

GC-MS investigation of VX stored in a steel container

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Sammendrag

En stålcontainer med innhold av det kjemiske stridsmidlet VX har vært lagret i mer enn 40 år ved FFI ved -18 °C. Innholdet ble analysert ved hjelp av GC-MS med hensyn på VX og VX nedbrytningsforbindelser i både EI- og CI mode. Prøven inneholdt 74 % VX. En vial med VX som sannsynligvis stammer fra samme VX-container og som har blitt brukt til uttak i mange år, hadde en mengde på 69 % VX. I tillegg til VX, ble femten andre forbindelser identifisert i vialen, mens fjorten av de femten forbindelsene ble identifisert i containeren. Identifikasjonen ble basert på tolking av EI spektra, molekylmasse bestemmelse ved hjelp av CI, retensjons indeks (RI) og beskrivelser og tolkninger i forskjellige publikasjoner. Mengden av de forskjellige nedbrytningsforbindelser er forholdsvis like i vialen og containeren bortsett fra Bis(2-diisopropylaminoethyl) disulfide som har økt fra ca 6 % til 13 % og 1,3-dicyclohexylcarbodiimide som har minket fra 5 % til 2 % i vialen.

English summary

A steel container containing the chemical agent VX which has been stored at $-18\text{ }^{\circ}\text{C}$ for more than forty years has been analysed for VX and VX degradation compounds with GC-MS both at EI- and CI mode. The content of VX is 74 % compared to the “daily use” vial which is 69 %. Fifteen VX degradation compounds were identified in the vial, while fourteen compounds in the container. The identification is based on interpretation of EI spectra, provided molecular ion in CI, retention indices (RI) and publications. The amount of the degradation compounds is almost the same in the two samples except Bis(2-diisopropylaminoethyl) disulfide which decreases from ca 6 % to 13 % and 1,3-dicyclohexylcarbodiimide which increases from 5 % to 2 % in the vial.

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1 Introduction

The organo phosphorous compounds known as V type nerve agents were discovered in the mid-fifties. The full-scale production of VX (O-Ethyl S-[2-(diisopropylamino) ethyl] methylphosphonothiolate) was commenced in April 1961, but the chemical structure of the compound was not made public until 1972.

At our laboratory, a steel container filled with VX (Figure 1.1), has been stored in a freezer for many years. The exact history of this container is not well known, but it is reason to believe that can be dated back to around 1964. It was probably supplied by US Army Chemical Corps Europe [1]. The primary purpose of this study was to investigate a long time stored VX sample as basic compounds and possible decomposition products using gas chromatograph- mass spectrometer (GC-MS) in electron impact (EI) and chemical ionization (CI) mode. Compound identification was based on information about the molecular size from CI spectra, MS spectral data and GC retention indices (RI) RI is based on calculation using n-alkanes ($C_8 - C_{22}$) as index standards and GC-columns with stationary phase 95 % dimetyl/5 % phenyl silicone; such as SE-54, CP-Sil 8 and DB-5.

The VX sample has been stored in a closed steel container for more than 40 years at $-18\text{ }^{\circ}\text{C}$ and has probably been opened only once since it arrived at the institute. A sample from a 5 ml Microflex glass vial with VX (“daily use”) was also analysed. This vial has been stored in a freezer and the VX content is probably taken from the same steel container.



Figure 1.1 Steel container where VX was stored for more than 40 years

2 Experimental

2.1 Chemicals

1 mg samples of VX from the steel container and the glass vial were dissolved in 10 ml dichloromethane (CAS No 75-09-2), ultra resi-analyzed from J Baker. Before analyses the VX sample was diluted to a concentration of 50 ng/ μ l.

2.2 Instrumentation

The analyses was performed with a Fisons MD800 mass spectrometer coupled to a Fisons 8060 gas chromatograph. The GC-column used for the instrument was 30 m x 0.25 mm with 0.25 μ m DB-5 MS stationary phase from J&W Inc.

The GC conditions for the analyses were an oven temperature programmed from 40°C (1 min) – 10 °C/min – 280 °C (10 min) and He (grade 6.0) used as carrier gas with a flow rate of 1 ml/min. 1 μ l of the sample was injected splitless for 1 minute. Other instrumental parameters used are shown in Table 2.1.

Parameter	GC: Fisons GC 8060 MS: Fisons MD800/250	
	EI	CI
Injector temp (°C)	220	220
Transfer line temp (°C)	260	260
Ion Source temp (°C)	190	150
Electron energy (eV)	70	70
Scan range (amu)	35 - 600	100 - 600
Scan time (sec)	0.6	0.6
Reagent gas		Ammonia or methane

Table 2.1 Instrumental parameters used for MS analysis

3 Results and discussion

Figure 3.1 illustrates an EI chromatogram of the VX sample taken from the vial. The total ion chromatogram (TIC) shows several impurities in the VX sample. A total of sixteen compounds were identified in the diluted sample from the vial and fifteen compounds were identified in the container. The compound No **10** was only detected in the vial. No derivatization of the sample was carried out for identifying possible polar degradation products from the stored VX sample. The identification was based on library EI spectra, CI, RI and publications.

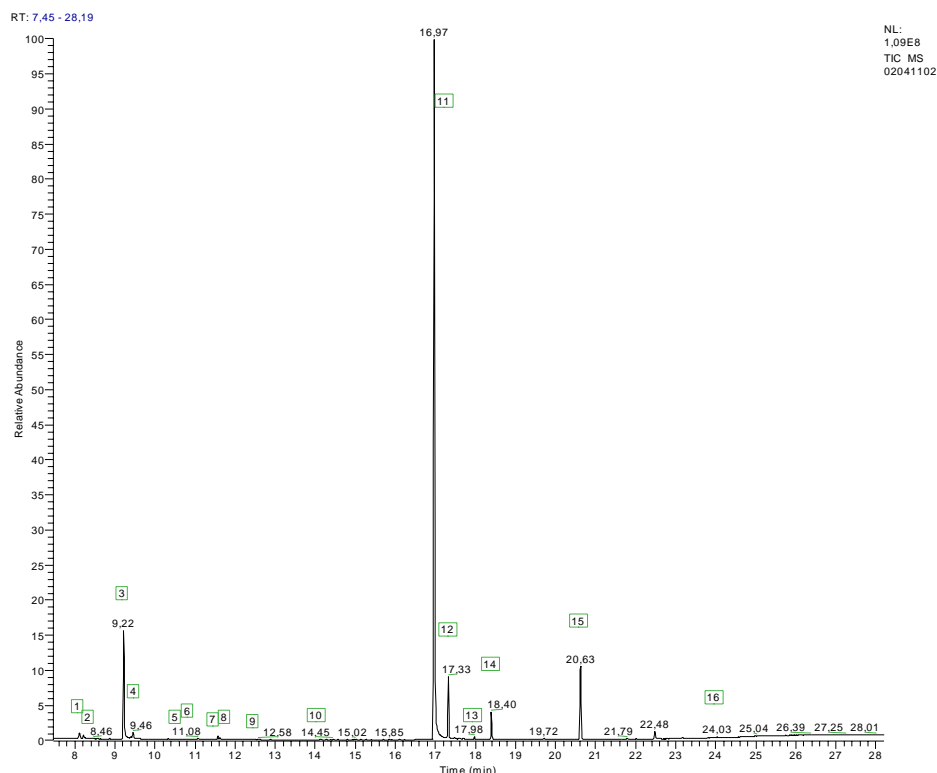


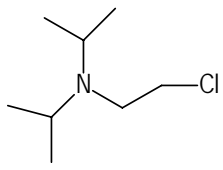
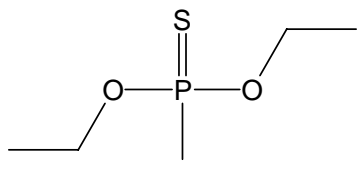
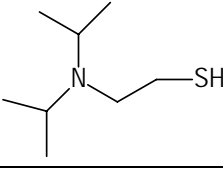
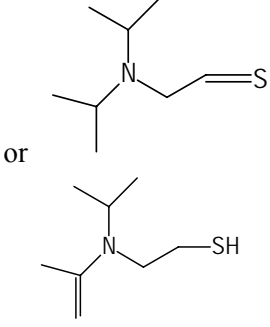
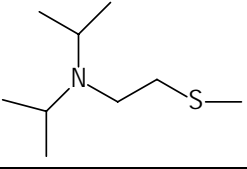
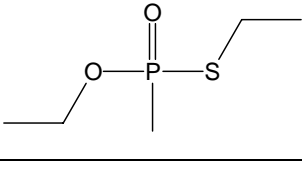
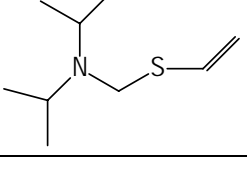
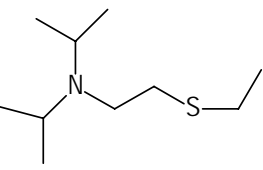
Figure 3.1 GC chromatogram of VX from vial. The numbers indicate the identified compounds

Compounds No 6 and 10 gave no CI spectra at the expected retention time. The EIMS- and CIMS- spectra from the sixteen compounds are given in Appendix A.

Identification of all the VX degradation products based on only EI is difficult. Many of the degradation products obtained in the chromatogram contain the diisopropylaminoethyl group with fragments dominated by the ion m/z 114, $[i\text{-Pr}_2\text{N}=\text{CH}_2]^+$. The EI-spectra are almost similar and show little or no molecular ion information for identification of the compounds. Use of CI reagent gases gives information of the molecular ions $(M+H)^+$ and some other characteristics fragment ions [2]. The molecular information from CI depends also on the molecular behaviour, the reagent gas and the concentration of the compounds. In this study both ammonia and methane were used as reagent gases. Ammonia is a “softer” reagent gas and will give less fragmentation and more information about the molecular ions than methane. In this experiment ammonia is the best reagent gas (Table 3.1).

The GC retention indices (RI) available in the literature are used to support the identification and confirmation of the suggested components in the VX samples. Compounds No 1, 2, 3, 8, 11-16 have matching RI with literature. Together with EI-spectra matched from library and molecular identification (CI) they were identified as listed in Table 3.1.

In the GC-chromatogram, compound No 6 has a low response and because of the tailing it is difficult to decide the exact RI. Because of the low concentration, there are also no CI responses with ammonia or methane at the expected retention time and this make the identification uncertain.

No	Compound	CI-gas	Structure	CAS #	MW	RI
1	2- <i>N,N</i> -Diisopropyl aminoethyl-chloride	NH ₃		96-79-7	163	1049 ¹ 1052 ³ 1039 ⁴
2	<i>O,O</i> -Diethyl methylphosphonothioate	NH ₃ CH ₄		6996-81-2	168	1056 ¹
3	2-(Diisopropylamino) ethanethiol (DESH)	NH ₃ CH ₄		5842-07-9	161	1120 ¹ 1114 ² 1120 ³
4 *	2-(Diisopropylamino)ethanethiol or 2-[isopropyl(prop-1-en-2-yl)amino]ethanethiol	NH ₃			159	1136 ¹
5 *	2-(Diisopropylamino)ethyl methyl sulfide	NH ₃		63346-69-0	175	1206 ¹
6 *	<i>O,S</i> -diethyl methylphosphonothioate	neg		2511-10-6	168	1200 ¹ 1174 ² 1174 ³ 1178 ⁴
7 *	2-(Diisopropylamino)ethyl vinyl sulfide	NH ₃			187	1277 ¹
8	2-(Diisopropylamino)ethyl ethyl sulfide	NH ₃		110501-54-7	189	1280 ¹ 1278 ²

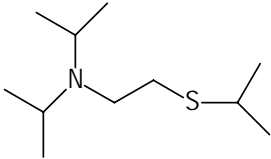
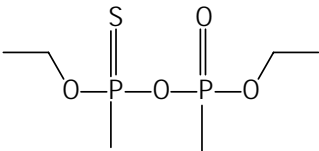
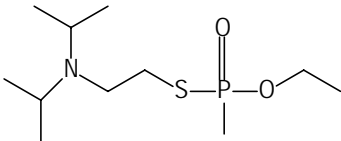
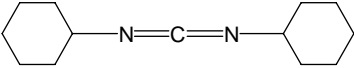
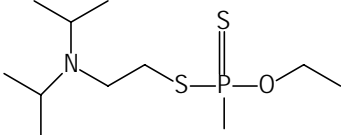
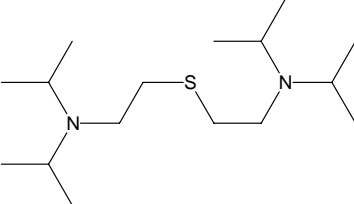
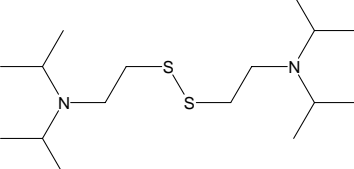
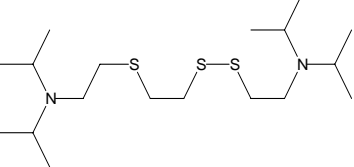
No	Compound	CI-gas	Structure	CAS #	MW	RI
9 *	2-(Diisopropylamino)ethyl isopropylsulfide	NH ₃			203	1348 ¹
10 *	O,O-Diethyl dimethylmonothionopyrophosphate	neg			246	1453 ¹
11	VX (O-ethyl S-2-diisopropylaminoethyl methylphosphonothiolate)	NH ₃ CH ₄		50782-69-9	267	1702 ¹ 1705/ 1713 ² 1713 ³ 1721 ⁴
12	1,3-dicyclohexylcarbodiimide	NH ₃ CH ₄		538-75-0	206	1734 ¹
13	O-Ethyl S-[2-(diisopropylamino)ethyl] methylphosphonodithiolate	NH ₃		161488-46-6	283	1793 ¹ 1793 ²
14	Bis(2-diisopropylaminoethyl) sulfide	NH ₃		110501-56-9	288	1831 ¹ 1836 ² 1855 ⁴
15	Bis(2-diisopropylaminoethyl) disulfide	NH ₃ CH ₄		65332-44-7	320	2053 ¹ 2058/ 2065 ²
16	1,9-Bis(diisopropylamino)-3,4,7-trithianonane	NH ₃		110501-59-2	380	2568 ²

Table 3.1 The names, molecular weights, structures, CAS No and RI related to VX and degradation products identified in the steel container and the daily use vial

¹RI calculated in this experiment

²RI from Nato (Canada, Denmark or Finland)

³RI from OPCW

⁴RI from FFI, MAT95Q

* suggested compound

Identification of compounds No **4**, **5**, **7** and **9** is based on CI spectra and presumptions and discussion in different publications [2-4].

CI spectra of compound No **4** gave 100 % of the protonated molecular ion together with typical fragmentation ions (m/z 100, 102, 128, 130) when using ammonia as reagent gas [2]. The spectral data is almost equal to what Rohrbaugh has reported. He suggest that the structure may be HSCH₂CH₂N(*i*-Pr)(C[Me]=CH₂) [3], while some years later [4] he suggested the structure to be *i*-Pr₂NCH₂CH₂CH=S both based on EI and CI mass spectral interpretation and retentions time behaviour. The compound in our experiment is probably *i*-Pr₂NCH₂CH₂CH=S because the compound is more similar to the other structures identified.

The compound No **7** is identified as 2-(Diisopropylamino)ethyl vinyl sulphide. This is based on EI spectra, a dominated pseudo-molecular ion in ammonia CI and a comparison with reported results [3;4].

Both compounds No **5** and **9** are dominated by the pseudo-molecular ions (M+1)⁺ in ammonia CI mass spectra. Compared to the identification of twenty-three different VX degradation compounds D'Agostino et al. [2] have reported using ammonia as reagent gas, it is probable that compound No **5** is 2-(Diisopropylamino)ethyl methyl sulfide and compound No **9** is 2-(Diisopropylamino)ethyl isopropylsulfide.

Compound No **10** (O,O-Diethyl dimethylmonothionopyrophosphate) is based on the EI spectra and publications [4;5]. This compound is a decomposition product in VX samples. The compound is only detected in the “daily use” vial (Table 4.1) at EI mode.

4 Conclusions

In addition to VX, fifteen (fourteen from the container) different compounds were identify based on GC-MS (EI and CI). A large number of compounds in the samples with mass 114 which were not identified. Table 4.1 gives a list of the amount of the different compounds identified in the samples.

Compound No	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Vial, %	0.3	0.3	9.8	0.8	<0.1	<0.1	0.2	0.1	0.2	<0.1	69	2	0.2	2.4	13.5	0.5
Container, %	0.5	0.4	9.2	0.5	<0.1	<0.1	0.3	0.2	<0.1	ND	74	5	0.2	1.9	6.3	0.1

Table 4.1 The percent amount of each compound in the container and the “daily use” VX vial
ND = not detected

After more than 40 years storage at – 18 °C in a steel container the contents of VX is 74 % compared to the “daily use” vial which is 69 %. The amount of the degradation compounds are comparable in the two

samples, except for Bis(2-diisopropylaminoethyl) disulfide (No **15**) which had an increase from about 6 % in the container to 13 % in the vial. Compound No **10** is observed only in the vial

Compound No **12**, 1,3-dicyclohexylcarbodiimide, is a stabilizer commonly added to VX [2]. The percent amount of carbodiimide has decreased in the vial compared to the container. Two degradation compounds from the carbodiimide were also identified. *N,N'*-dicyclohexylthiourea were detected in both samples while 1,3-dicyclohexylurea was detected only in the vial.

References

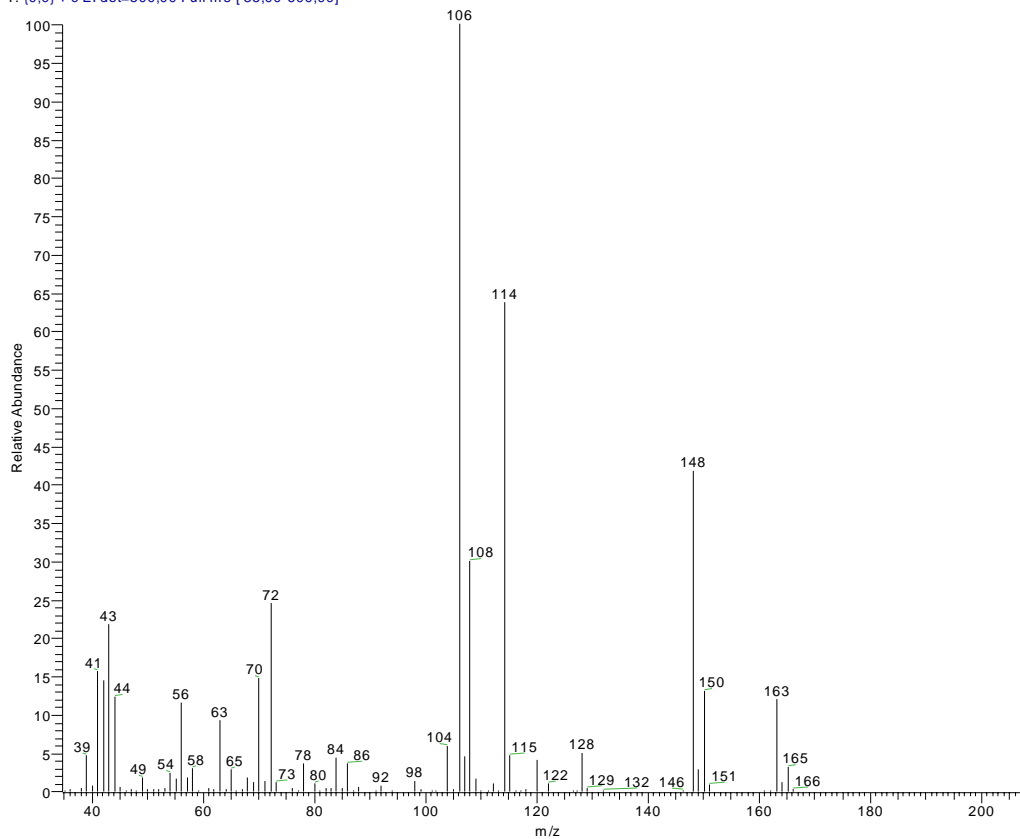
- [1] J. A. B. Barstad and F. Fonnum, "Technical note on reactivation and ageing of acetylcholinesterase inhibited by VX," Nov. 1964.
- [2] P. A. D'Agostino, L. R. Provost, and J. Visentini, "Analysis of *O*-ethyl *S*-(2-diisopropylamino)ethyl) methylphosphonothiolate (VX) by capillary column gas chromatography-mass spectrometry," *Journal of Chromatography*, vol. 402, pp. 221-232, 1987.
- [3] D. K. Rohrbaugh, "Characterization of equimolar VX-water reaction product by gas chromatography-mass spectrometry," *Journal of Chromatography*, vol. 809, pp. 131-139, 1998.
- [4] D. K. Rohrbaugh, "Methanol chemical ionization quadrupole ion mass spectrometry of *O*-ethyl *S*-(2-diisopropylamino)ethyl) methylphosphonothiolate (VX) and its degradation products," *Journal of Chromatography*, vol. 893, no. 2, pp. 393-400, 2000.
- [5] C. A. Boulet and P. A. D'Agostino, "Analysis of dimethylpyrophosphate decomposition products of VX by GC-MS/MS and ³¹P NMR," *Phosphorus, Sulfur, and Silicon*, vol. 104, pp. 93-101, 1995.

Appendix A MS-spectra

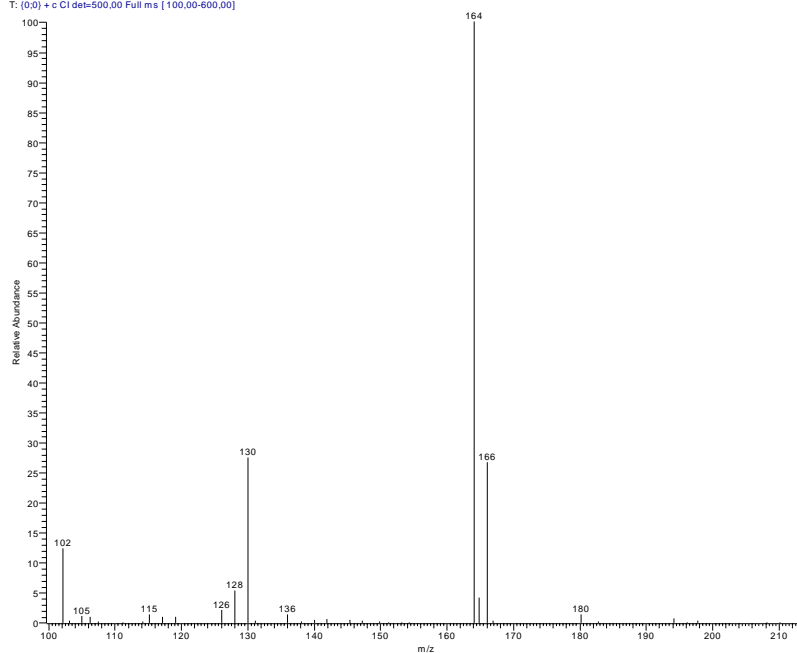
There is a difference in about 0.3 min between all the EI- and CI retention times because the column has been cut during the analysis.

- 1) 2-*N,N*-Diisopropyl aminoethyl-chloride (MW 163),
EIMS (upper) CIMS-ammonia (lower)

02041102 #560 RT: 8.11 AV: 1 SB: 15 7,98-8,06, 8,32-8,37 NL: 1,71E5
T: {0;0} + c EI det=500,00 Full ms [35,00-600,00]



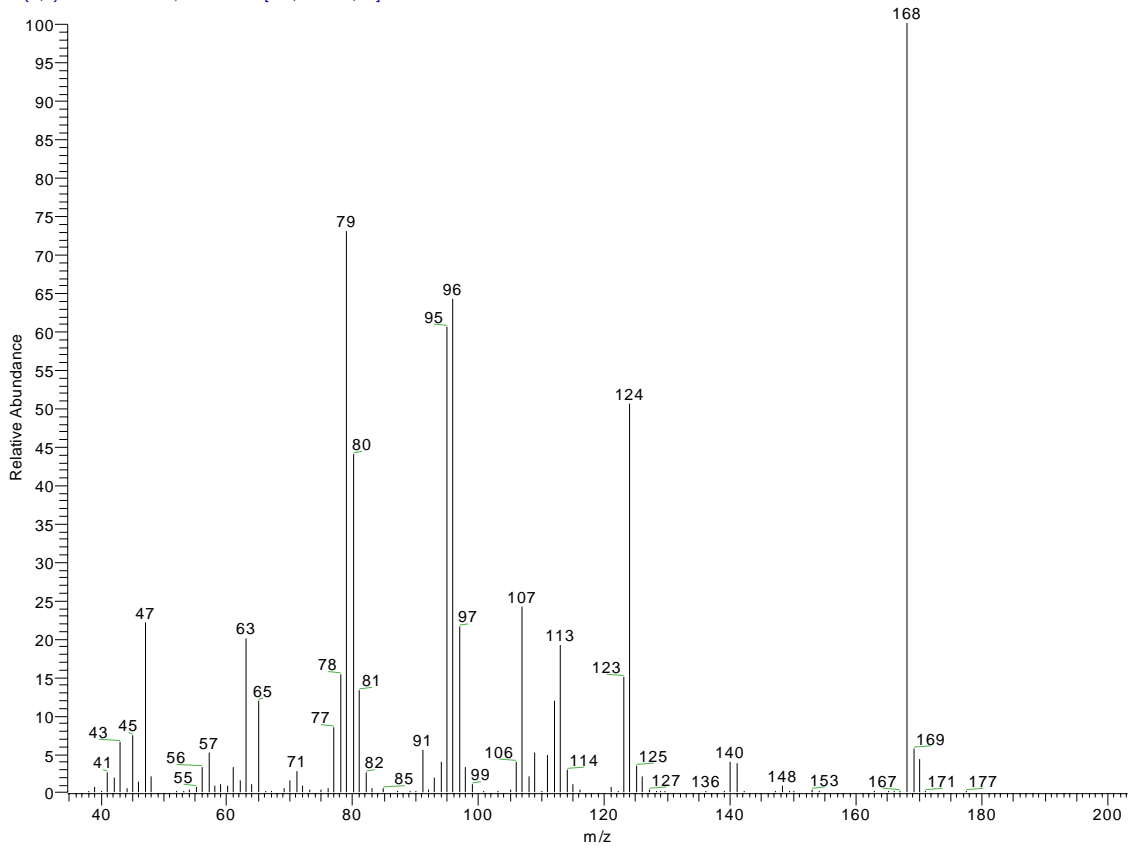
02053005 #538 RT: 7.88 AV: 1 SB: 23 7,64-7,74, 8,12-8,23 NL: 6,25E3
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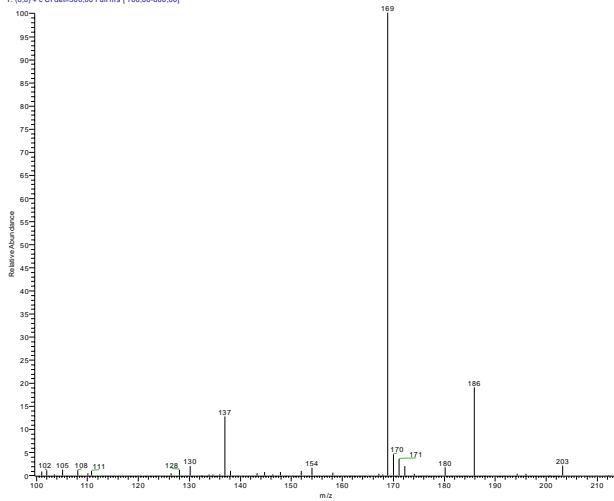
2) *O,O*-Diethyl methylphosphonothioate (MW 168)

EIMS (upper) CIMS-ammonia (lower right) CIMS-methane (lower left)

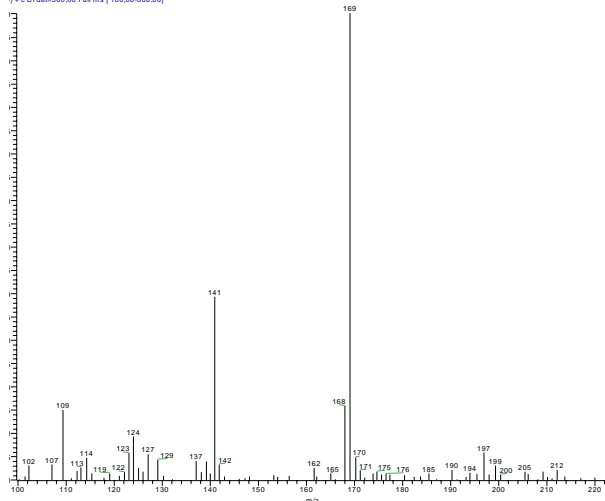
02041102 #570-574 RT: 8,21-8,25 AV: 5 SB: 23 7,90-8,02, 8,32-8,41 NL: 4,78E4
T: {0;0} + c EI det=500,00 Full ms [35,00-600,00]



02053005 #548 RT: 7,98 AV: 1 SB: 23 7,64-7,74, 8,12-8,23 NL: 6,88E3
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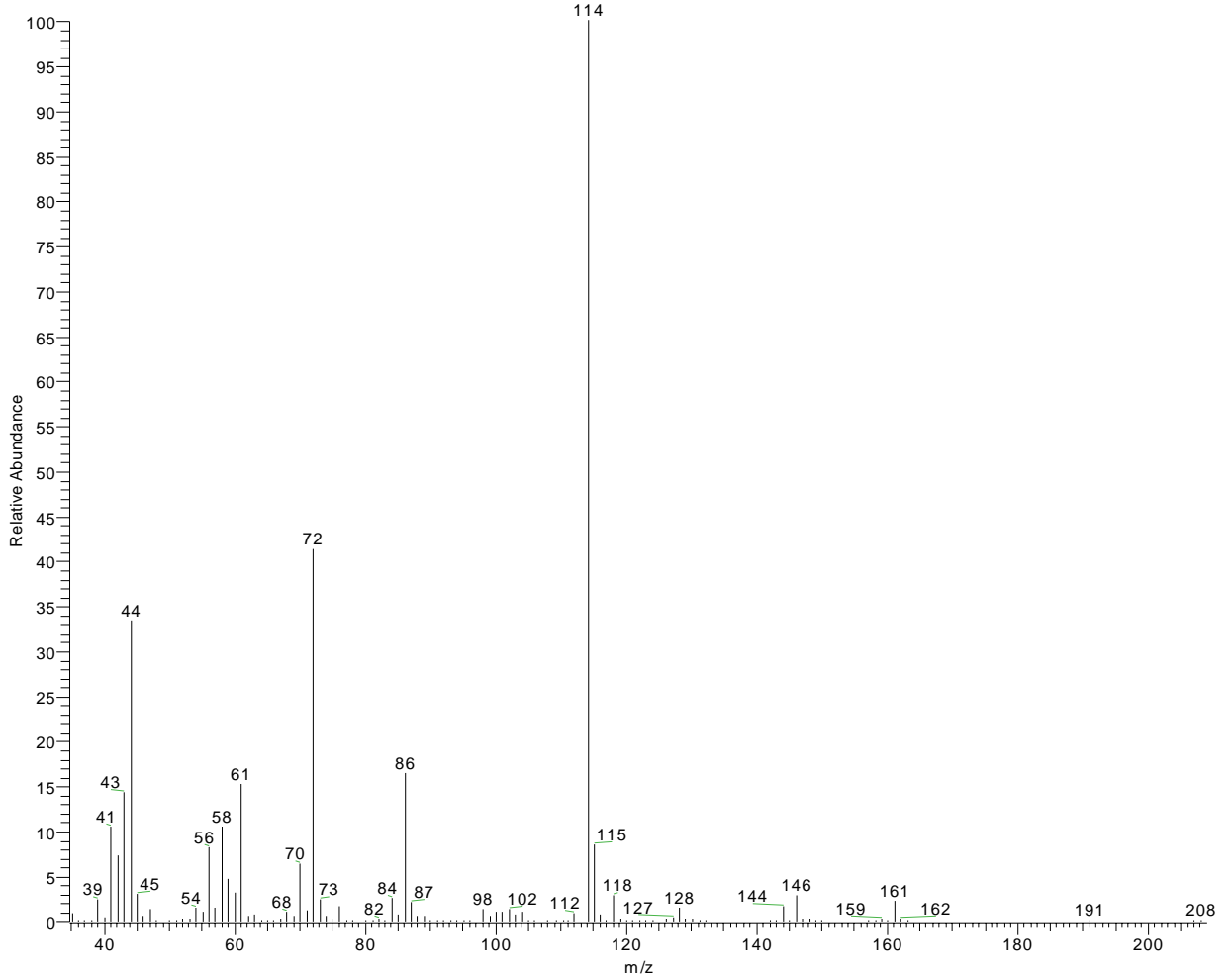
105 #548 RT: 7,98 AV: 1 SB: 33 7,58-7,75, 8,09-8,23 NL: 5,29E3
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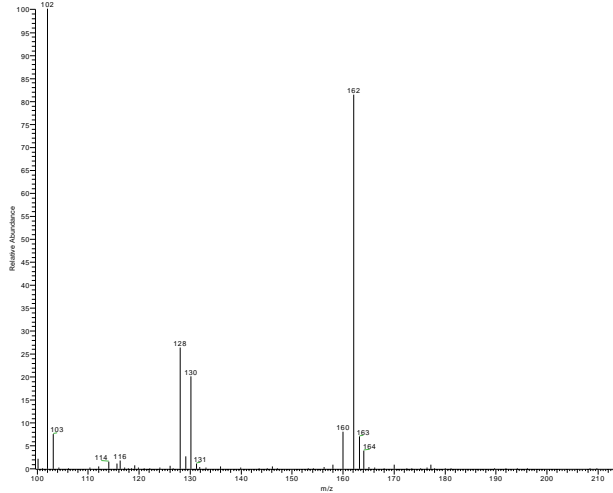
3) 2-(Diisopropylamino) ethanethiol (MW 161)

EIMS (upper) CIMS-ammonia (lower right) CIMS-methane (lower left)

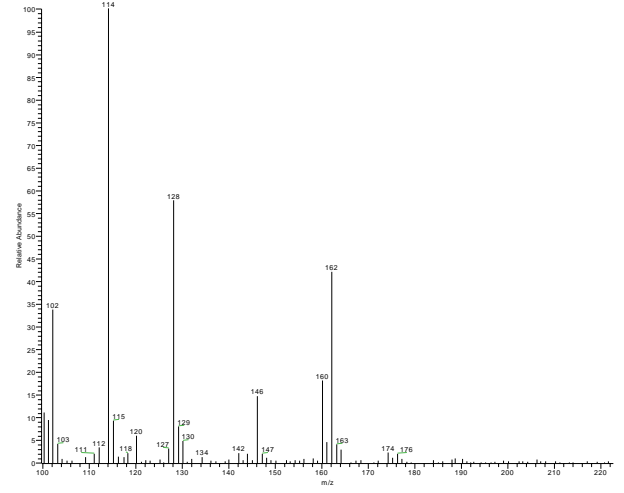
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02053005 #647 RT: 8,97 AV: 1 SB: 23 7,64-7,74, 8,12-8,23 NL: 6,10E4
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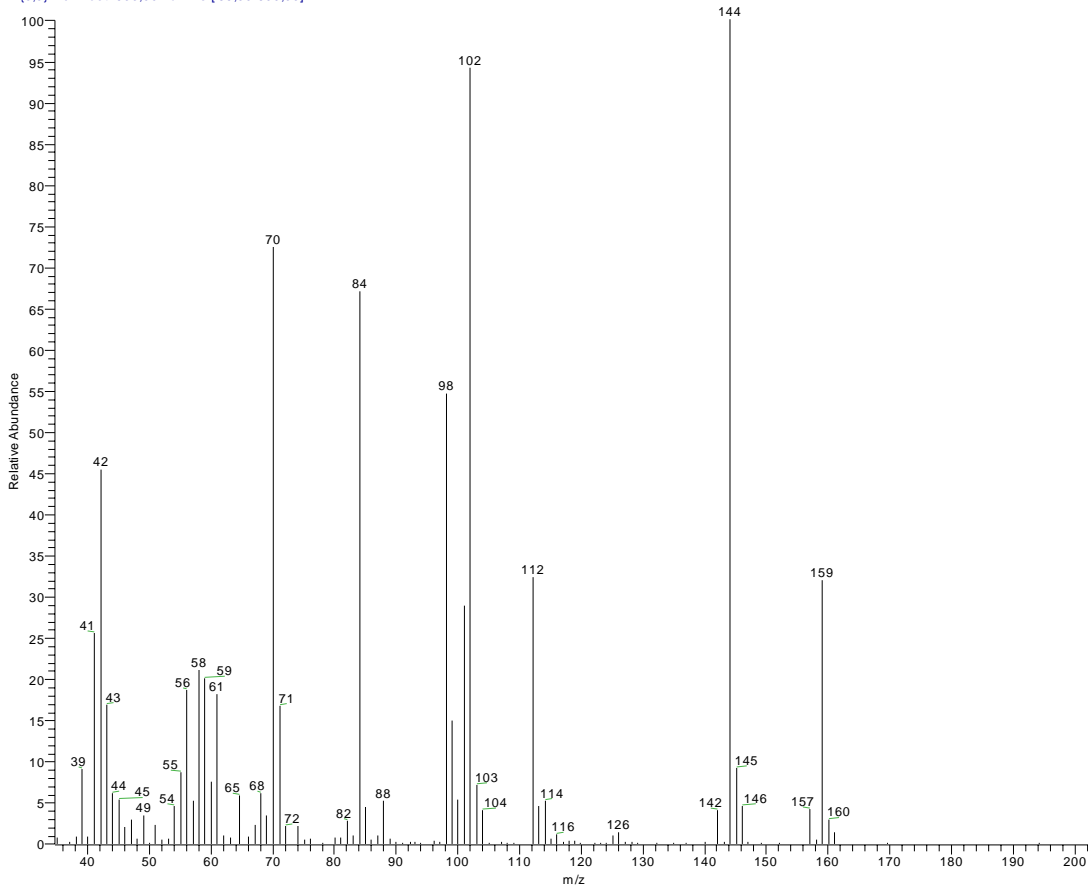


02053105 #646 RT: 8,96 AV: 1 SB: 33 7,58-7,75, 8,09-8,23 NL: 2,25E4
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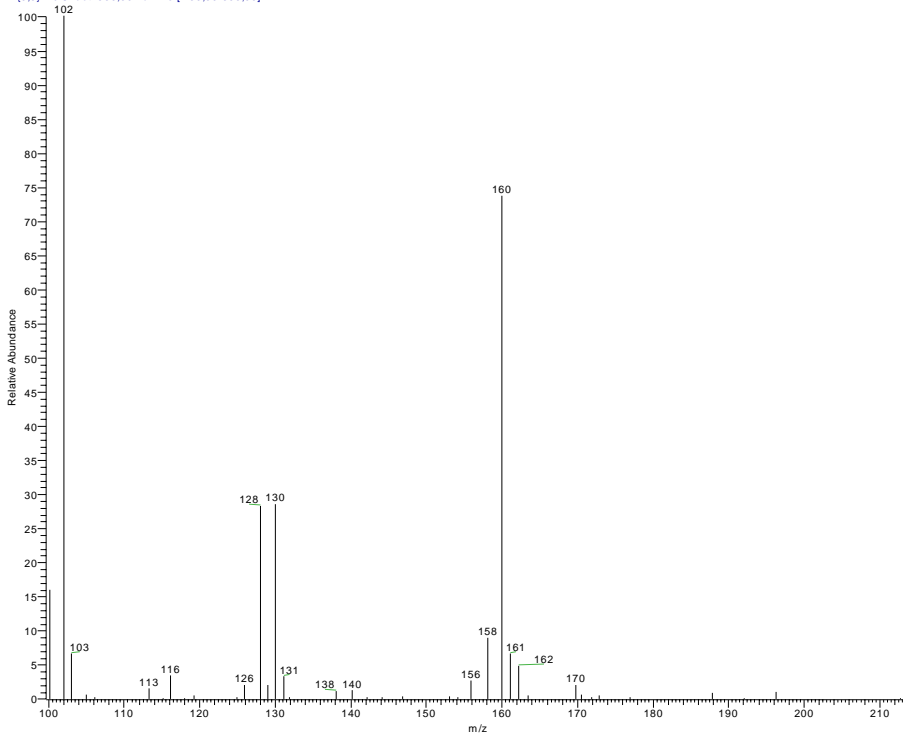


4) 2-(Diisopropylamino)ethanethiol (MW 159) EIMS (upper) CIMS-ammonia (lower)

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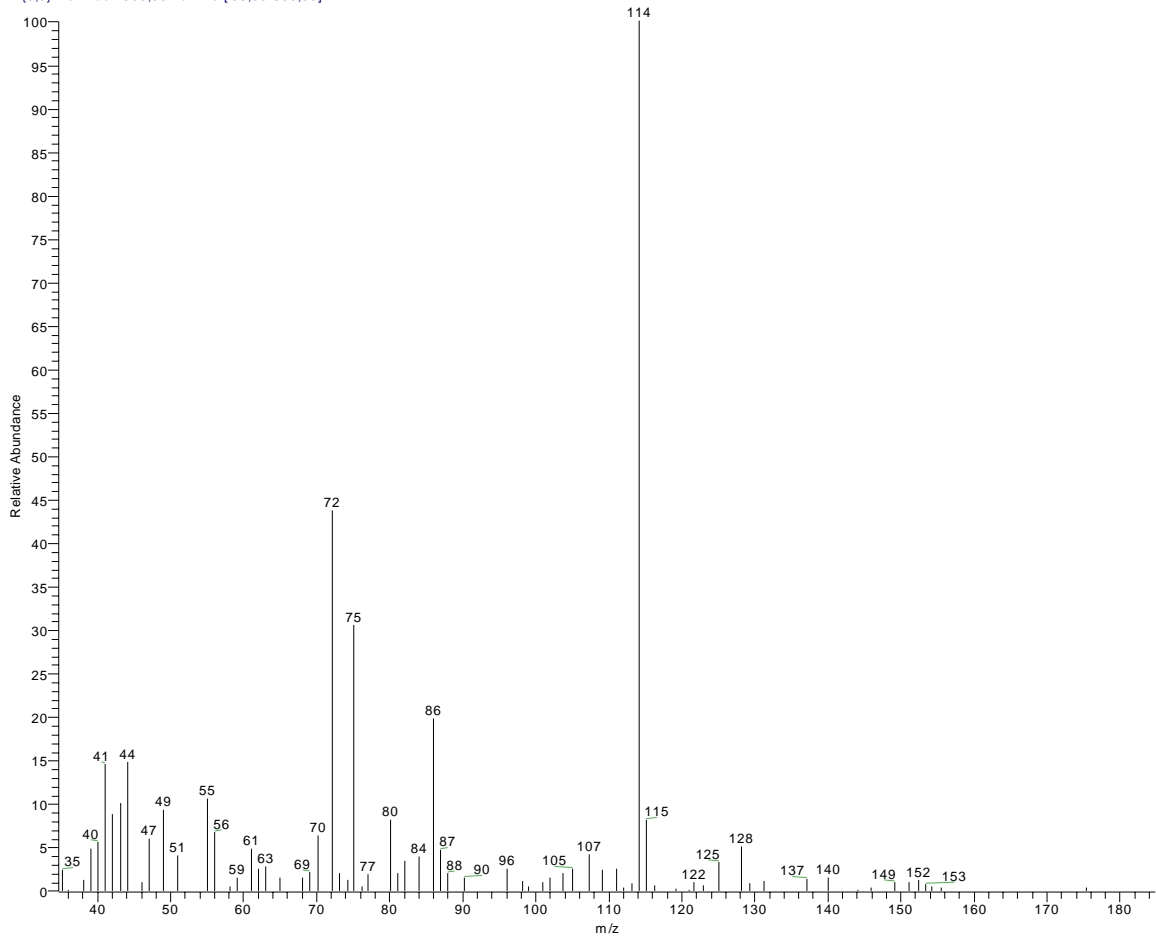


02053005 #670 RT: 9.20 AV: 1 SB: 23 7.64-7.74, 8.12-8.23 NL: 6.85E3
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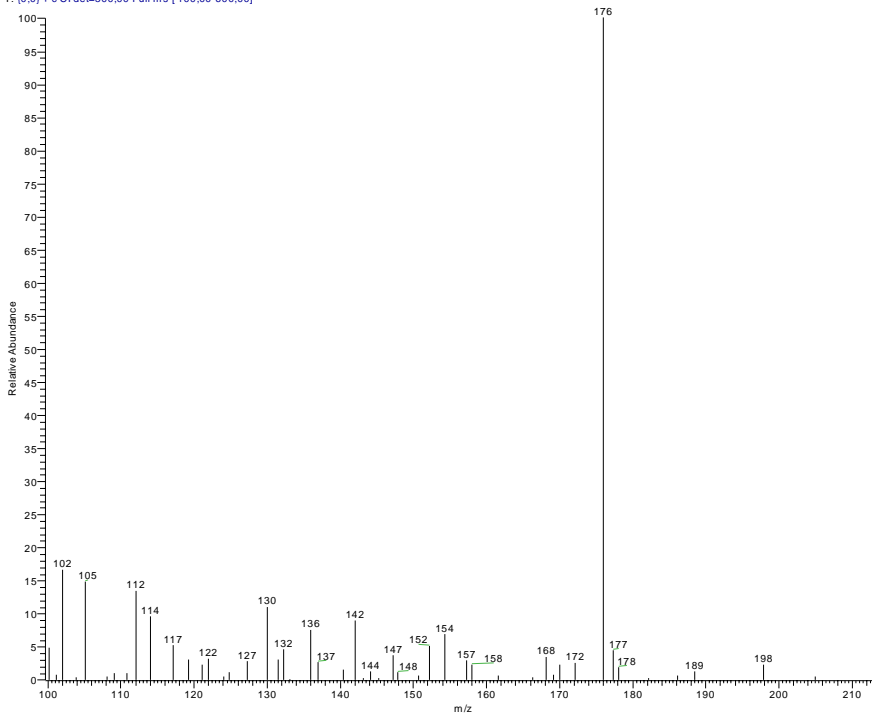


5) 2-(Diisopropylamino)ethyl methyl sulfide (MW 175)
EIMS (upper) CIMS-ammonia (lower)

02041205 #807 RT: 10.58 AV: 1 SB: 10 10.53-10.56, 10.62-10.67 NL: 8,25E3
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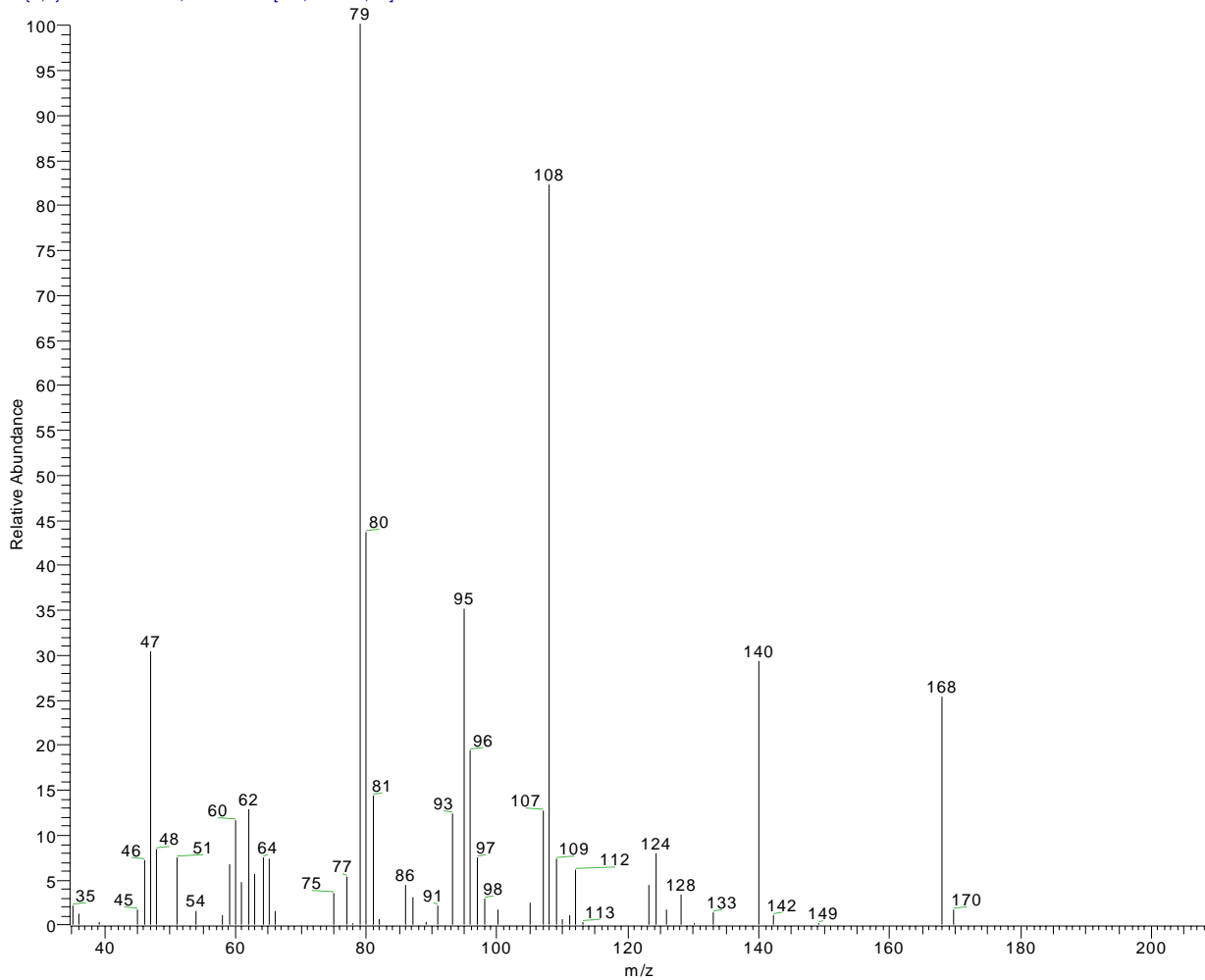
02053005 #780-782 RT: 10.30-10.32 AV: 3 SB: 13 10.22-10.28, 10.39-10.44 NL: 8,87E2
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6) *O,S*-diethyl methylphosphonothioate (MW 168)

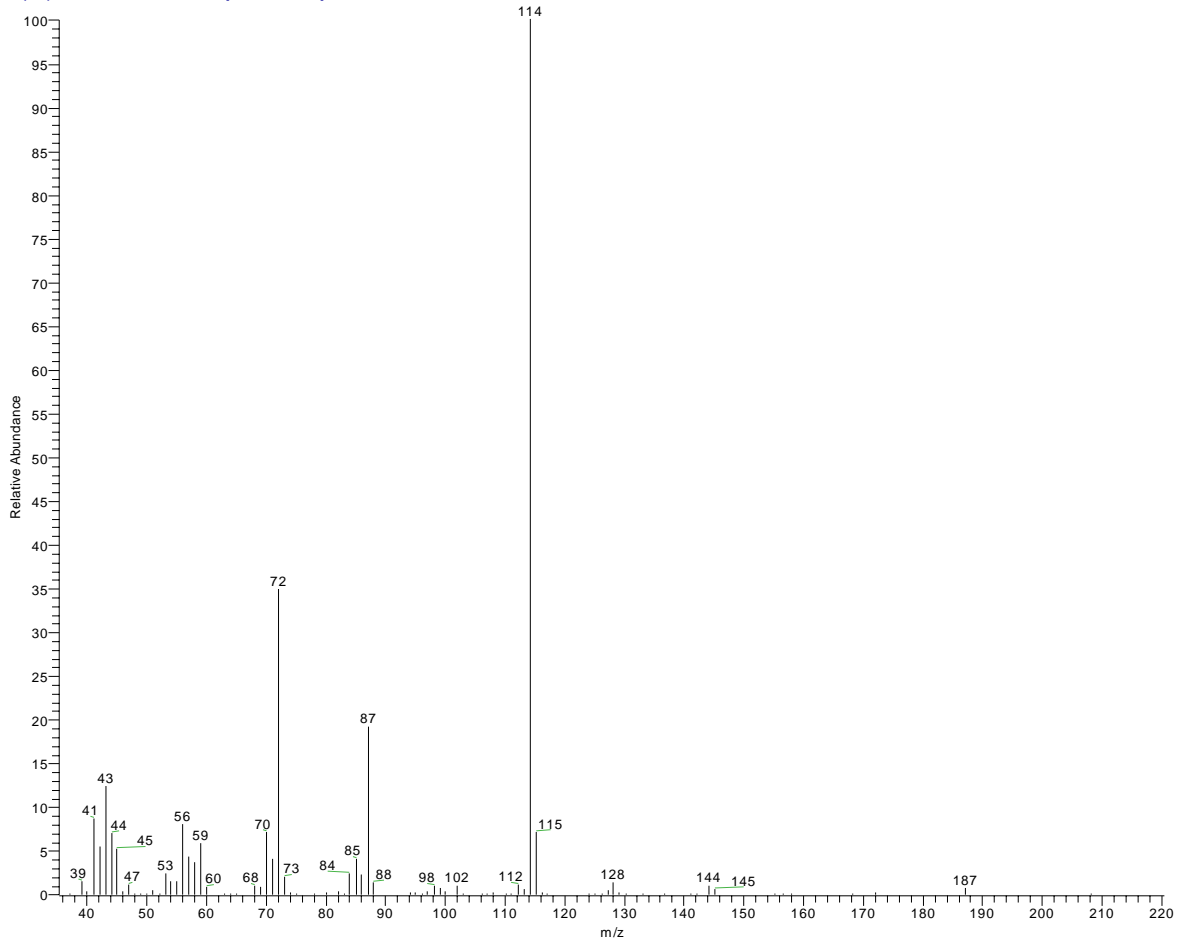
EIMS

02041102 #827 RT: 10,78 AV: 1 SB: 99 9,68-10,17, 12,14-12,62 NL: 6,50E3
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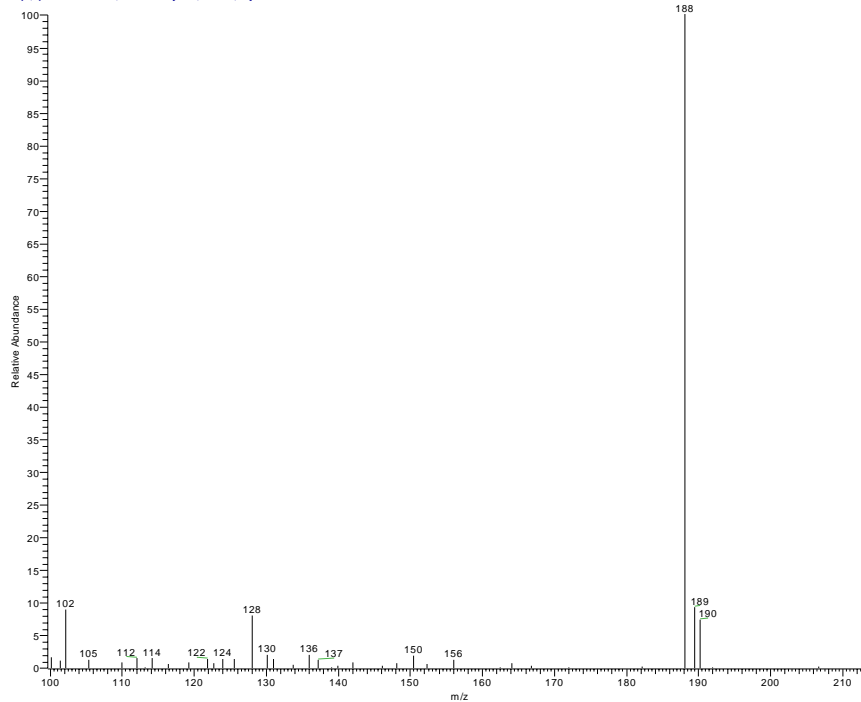


7) 2-(Diisopropylamino)ethyl vinyl sulfide (MW 187)
EIMS (upper) CIMS-ammonia (lower)

02041102 #906 RT: 11.57 AV: 1 SB: 16 11.45-11.54, 11.61-11.66 NL: 1.85E5
T: (0;0) + c EI det=500,00 Full ms [35,00-600,00]

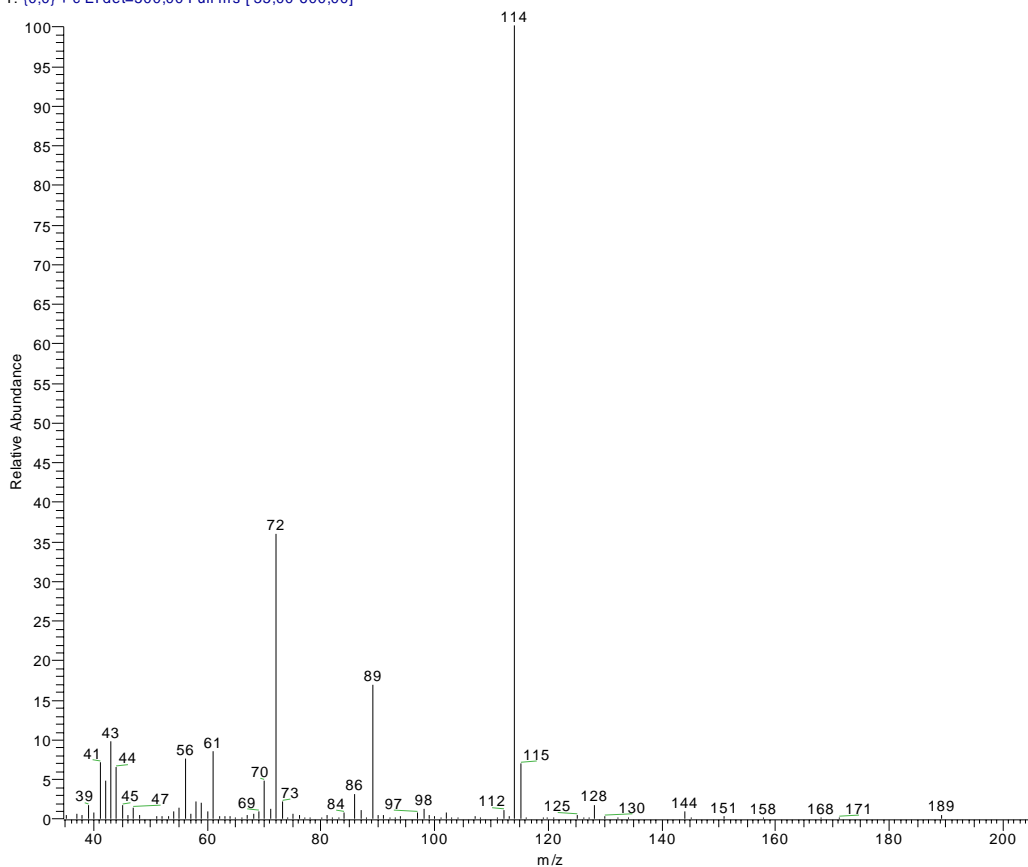


02053005 #880 RT: 11.30 AV: 1 SB: 13 10.22-10.28, 10.39-10.44 NL: 6.40E3
T: (0;0) + c CI det=500,00 Full ms [100,00-600,00]

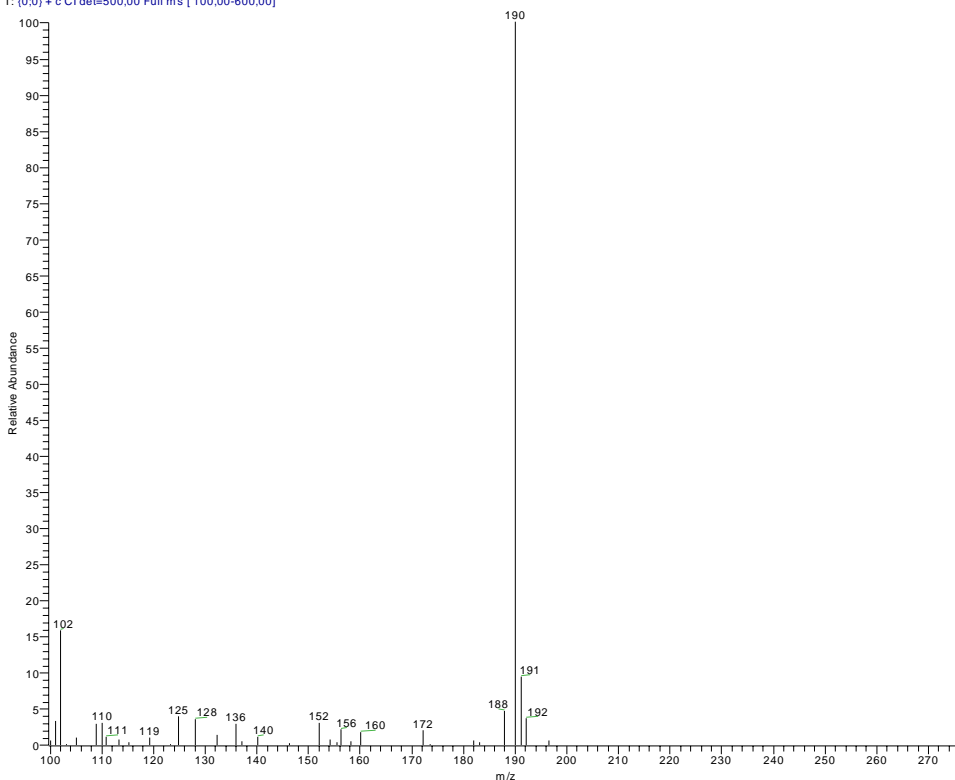


8) 2-(Diisopropylamino)ethyl ethyl sulfide (MW 189)
EIMS (upper) CIMS-ammonia (lower)

02041102 #912 RT: 11,63 AV: 1 SB: 27 11,28-11,42, 11,73-11,84 NL: 9,34E4
T: {0:0} + c EI det=500,00 Full ms [35,00-600,00]



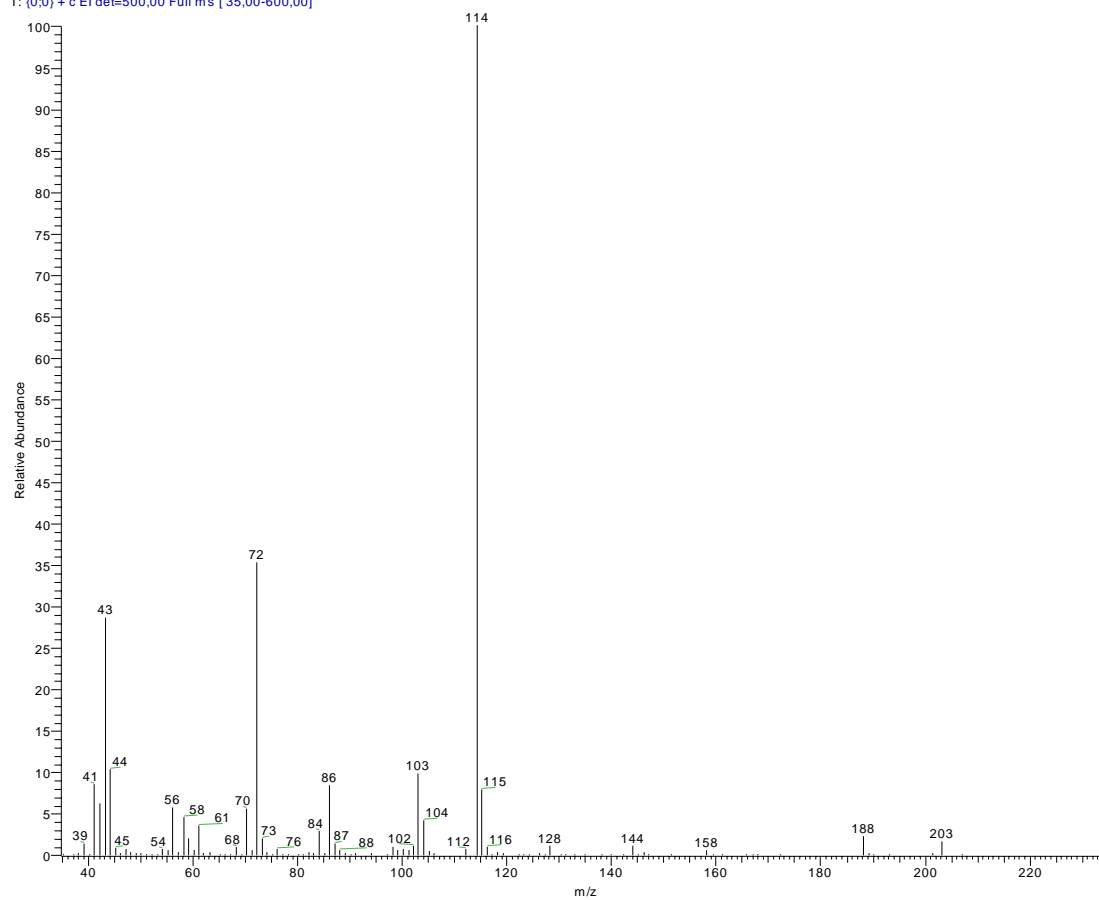
02053005 #885 RT: 11,35 AV: 1 SB: 13 10,22-10,28, 10,39-10,44 NL: 2,39E3
T: {0:0} + c CI det=500,00 Full ms [100,00-600,00]



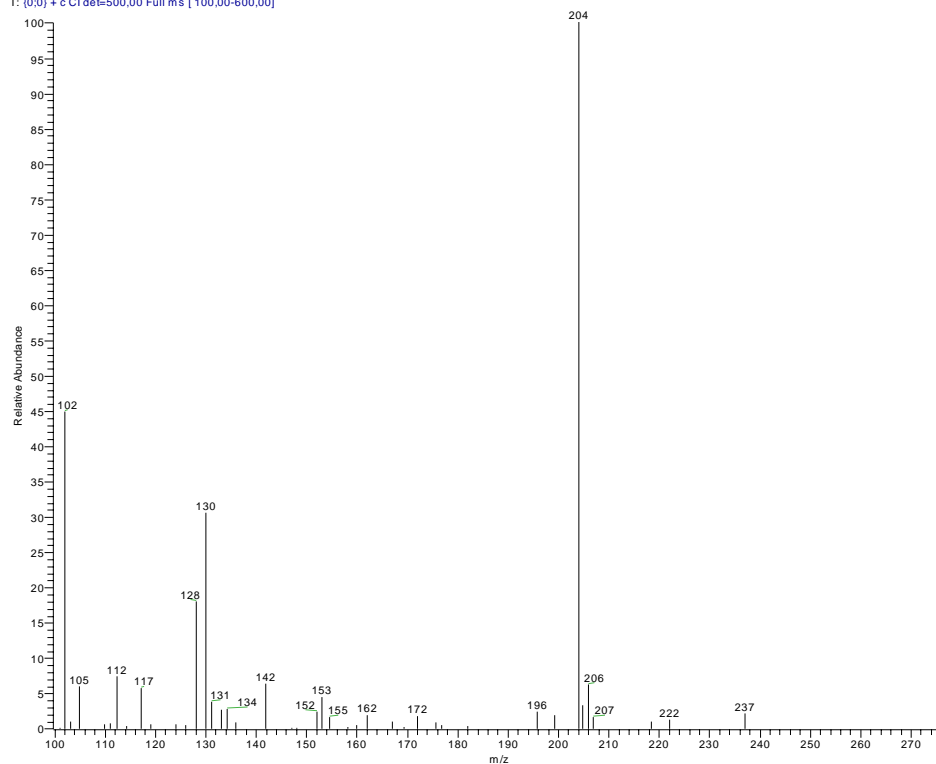
9) 2-(Diisopropylamino)ethyl isopropylsulfide (MW 203)

EIMS (upper) CIMS-ammonia (lower)

02041205 #1008 RT: 12.59 AV: 1 SB: 26 12,43-12,55, 12,67-12,79 NL: 1,35E5
T: (0;0) + c EI det=500,00 Full ms [35,00-600,00]



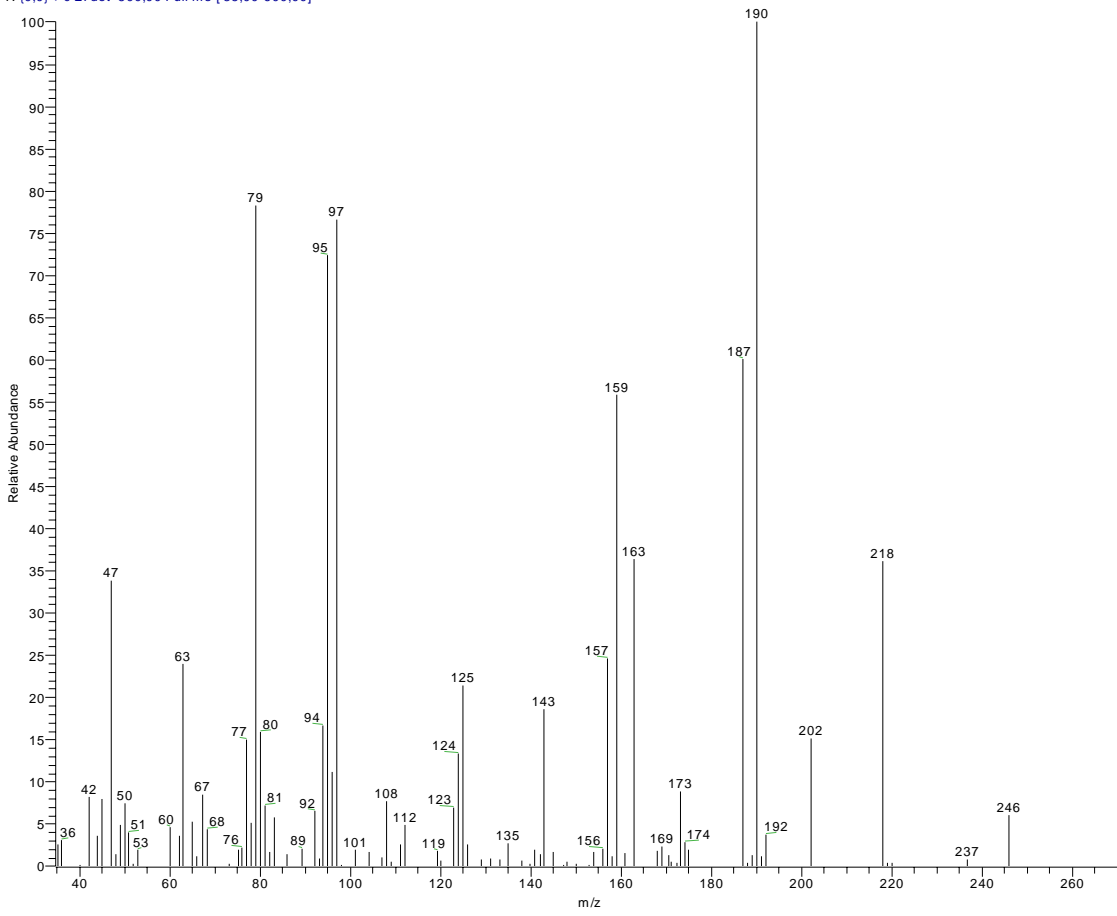
02053005 #981 RT: 12.31 AV: 1 SB: 13 10,22-10,28, 10,39-10,44 NL: 2,30E3
T: (0;0) + c CI det=500,00 Full ms [100,00-600,00]



10) *O,O*-Diethyl dimethylmonothionopyrophosphate (MW 246)

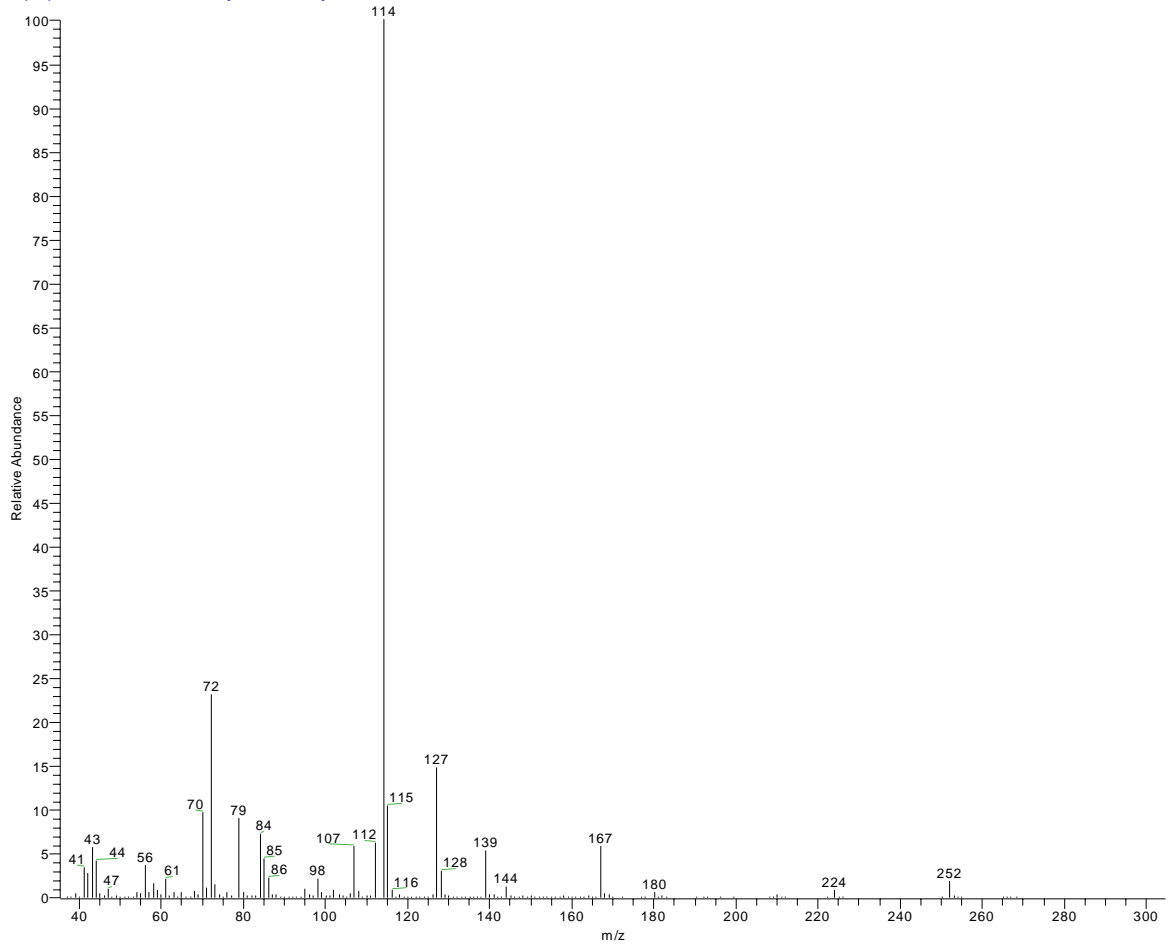
EIMS

02041205 #1149 RT: 14.00 AV: 1 SB: 47 13,71-13,93, 14,33-14,56 NL: 5,90E3
T: [0:0] + c El det=500,00 Full ms [35,00-600,00]

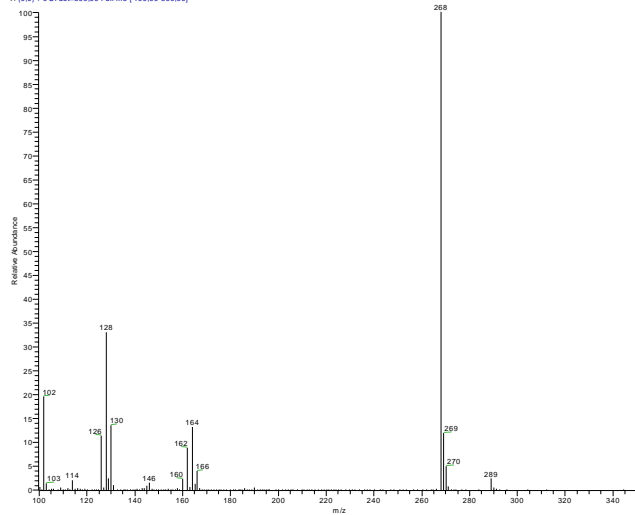


11) VX (*O*-ethyl *S*-2-diisopropylaminoethyl methylphosphonothiolate) (MW 267)
EIMS (upper) CIMS-ammonia (under right) CIMS-methane (lower left)

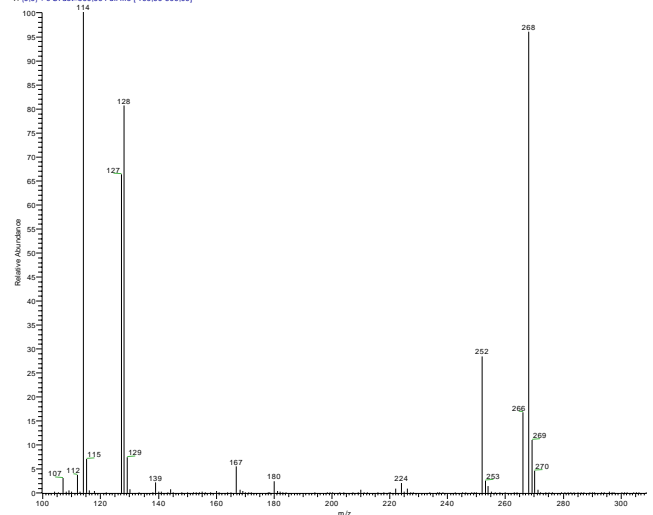
02041102 #1443 RT: 16.94 AV: 1 SB: 15 16,84-16,91, 17,08-17,14 NL: 3,24E6
T: (0;0) + c Et det=500,00 Full ms [35,00-600,00]



02053005 #1416 RT: 16.66 AV: 1 SB: 13 10,23-10,28, 10,39-10,44 NL: 4,77E5
T: (0;0) + c Cl det=500,00 Full ms [100,00-600,00]



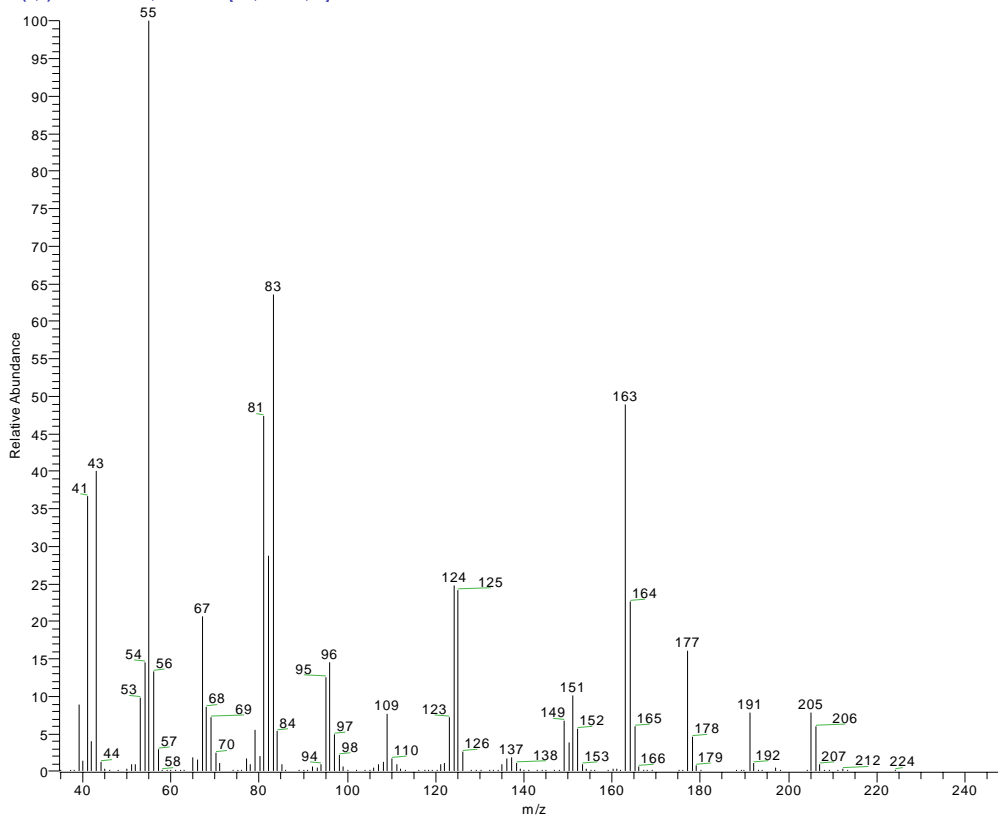
02053105 #1417 RT: 16.67 AV: 1 SB: 17 8,93-9,02, 9,13-9,19 NL: 1,38E5
T: (0;0) + c Cl det=500,00 Full ms [100,00-600,00]



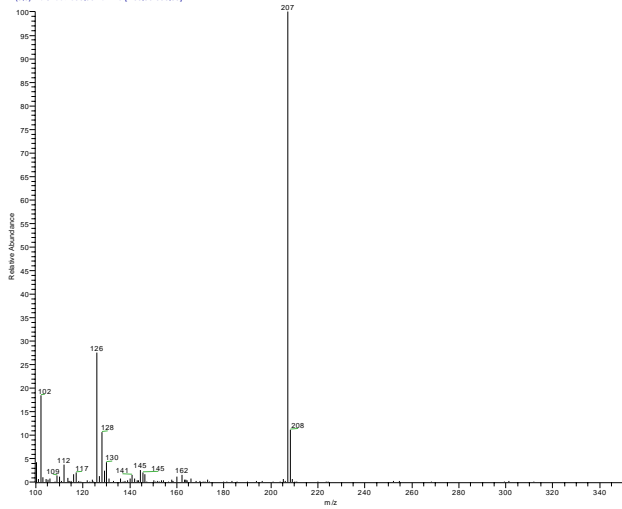
12) 1,3-dicyclohexylcarbodiimide (mw 206)

EIMS (upper) CIMS-ammonia (lower right) CIMS-methane (lower left)

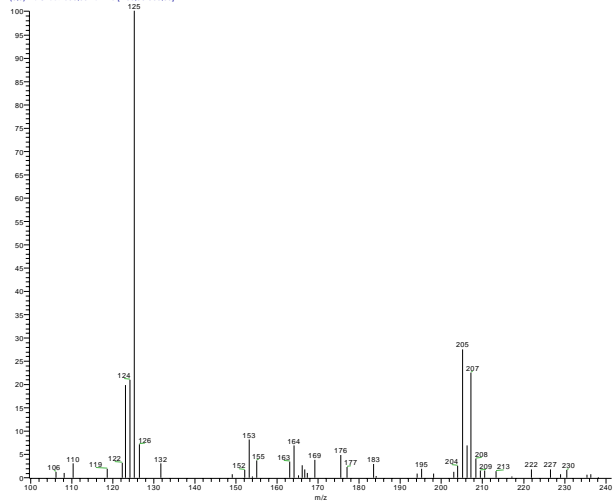
02041102 #1480 RT: 17,31 AV: 1 SB: 9 17,24-17,28, 17,38-17,41 NL: 4,77E5
T: {0;0} + c EI det=500,00 Full ms [35,00-600,00]



02053005 #1452 RT: 17,02 AV: 1 SB: 13 10,22-10,28, 10,39-10,44 NL: 3,02E4
T: {0;0} + c CI det=500,00 Full ms [100,00-600,00]

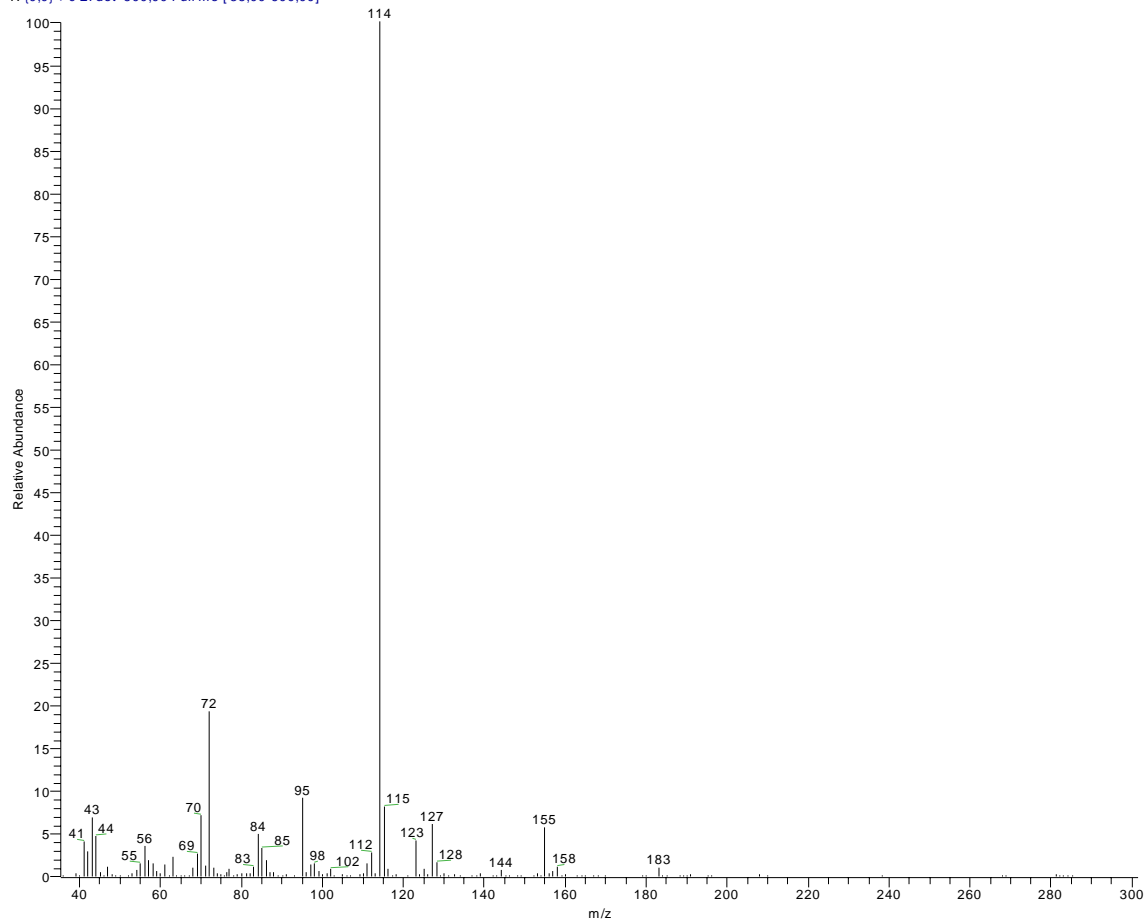


053105 #1452 RT: 17,02 AV: 1 SB: 17 8,93-9,02, 9,13-9,19 NL: 2,92E3
T: {0;0} + c CI det=500,00 Full ms [100,00-600,00]

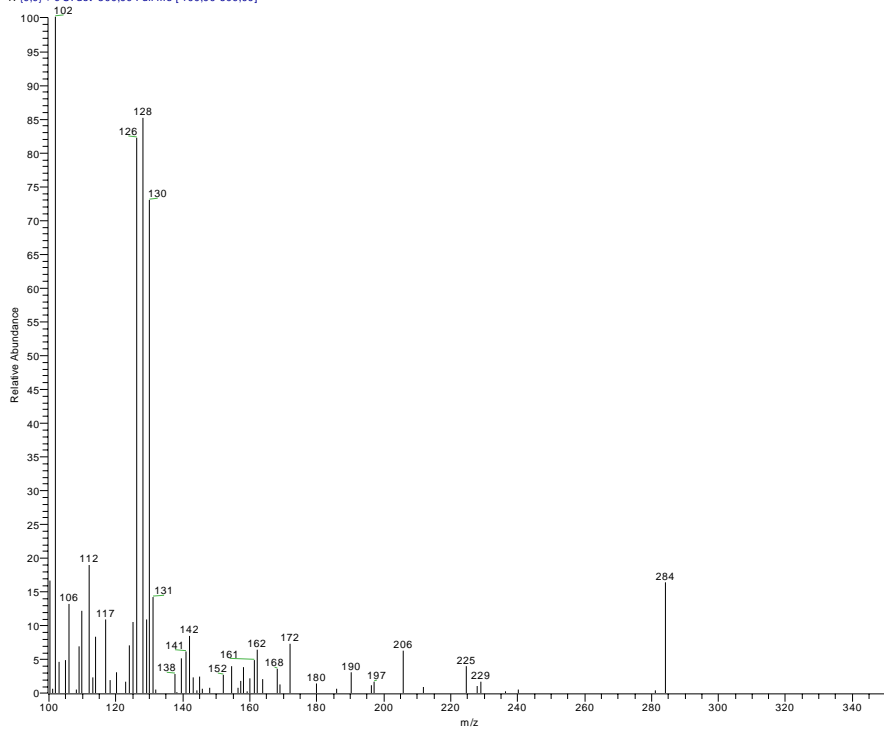


13) *O*-Ethyl S-[2-(diisopropylamino)ethyl] methylphosphonodithiolate (MW 283)
EIMS (upper) CIMS-ammonia (lower)

02041205 #1547 RT: 17,98 AV: 1 SB: 12 17,90-17,95, 18,04-18,09 NL: 1,74E5
T: {0,0} + c EI det=500,00 Full ms [35,00-600,00]

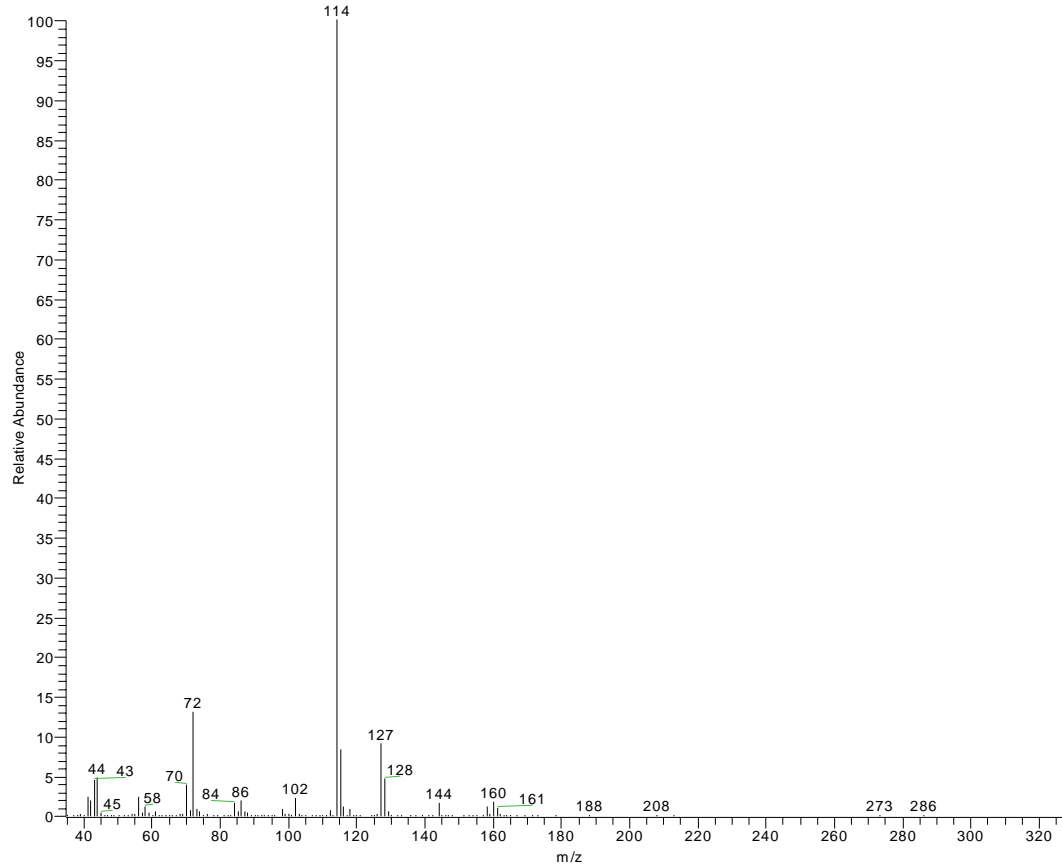


02053005 #1517 RT: 17.67 AV: 1 SB: 13 10,22-10,28, 10,39-10,44 NL: 1,76E3
T: (0,0) + c CI det=500,00 Full ms [100,00-600,00]

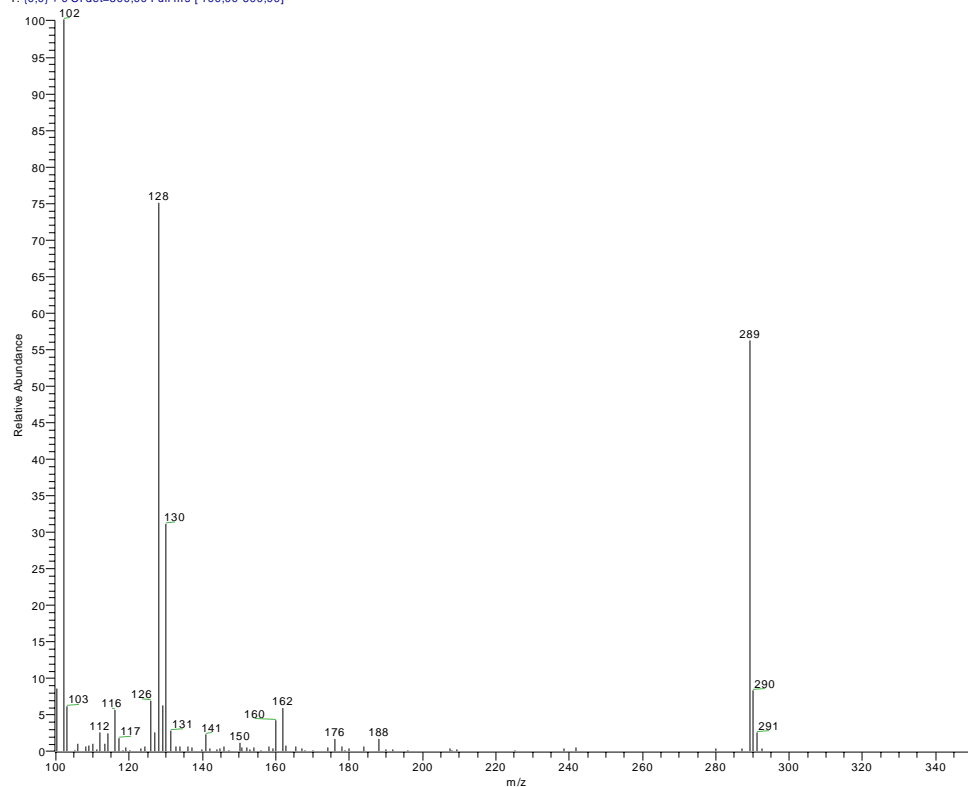


14) Bis(2-diisopropylaminoethyl) sulfide (MW 288)
EIMS (upper) CIMS-ammonia (lower)

02041102 #1588 RT: 18.39 AV: 1 SB: 10 18,30-18,35, 18,48-18,51 NL: 1,25E6
T: (0,0) + c EI det=500,00 Full ms [35,00-600,00]

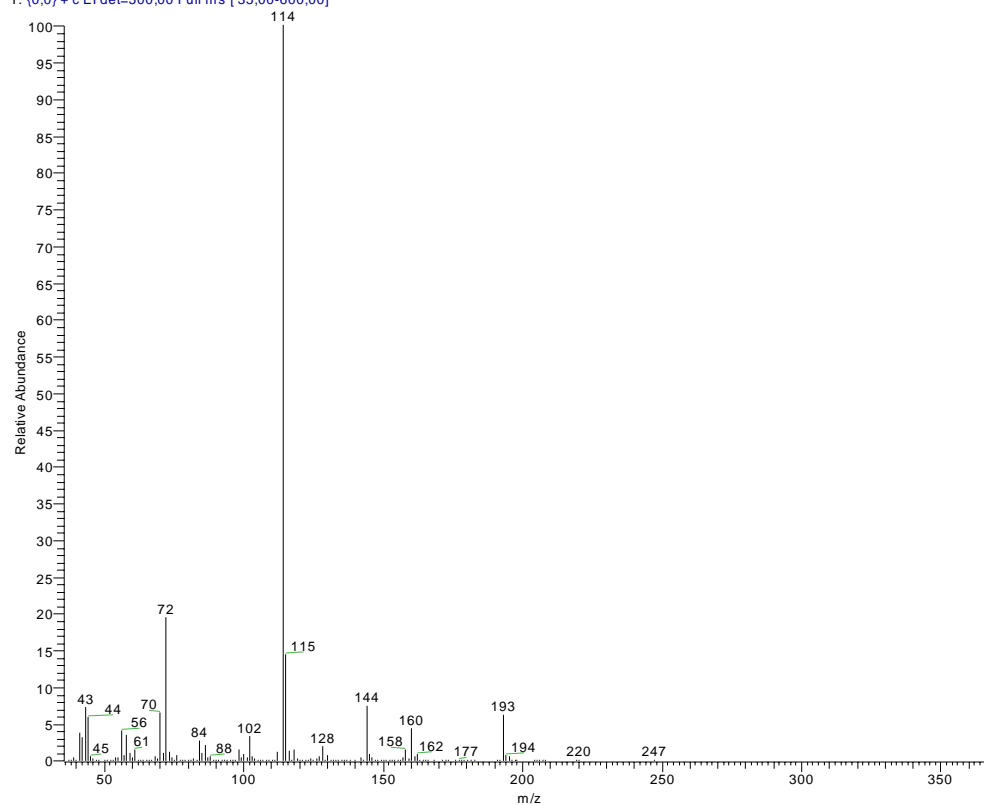


02053005 #1560 RT: 18,10 AV: 1 SB: 13 10,22-10,28, 10,39-10,44 NL: 1,22E4
T: {0;0} + c Cl det=500,00 Full ms [100,00-600,00]

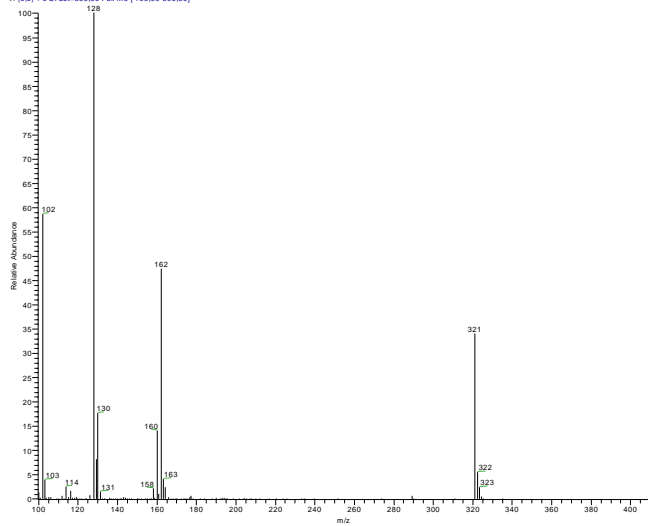


15) Bis(2-diisopropylaminoethyl) disulfide (MW 320)
EIMS (upper) CIMS-ammonia (lower right) CIMS-methane (lower left)

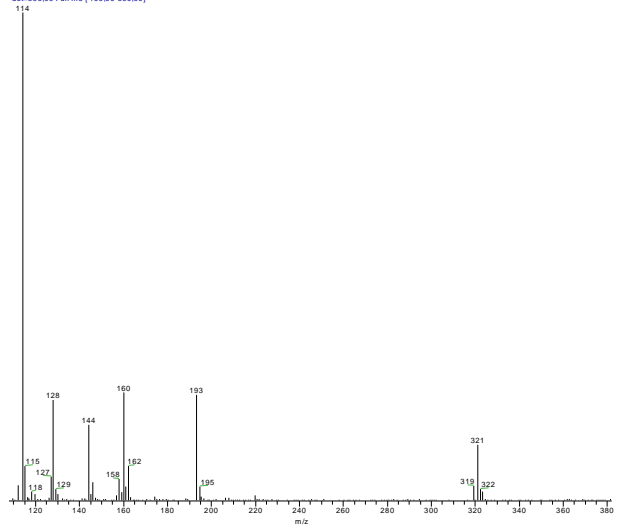
02041102 #1809-1811 RT: 20,60-20,62 AV: 3 SB: 10 20,51-20,55, 20,71-20,75 NL: 2,44E6
T: {0;0} + c El det=500,00 Full ms [35,00-600,00]



02053005#1781 RT: 20.31 AV: 1 SB: 13 10.22-10.28, 10.39-10.44 NL: 1.49E5
T: (2) + e Cl det=600.00 Full ms [100.00-600.00]

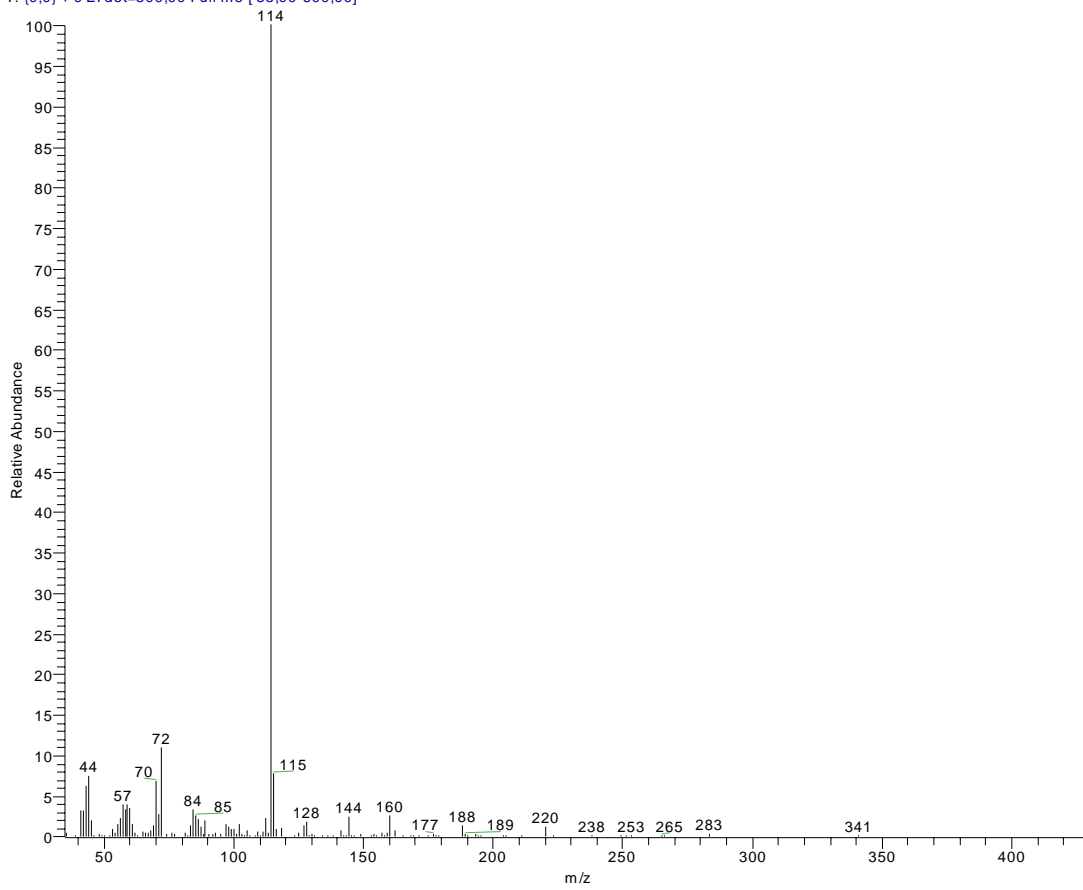


781 RT: 20.31 AV: 1 SB: 35 17.83-18.03, 18.21-18.34 NL: 4.50E4
det=500.00 Full ms [100.00-600.00]



16) 1,9-Bis(diisopropylamino)- 3,4,7-trithianonane (MW 380)
EIMS (upper) CIMS-ammonia (lower)

02041102 #2151-2152 RT: 24,02-24,03 AV: 2 SB: 32 23,83-23,96, 24,12-24,29 NL: 5,61E4
T: {0;0} + c EI det=500,00 Full ms [35,00-600,00]



02053005 #2120 RT: 23,70 AV: 1 SB: 13 10,22-10,28, 10,39-10,44 NL: 2,62E3
T: {0;0} + c CI det=500,00 Full ms [100,00-600,00]

