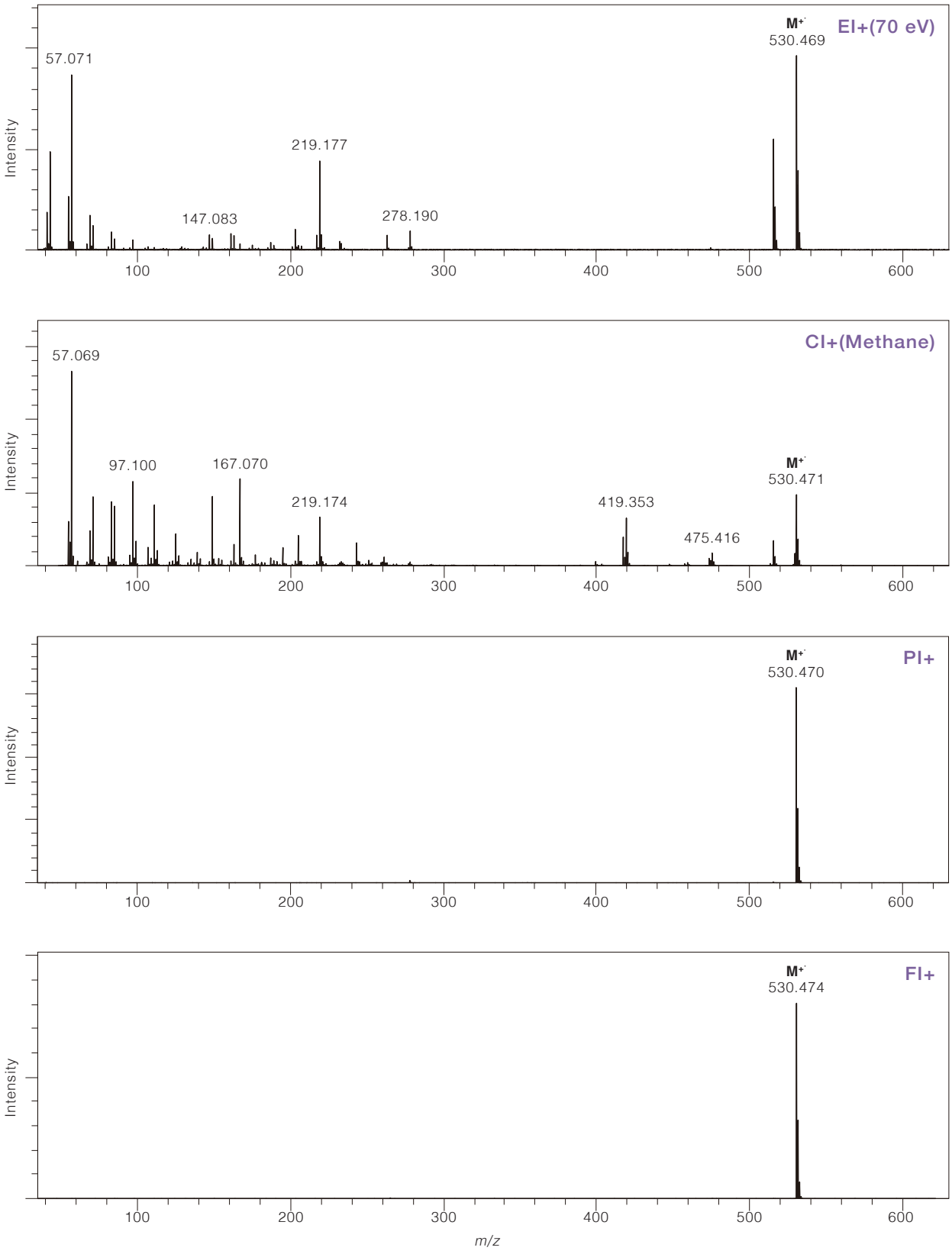


2,2-Bis(4-hydroxyphenyl)propane [Irganox 1076]

CAS No.2082-79-3

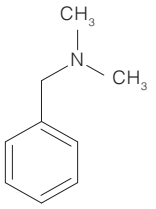


$C_{35}H_{62}O_3$=530

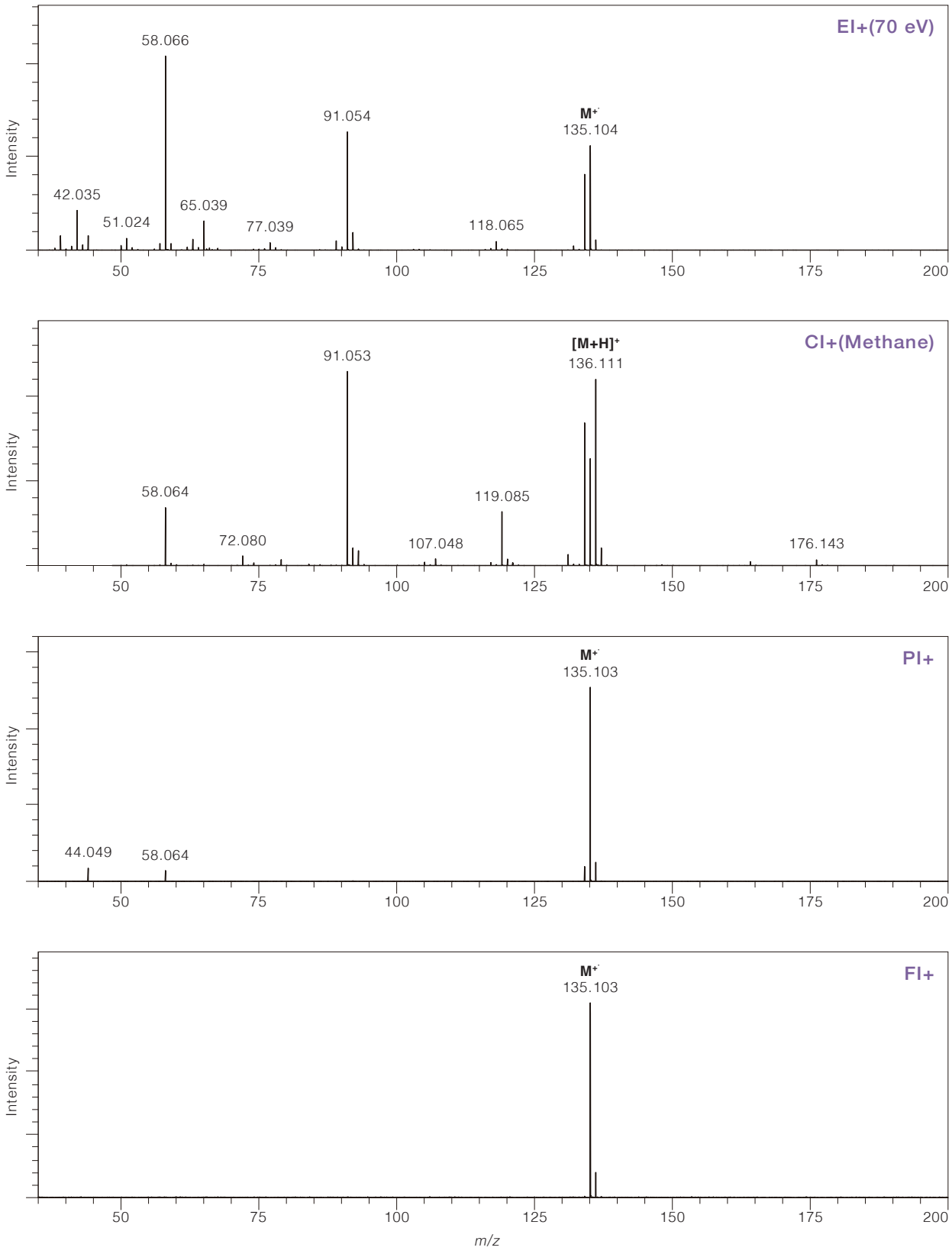


N,N-Dimethylbenzylamine

CAS No.103-83-3

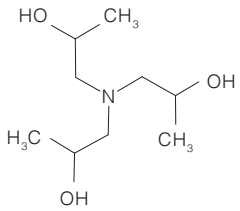


$C_9H_{13}N$=135

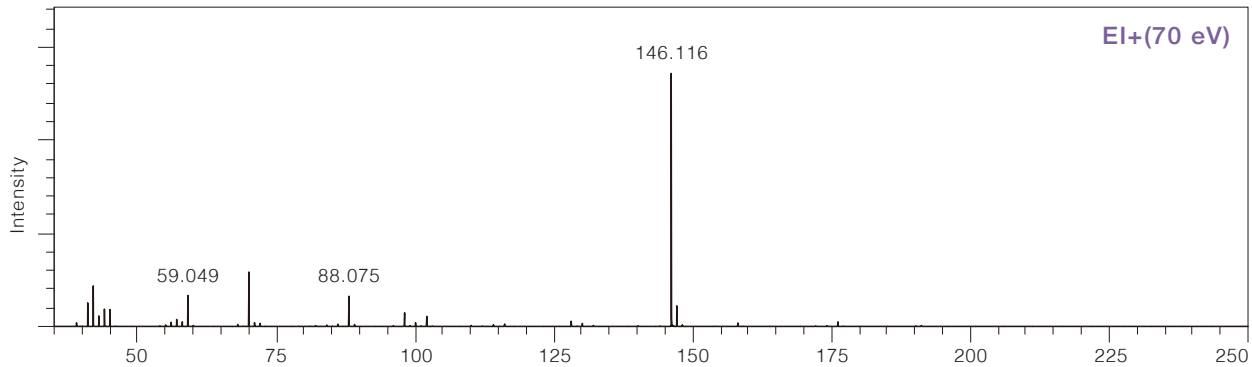


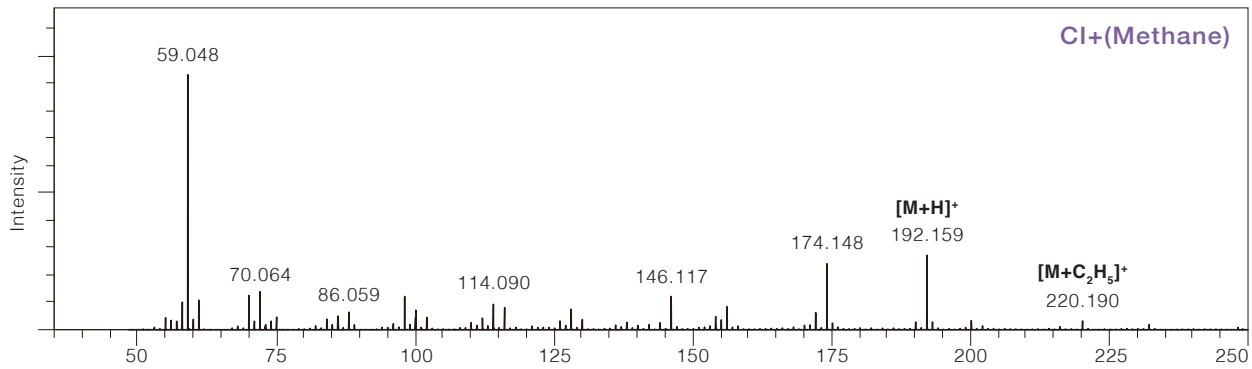
Triisopropanolamine

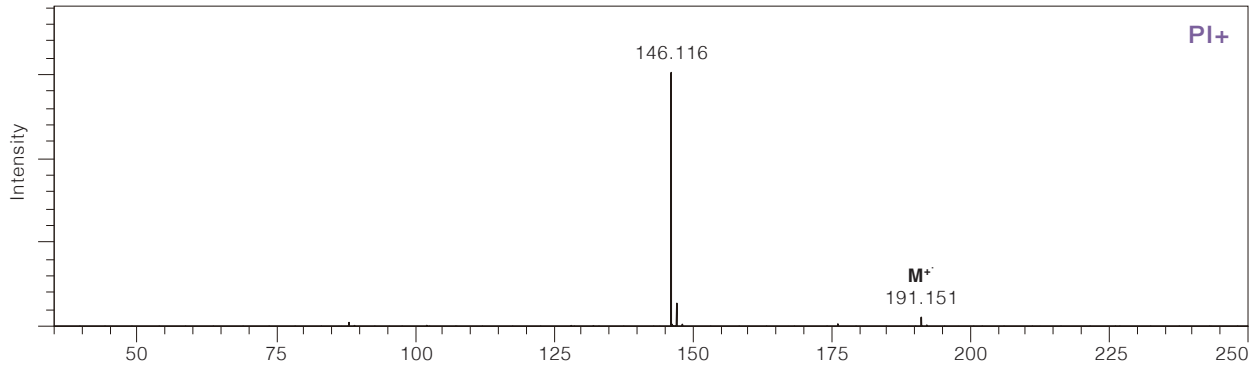
CAS No.122-20-3

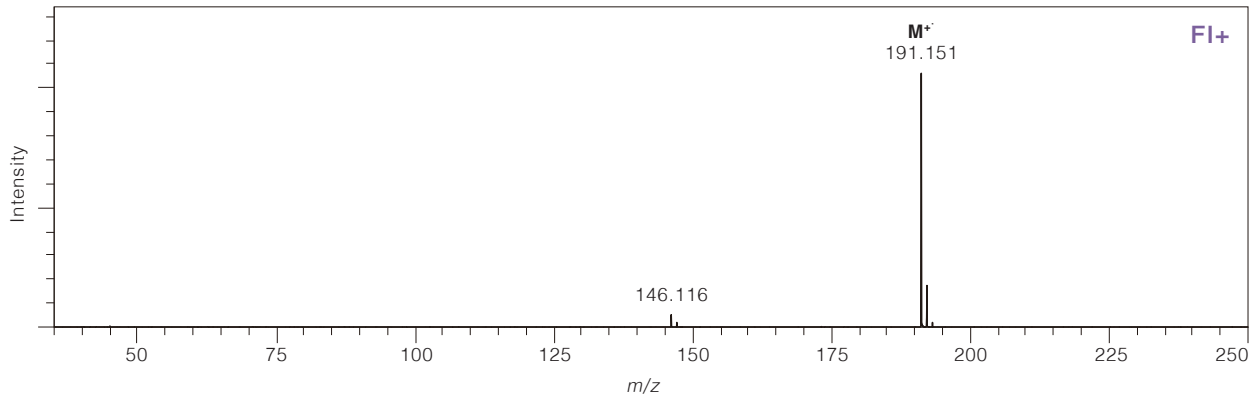


$C_9H_{21}NO_3$=191





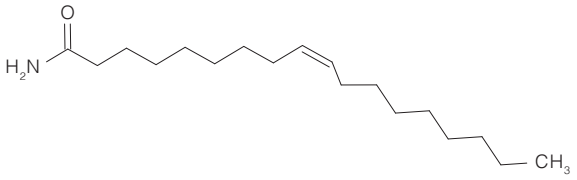




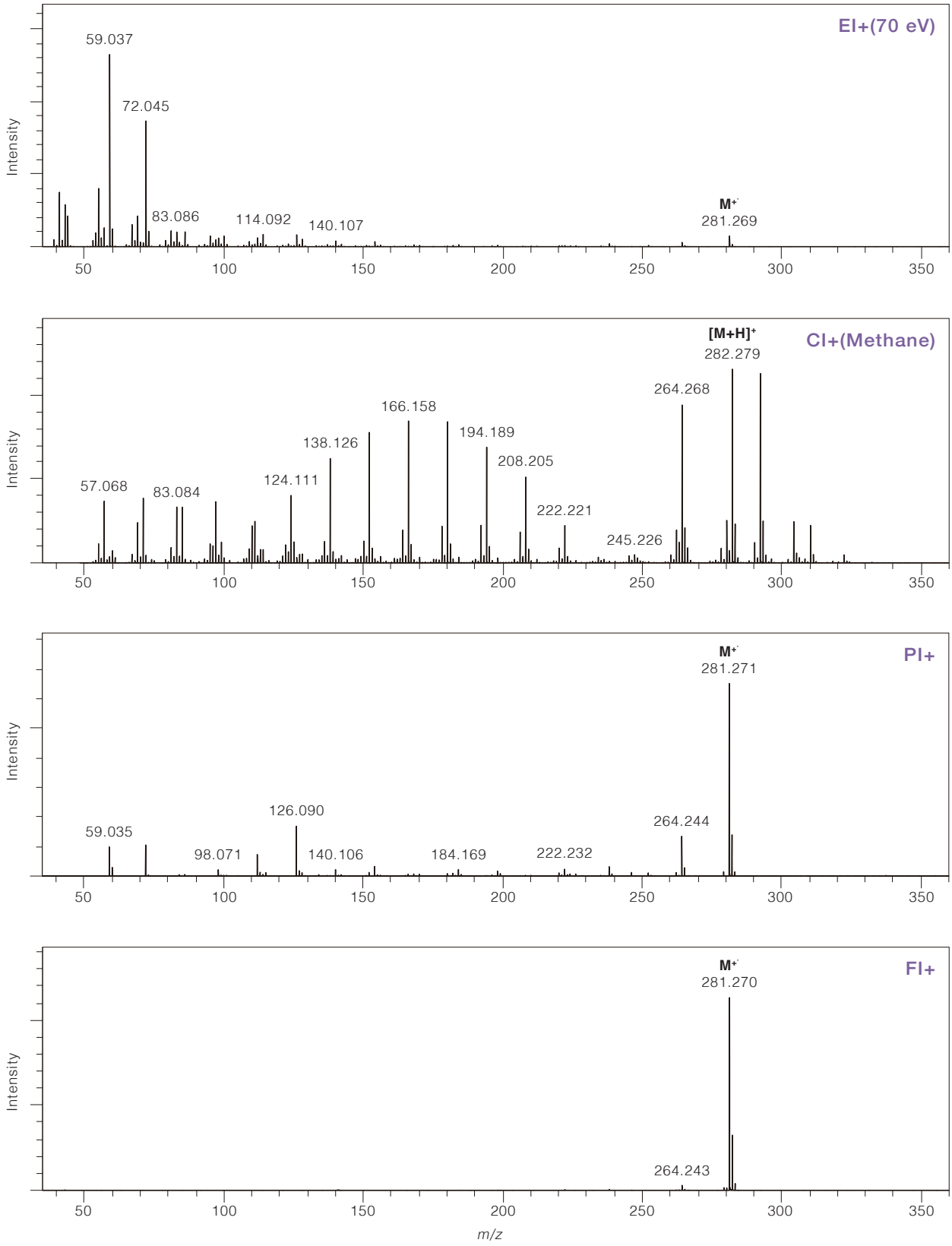
Fatty acid amides

Oleamide

CAS No.301-02-0



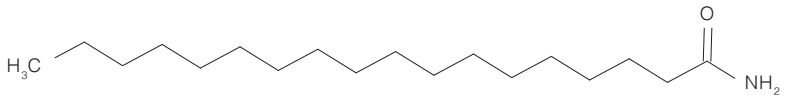
$C_{18}H_{35}NO$=281



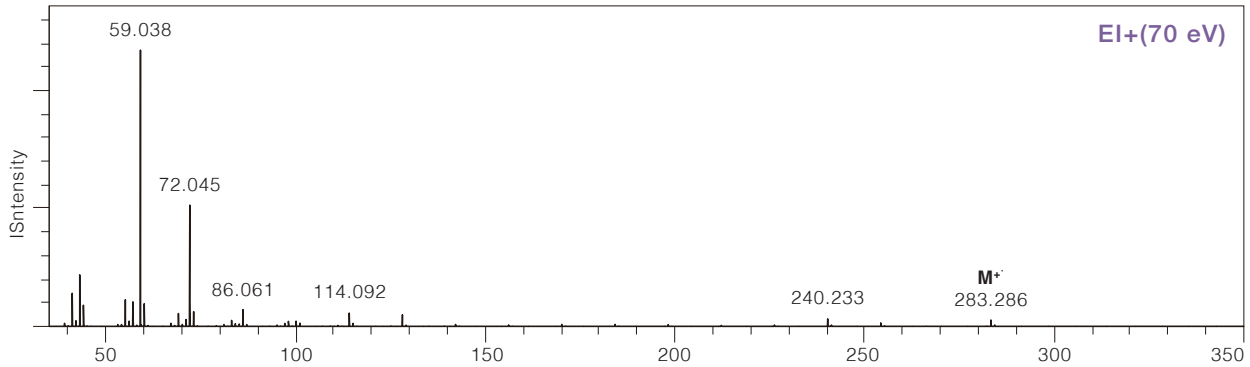
Fatty acid amides

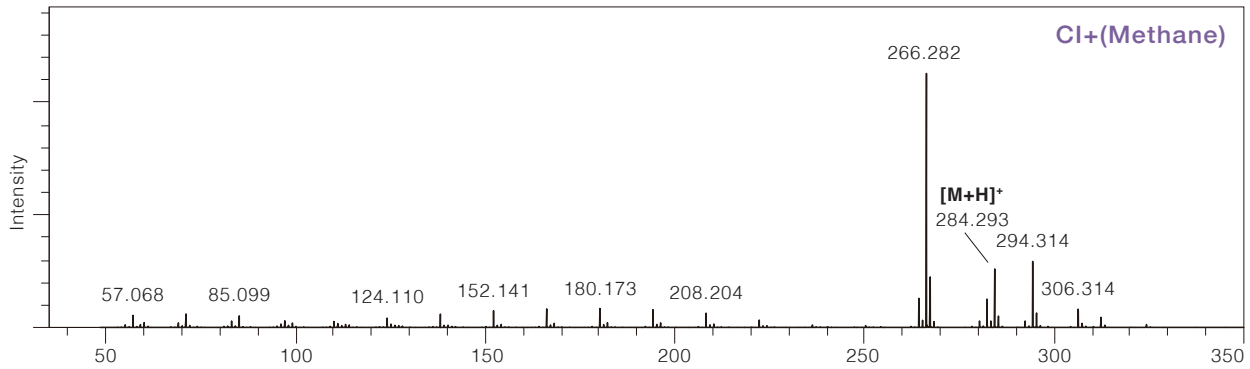
Stearamide

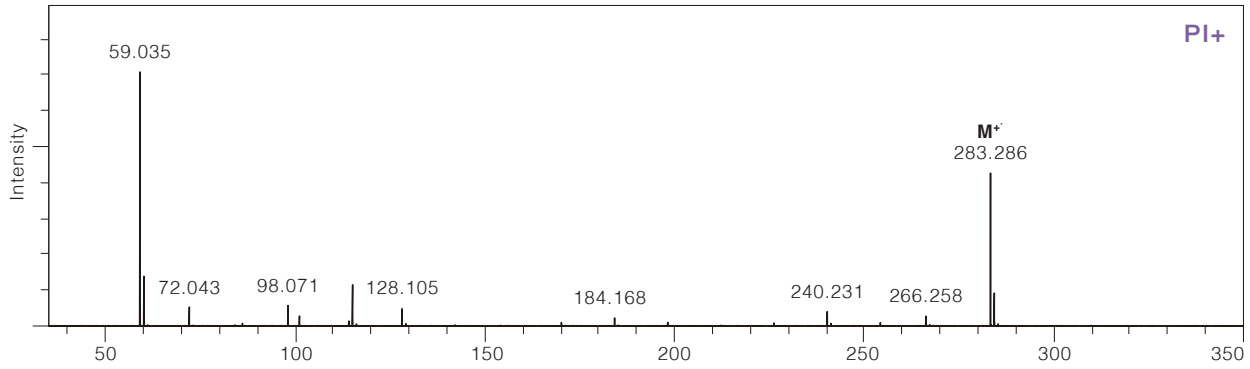
CAS No.124-26-5

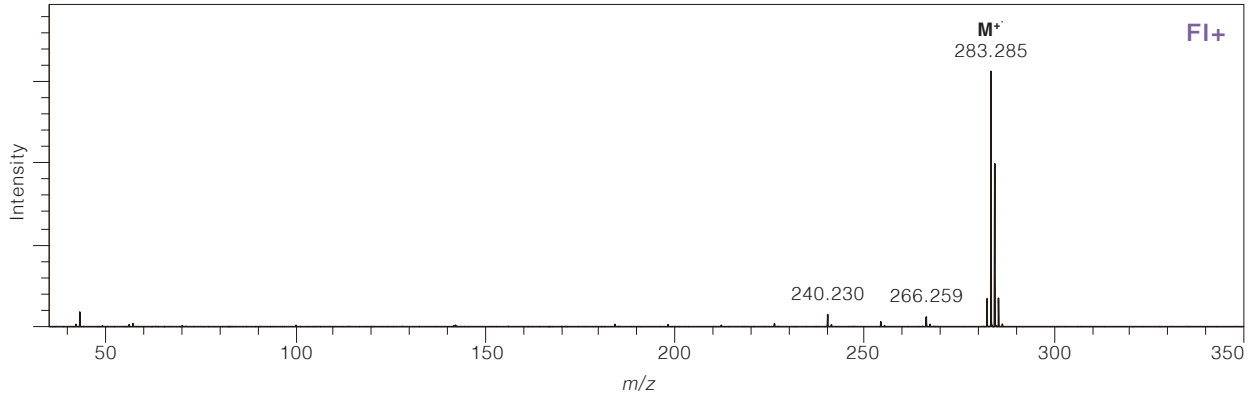


$C_{18}H_{37}NO$=283





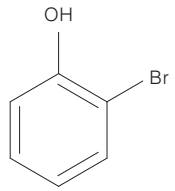




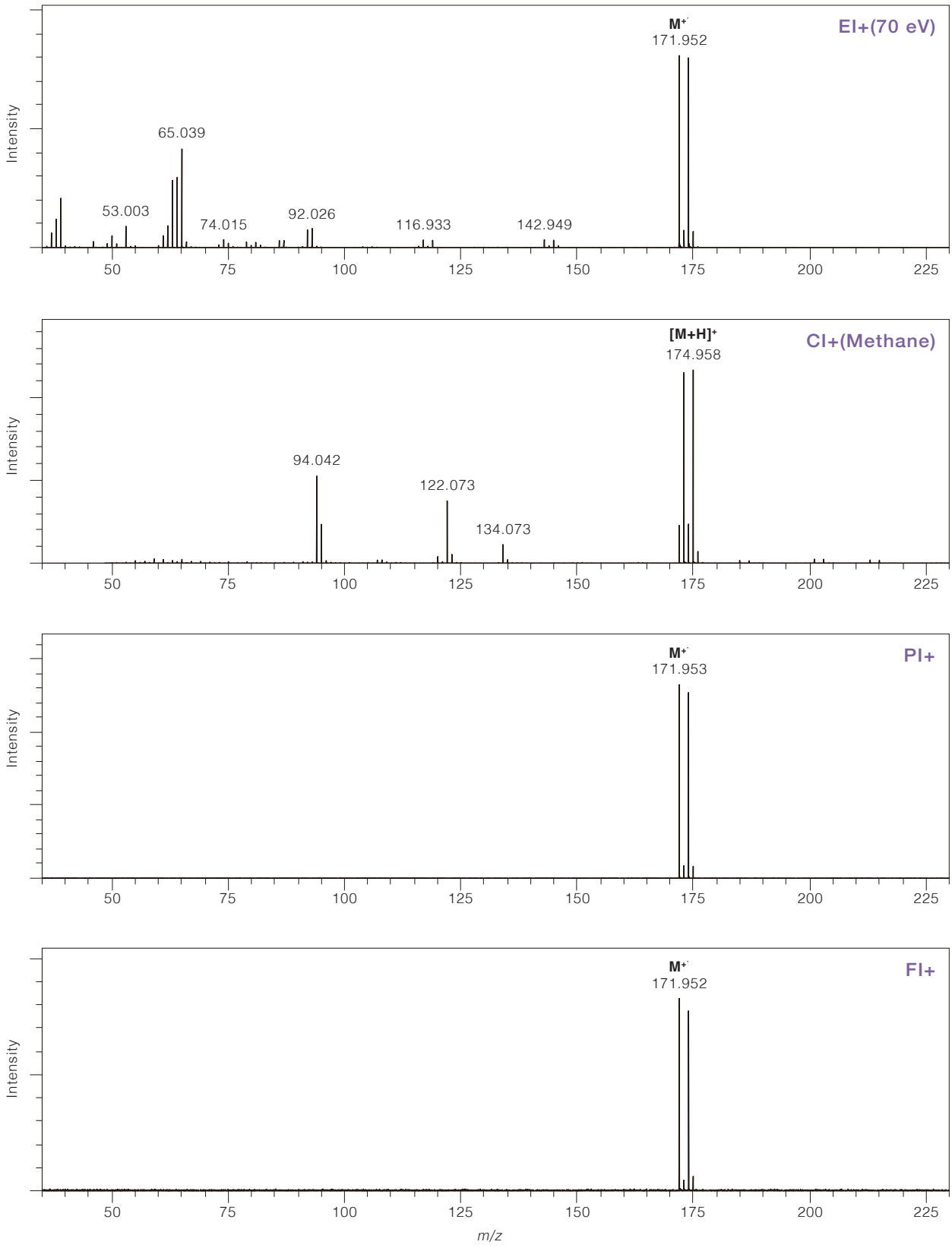
Halogen compounds

2-Bromophenol

CAS No.95-56-7

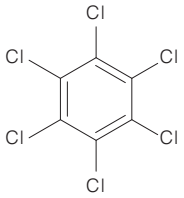


C_6H_5BrO=173

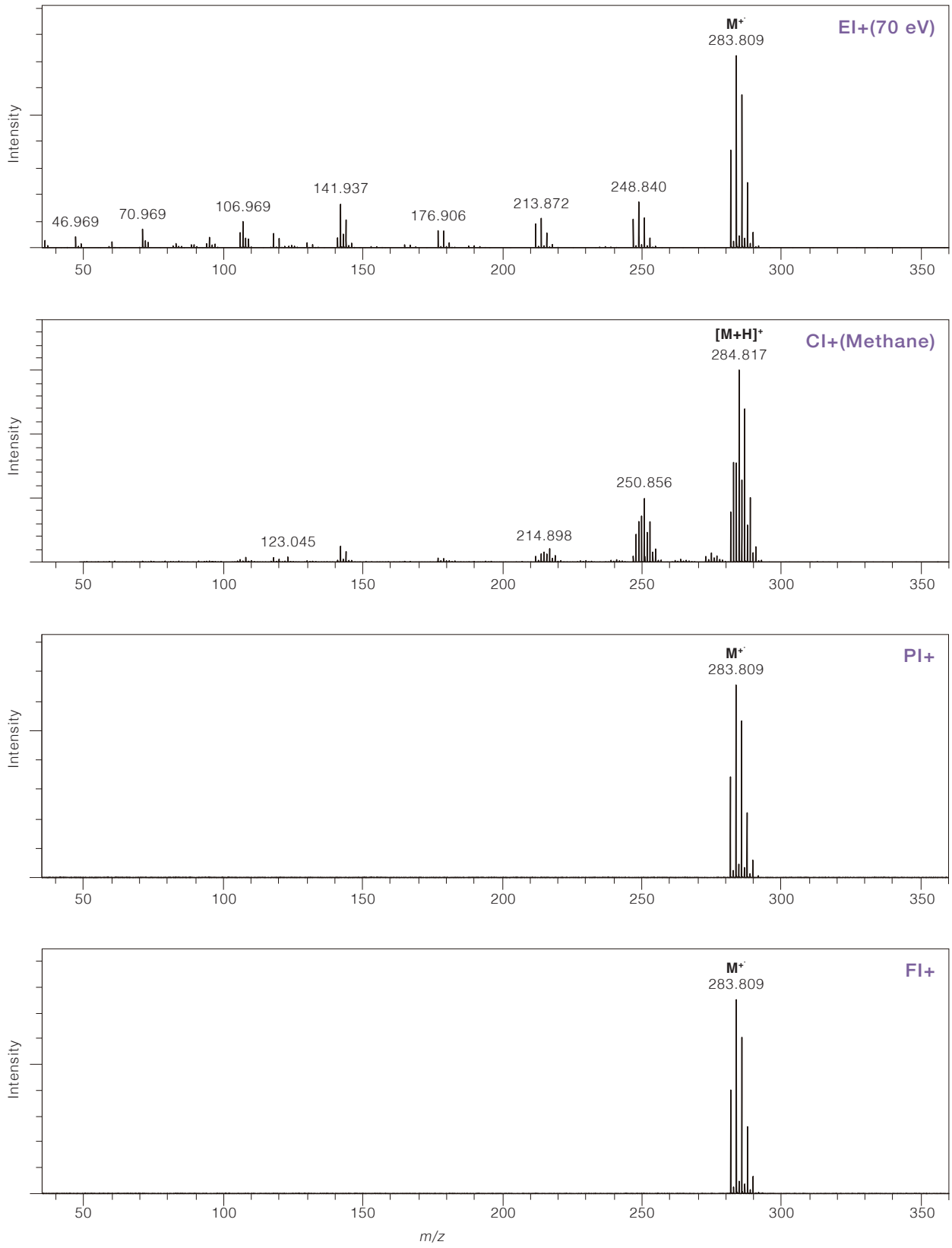


Hexachlorobenzene

CAS No.124-26-5



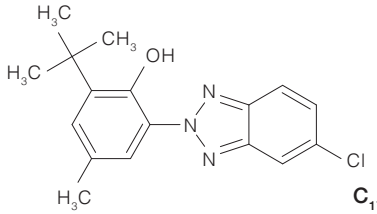
C_6Cl_6=284



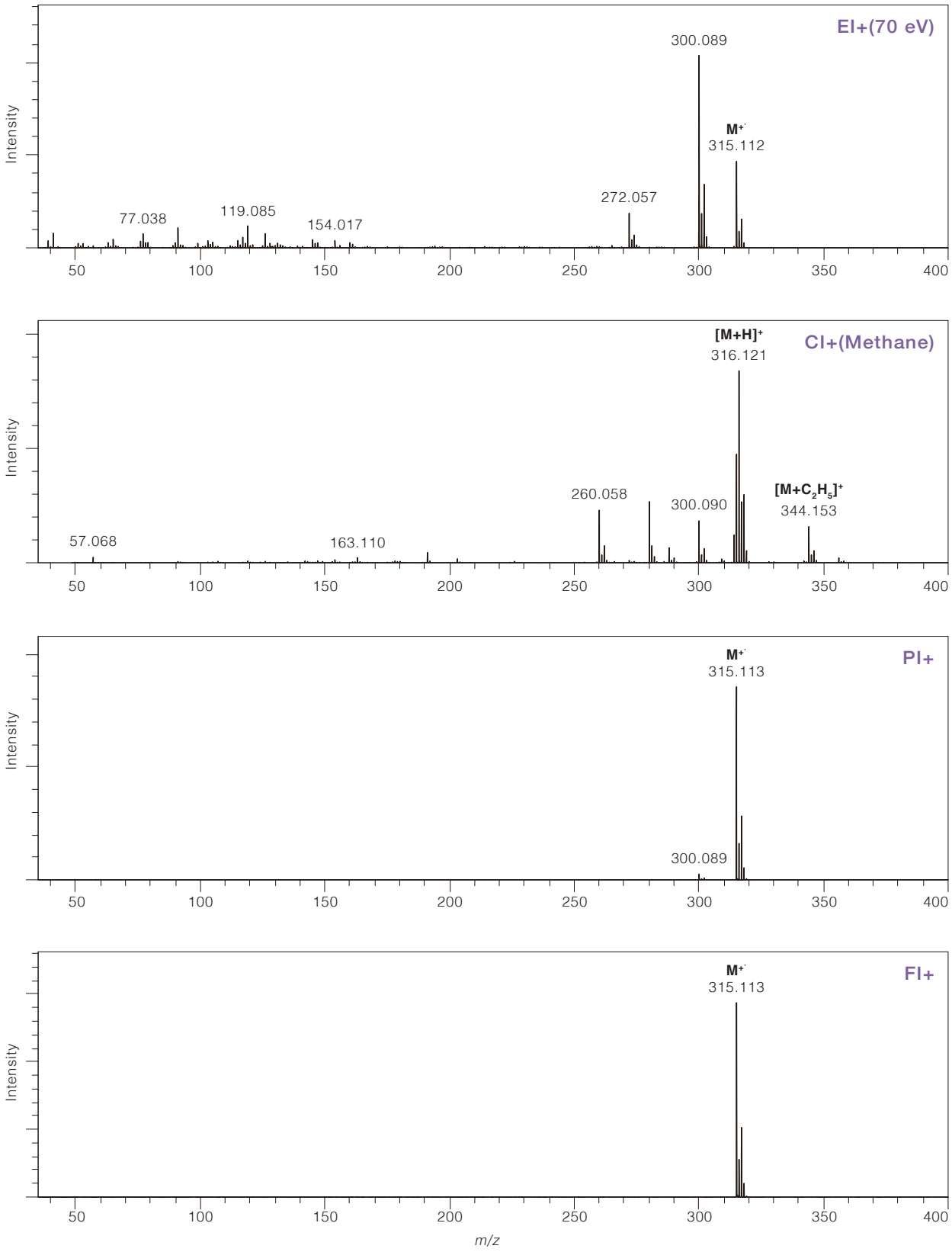
Halogen compounds

2-t-Butyl-6-(5-chloro-2 H-benzotriazol-2-yl)-4-methylphenol [Tinuvin326]

CAS No.3896-11-5



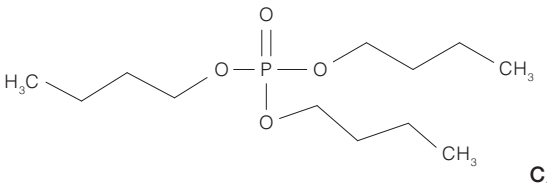
$C_{17}H_{18}ClN_3O$=315



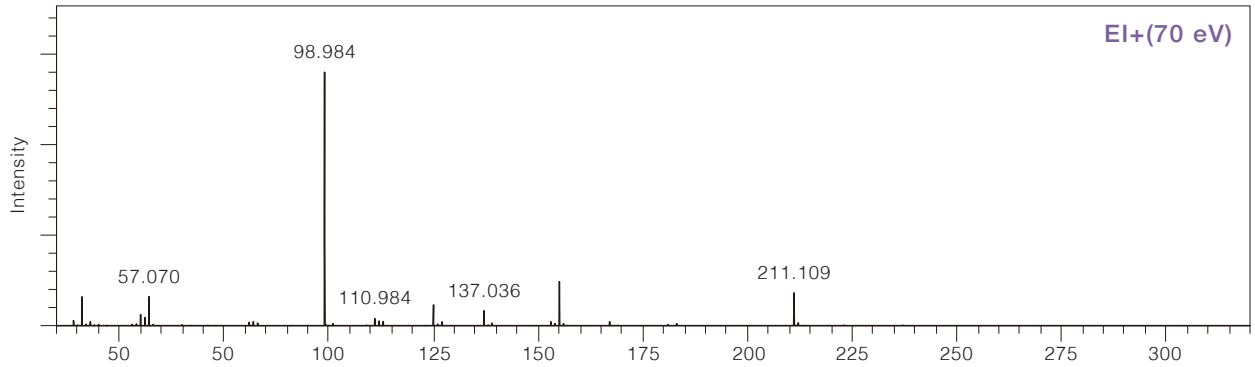
Phosphorus compounds

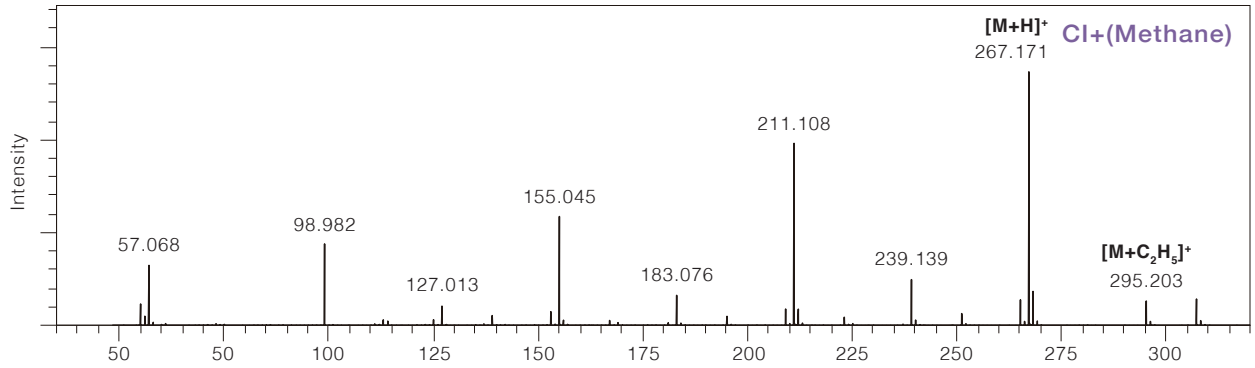
Tributyl Phosphate

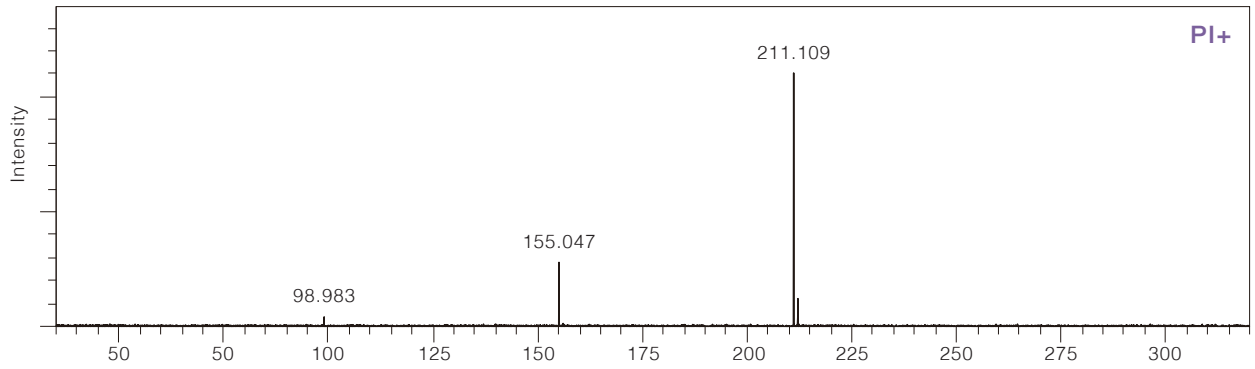
CAS No.126-73-8

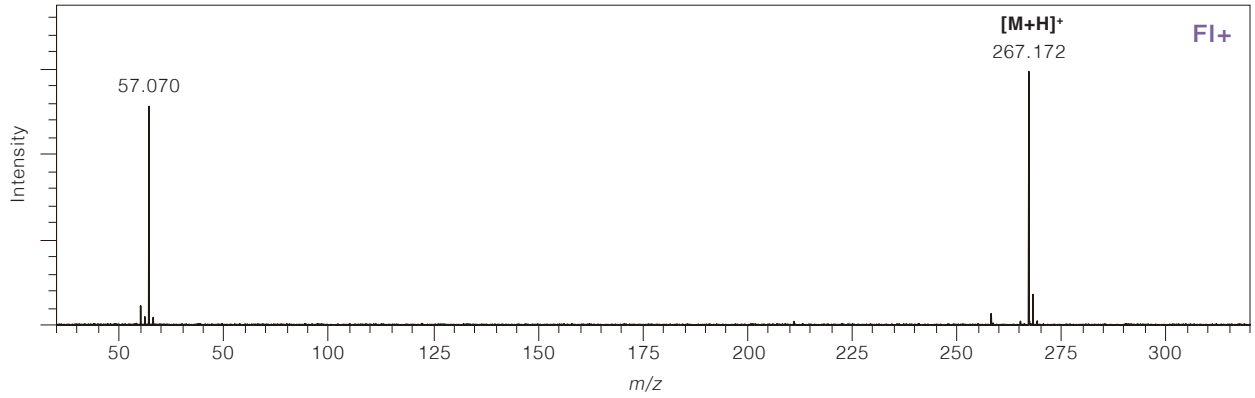


$C_{12}H_{27}O_4P$=266





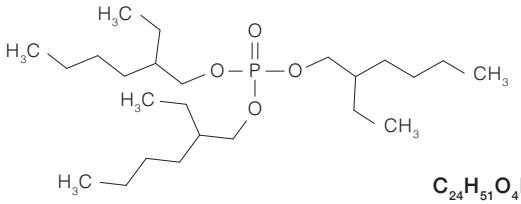




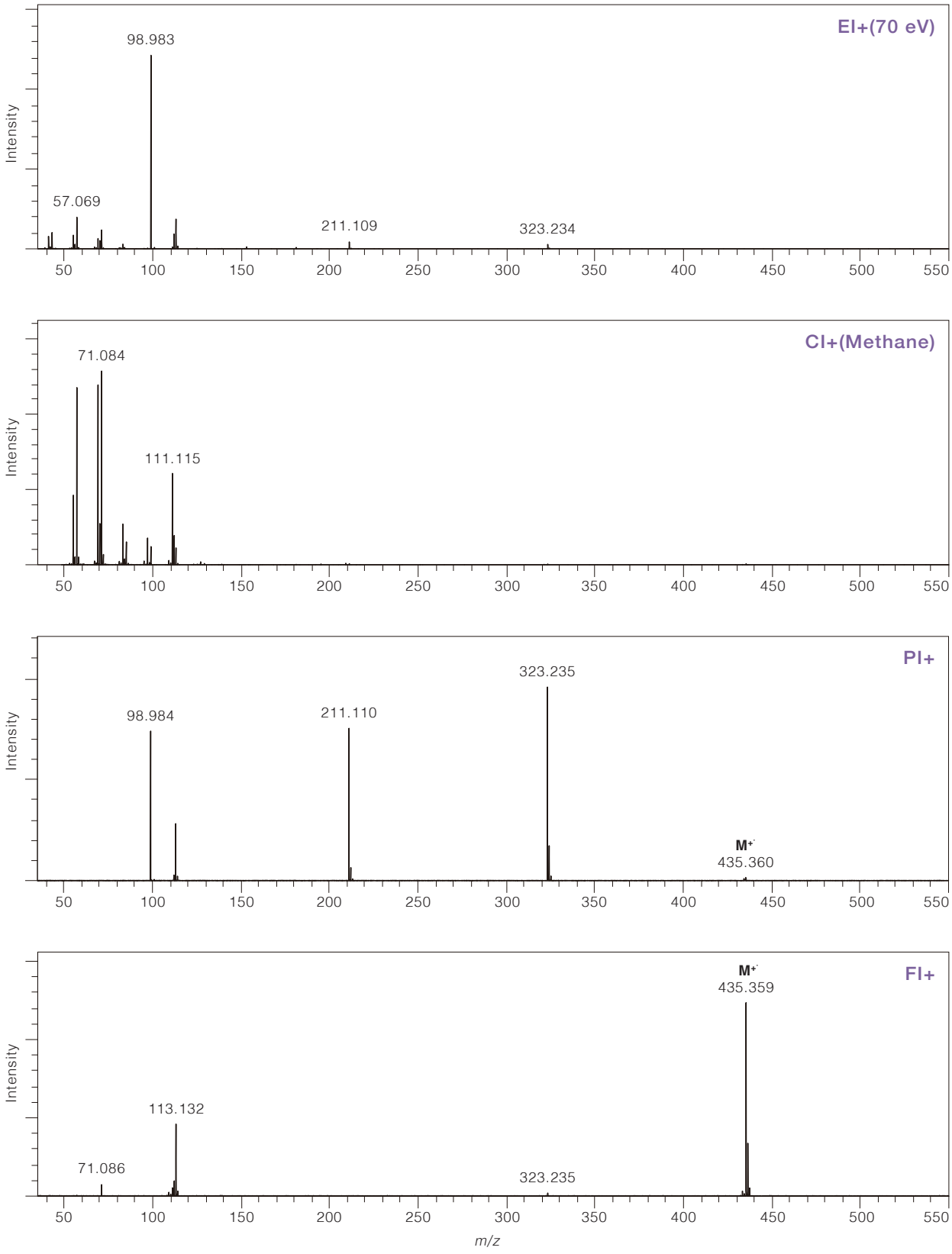
Phosphorus compounds

Tris(2-ethylhexyl) Phosphate

CAS No.78-42-2



$C_{24}H_{51}O_4P$=434



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