Application of Gas chromatography Mass Spectrometry (GC MS) in Food Science and Biotechnology

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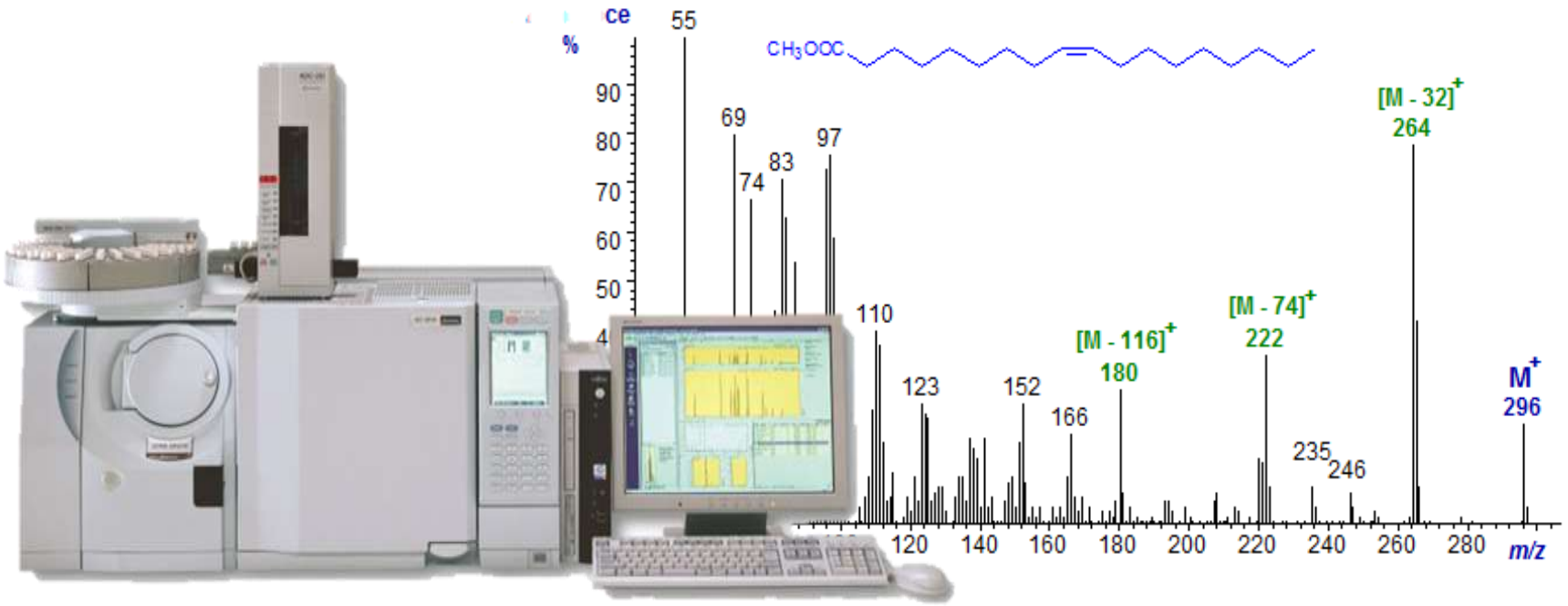
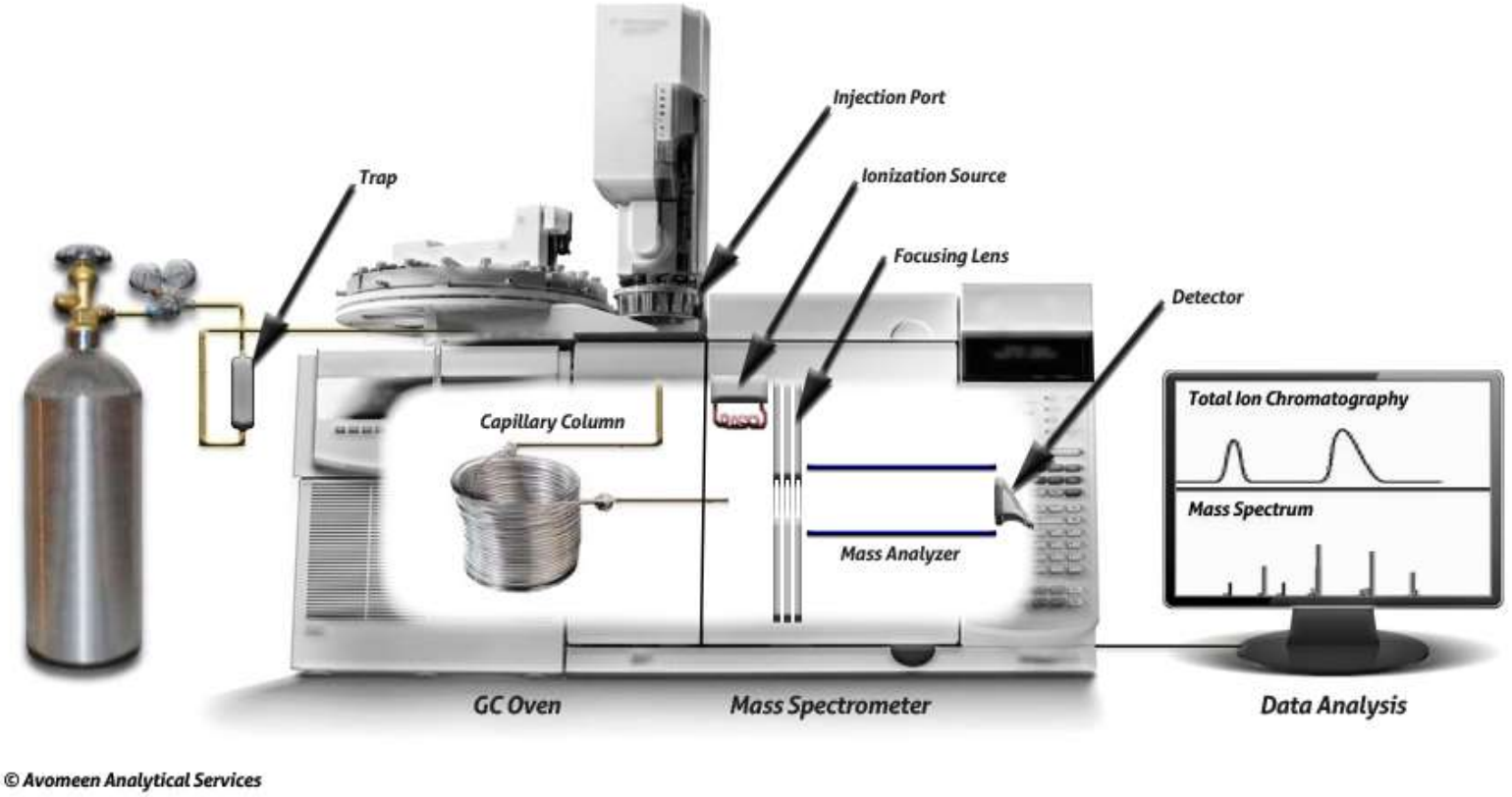


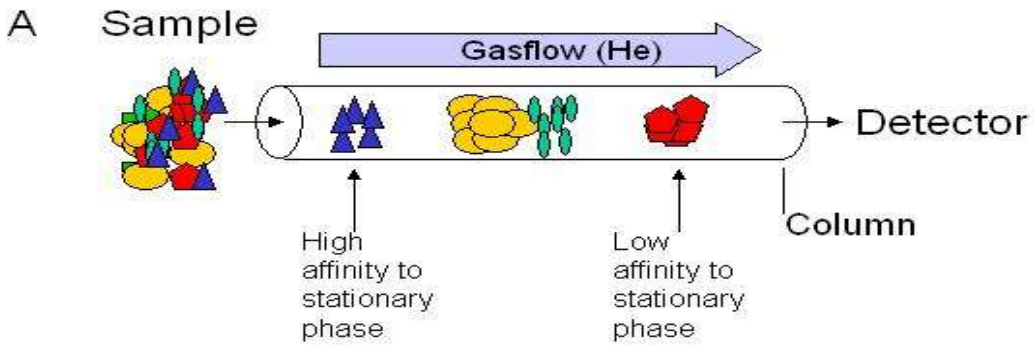
Gas chromatography mass spectrometry (GC/MS) is an instrumental technique, comprising a gas chromatograph (GC) coupled to a mass spectrometer (MS), by which complex mixtures of chemicals may be separated, identified and quantified.



How GC/MS works - two part analysis

1-The GC separates mixes of chemicals into individual components

2-The MS fragments the chemicals into unique patterns or spectra.



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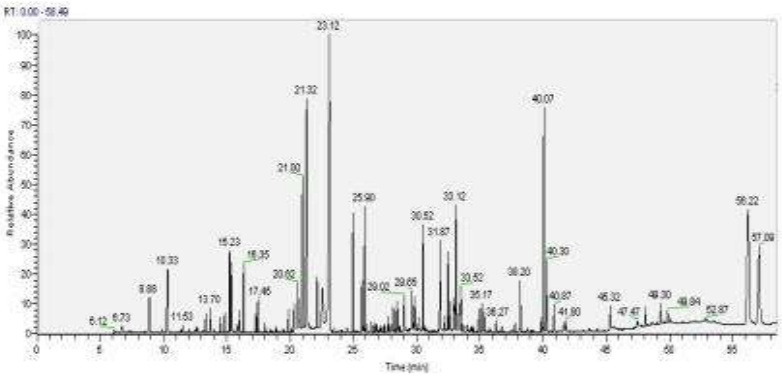
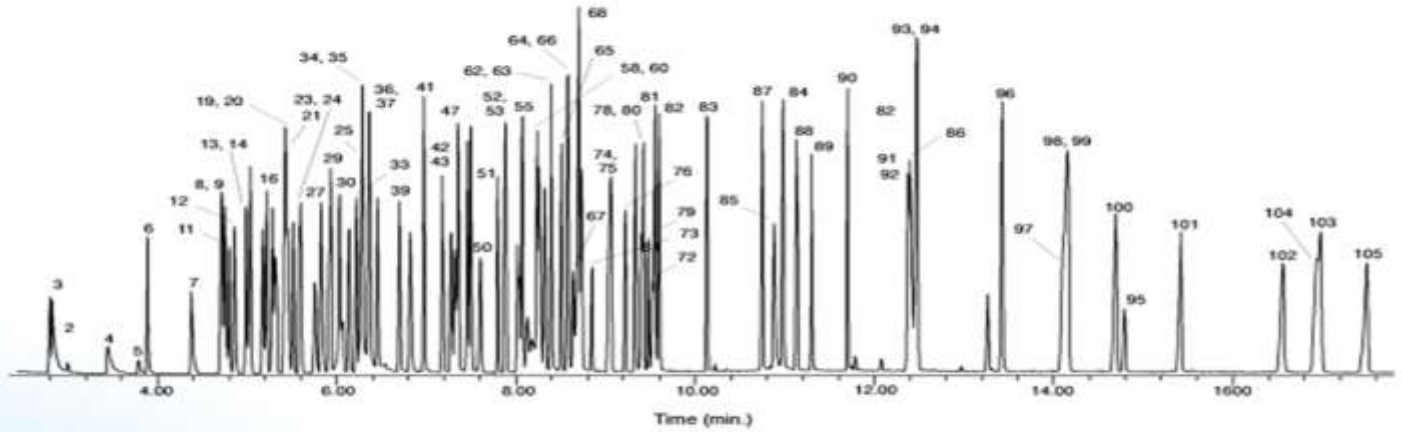


Semivolatiles—Solid Waste Analysis, GC/MS

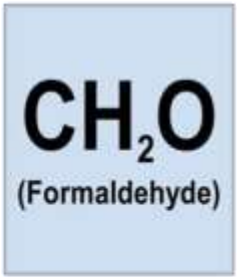
1. 1,4-Dichlorobenzene-d4
2. Pyridine
3. N-Nitrosodimethylamine
4. 2-Picoline
5. Methyl methanesulfonate
6. 2-Fluorophenol
7. Ethyl methanesulfonate
8. Phenol-d5
9. Phenol
10. Aniline
11. bis(2-Chloroethyl)ether
12. 2-Chlorophenol
13. 1,3-Dichlorobenzene
14. 1,4-Dichlorobenzene
15. Benzyl alcohol
16. 1,2-Dichlorobenzene
17. 2-Methylphenol
18. bis(2-chloro-isopropyl)ether
19. 4-Methylphenol
20. Acetophenone
21. n-Nitroso-di-n-propylamine
22. Hexachloroethane
23. Nitrobenzene-d5
24. Nitrobenzene
25. Naphthalene-d8
26. N-Nitrosopiperidine
27. Isophorone
28. 2-Nitrophenol
29. 2,4-Dimethylphenol
30. bis(2-Chloroethoxy)methane
31. 2,4-Dichlorophenol
32. Benzoic acid
33. 1,2,4-Trichlorobenzene
34. a-,a-Dimethylphenethylamine
35. Naphthalene
36. 4-Chloroaniline
37. 2,6-Dichlorophenol
38. Hexachlorobutadiene
39. N-Nitroso-di-n-butylamine
40. 4-Chloro-3-methylphenol
41. 2-Methylnaphthalene
42. 1,2,4,5-Tetrachlorobenzene
43. Hexachlorocyclopentadiene
44. Acenaphthene-d10
45. 2,4,6-Trichlorophenol
46. 2,4,5-Trichlorophenol
47. 2-Fluorobiphenyl
48. 2-Chloronaphthalene
49. 1-Chloronaphthalene
50. 2-Nitroaniline
51. Dimethylphthalate
52. Acenaphthylene
53. 2,6-Dinitrotoluene
54. 3-Nitroaniline
55. Acenaphthene
56. 2,4-Dinitrophenol
57. Dibenzofuran
58. Pentachlorobenzene
59. 4-Nitrophenol
60. 2,4-Dinitrotoluene
61. 1-Napthylamine
62. 2-Napthylamine
63. 2,3,4,6-Tetrachlorophenol
64. Fluorene
65. Diethylphthalate
66. 4-Chlorophenyl-phenylether
67. 4-Nitroaniline
68. Diphenylamine
69. n-Nitrosodiphenylamine
70. Diphenylhydrazine
71. 4,6-Dinitro-2-methylphenol
72. Phenanthrene-d10
73. 2,4,6-Tribromophenol
74. 4-Bromophenyl-phenyl ether
75. Phenacetin
76. Hexachlorobenzene
77. 4-Aminobiphenyl
78. Pentachlorophenol
79. Pentachloronitrobenzene
80. Pronamide
81. Phenanthrene
82. Anthracene
83. Di-n-butylphthalate
84. Fluoranthene
85. Benzidine
86. Chrysene-d12
87. Pyrene
88. Terphenyl-d14
89. p-Dimethylaminoazobenzene
90. Butylbenzyl phthalate
91. Benzo[a]anthracene
92. 3,3'-Dichlorobenzidine
93. Chrysene
94. bis(2-Ethylhexyl)phthalate
95. Perylene-d12
96. Di-n-octylphthalate
97. Benzo[b]fluoranthene
98. 7,12-Dimethylbenz(a) anthracene
99. Benzo (k) fluoranthene
100. Benzo[a]pyrene
101. 3-Methylcholanthrene
102. Dibenzo(a,j)acridine
103. Dibenz[a,h]anthracene
104. Indeno (1,2,3-cd) pyrene
105. Benzo[g,h,i]perylene



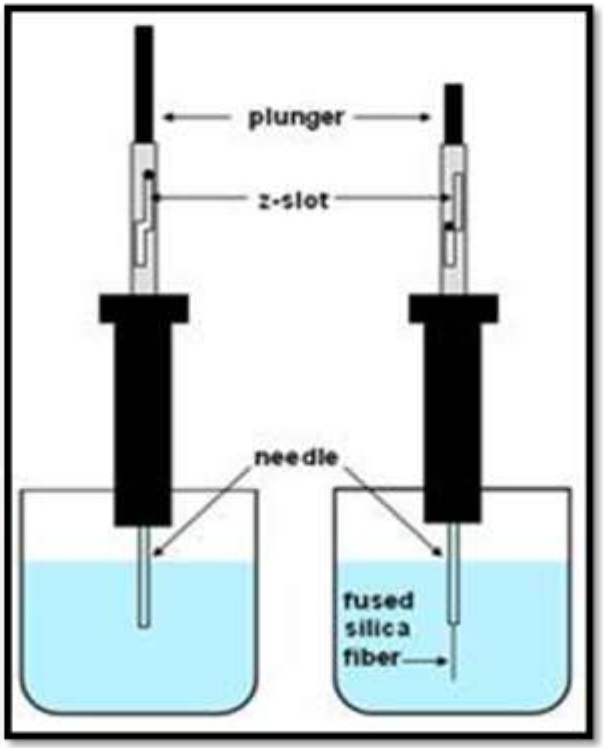
Conditions:
Column: HP-5MS, 30 m x 0.25 mm x 0.25 µm (Part No. 14091S-433)
Carrier: Helium, pressure program 0.1 psi (0.1 min) at 99 psi/min to 7.4 psi
Injection: 0.1 µl, 250°C
Oven: Termperature program listed above
Detector: MSD, 280°C

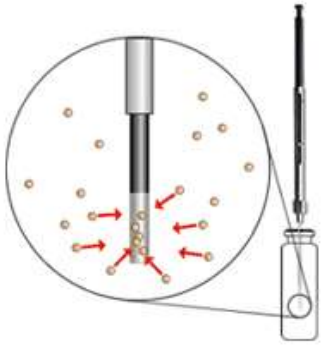
Fish and food safety: Determination of formaldehyde in 12 fish species by SPME extraction and GC–MS analysis

- The formaldehyde (FA) content in different fish products was evaluated using a solid phase micro extraction (SPME)-GC–MS method based on fiber derivatisation with pentafluorobenzyl-hydroxyl-amine hydrochloride. LOD and LOQ values of 17 and 28 μg kg−1, respectively were calculated. Fish quality was assessed by the analysis of 12 species (sea-fish, freshwater-fish and crustaceans), revealing variable FA levels. Fresh, deep frozen, canned, boiled and roasted fish were analysed; cooking always produced a decrease in the analyze content. Fish belonging to the Gadidae family were the samples with the highest FA concentration (from 6.4 ± 1.2 mg kg−1 to 293 ± 26 mg kg−1), in four cases out of 14 exceeding the value of 60 mg kg−1 proposed by the Italian Ministry of Health. Storage on ice was also investigated, showing moderate FA production also at temperature around 0 °C. FA contents lower than 22 mg kg−1 were finally found in all the other samples.



Solid- phase microextraction SPME





Determination of the Food Colorant, Chrysoidine, in Fish by GC–MS

chrysoidine was reported for its possible illegal applications. In Asian countries, fish traders have already used chrysoidine to resemble lower quality fish to expensive yellowfin

A method has been developed for confirmatory determination of chrysoidine in fish by GC–MS. Samples were extracted with methanol, and an aliquot was subjected to dispersive solid-phase extraction clean-up with octadecyl sorbent. After centrifuging and filtering, extracts were evaporated to dryness and derivatized with acetic anhydride. The detection and quantification limits were 2.3 and 7.7 μg kg^{-1} respectively, demonstrating the potential of the method for quality control of food.

Punicic acid is an omega-5 long chain polyunsaturated fatty acid found in pomegranate seed oil.

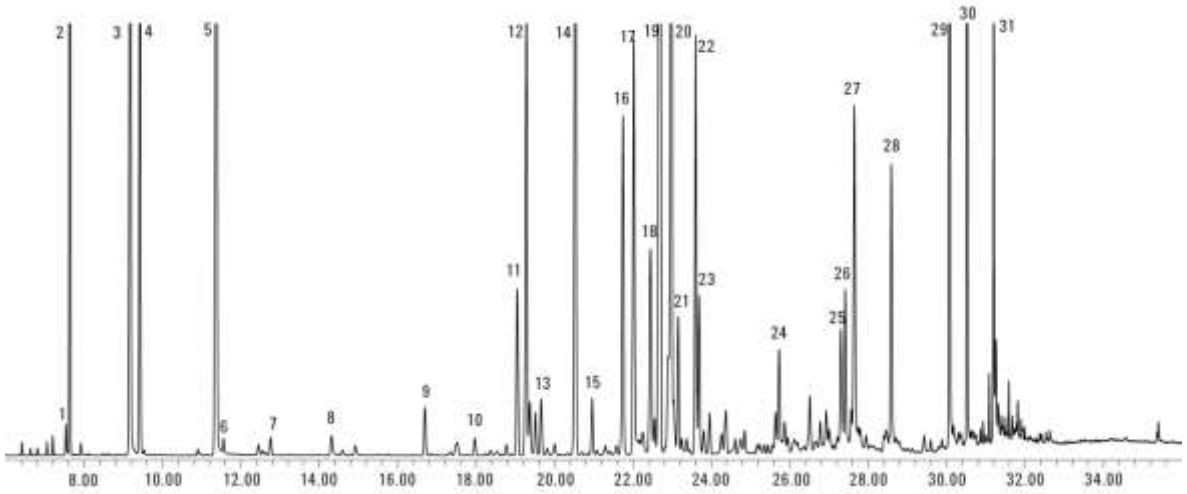
Solid-phase micro-extraction (SPME) sample collection

SPME experiments were performed at ambient temperature. A mouse carcass (laboratory mice, *Mus musculus*) was placed on a glass rectangular plate (10 cm × 10 cm) and covered with an oval glass cover lid (10 cm dia, 7 cm height). The centre of the glass lid protrudes up to form a standard glass screw joint (8 mm dia). The joint was closed using a corresponding plastic cap with a PTFE septum. The SPME holder with CAR/PDMS fibre (Supelco, previously desorbed for 5 min in GC injection port heated to 200 °C) was inserted through the PTFE septum into the atmosphere surrounding the mouse carcass and the fibre was exposed for 15 min and immediately GC×GC-TOFMS analysed. 10 mouse carcasses (*Mus musculus*) were used. During the first 24 h, SPME samplings were performed at every hour. Later on, samplings were repeated at longer intervals

Identification of Essential Oil Components by GC-MS

- At Aromatics International every batch of oil purchased from a distiller or distributor is tested with GC/MS
- This process is used to identify any adulteration of the essential oil tested and Purity

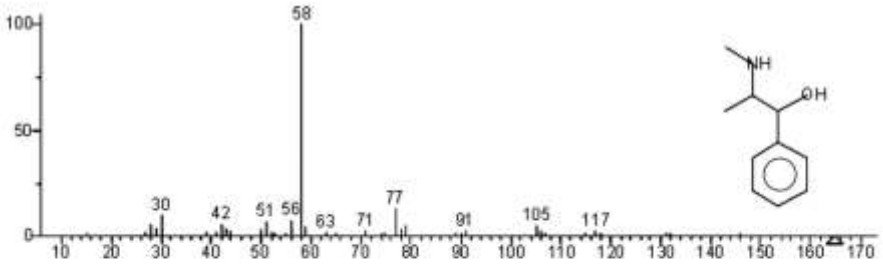
Ylang Ylang Oil Major Components - 4 EU Allergens Observed



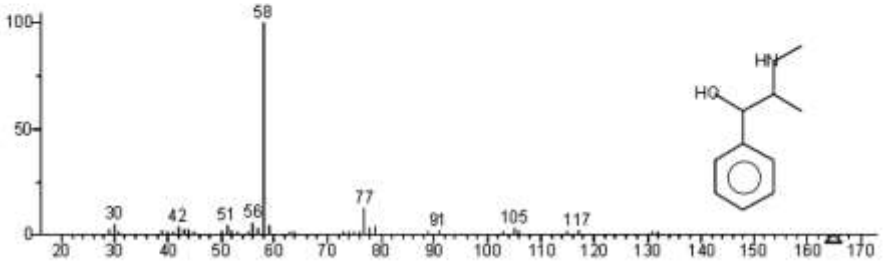
Ylang Ylang Oil Major Components include 4 EU Allergens

1 Eucolyptol	9 p-Propyl anisol	17 Cinnamyl acetate	25 δ-Muurolene
2 p-Methyl anisol	10 α-Cubebene	18 t-Muurolene	26 τ-Cardinol
3 ***Linalool***	11 Copaene	19 Germacrene D	27 τ-Muurolol
4 Methyl benzoate	12 β-Myrcene	20 α-Farnesene	28 b-Farnesene
5 Benzyl acetate	13 β-Elemene	21 α-Muurolene	29 ***Benzyl benzoate***
6 Ethyl benzoate	14 Caryophyllene	22 δ-Cadinene	30 Caryophyllene
7 Di-bromo benzene (ISTD)	15 β-Cubebene	23 γ-Cadinene	31 ***Benzyl salicylate***
8 Cic-gernaniol	16 α-Caryophyllene	24 Carphyllene oxide	

We can distinguish between isomers by using GC MS



Ephedrine



Pseudoephedrine

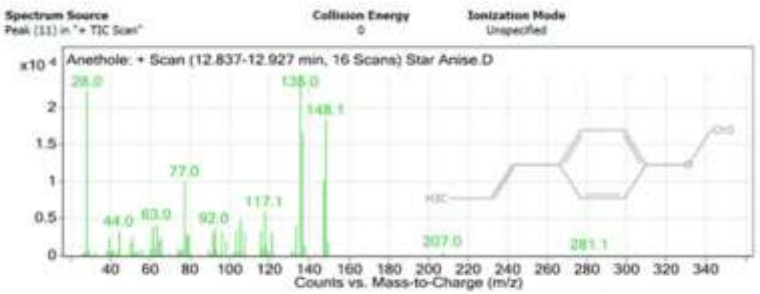


Figure 15: GC-MS spectrum source of Anethole at peak 11.

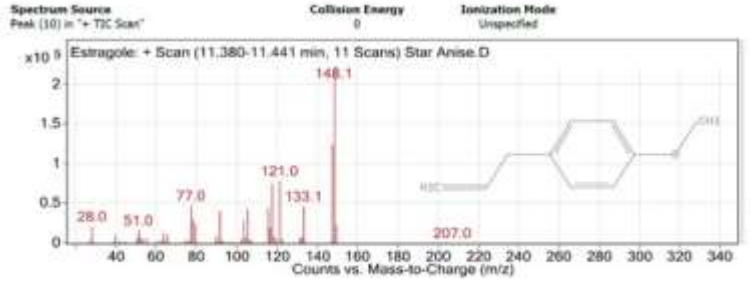


Figure 14: GC-MS spectrum source of Estragole at peak 10.

GC-MS uses to Detection and Identification the Antioxidant Compounds

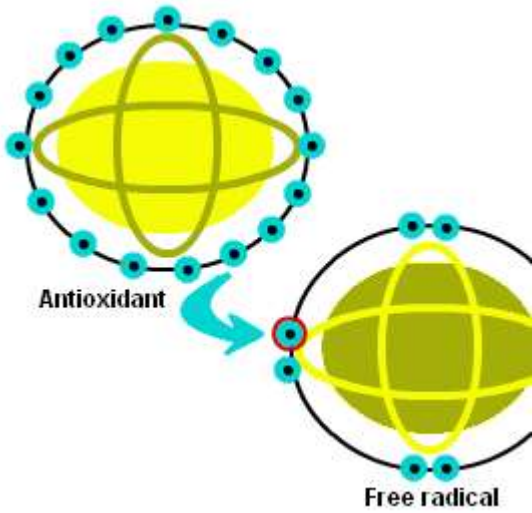
Gas Chromatography-Mass Spectrometry (GC-MS) and evaluation of antioxidant and antimicrobial activities of essential oil of Campomanesia adamantium (Cambess.) O. Berg (Guavira)

Volatile Compounds and Antioxidant Capacity of the Bio-Oil Obtained by Pyrolysis of Japanese Red Pine (Pinus Densiflora Siebold and Zucc.)

Antioxidant and Antimicrobial Activities with **GC/MS** Analysis of the Morus alba L. Leaves

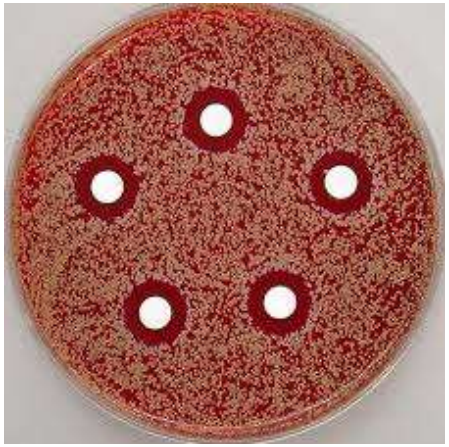
GC-MS ANALYSIS OF PHYTOCOMPONENTS AND TOTAL ANTIOXIDANT ACTIVITY OF HEXANE EXTRACT OF SINAPIS ALBA

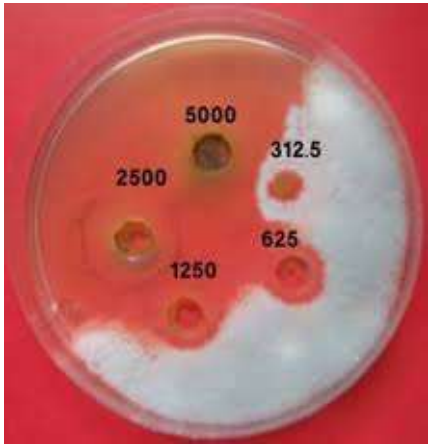
Butylated Hydroxytoluene in Edible Vegetable Oils

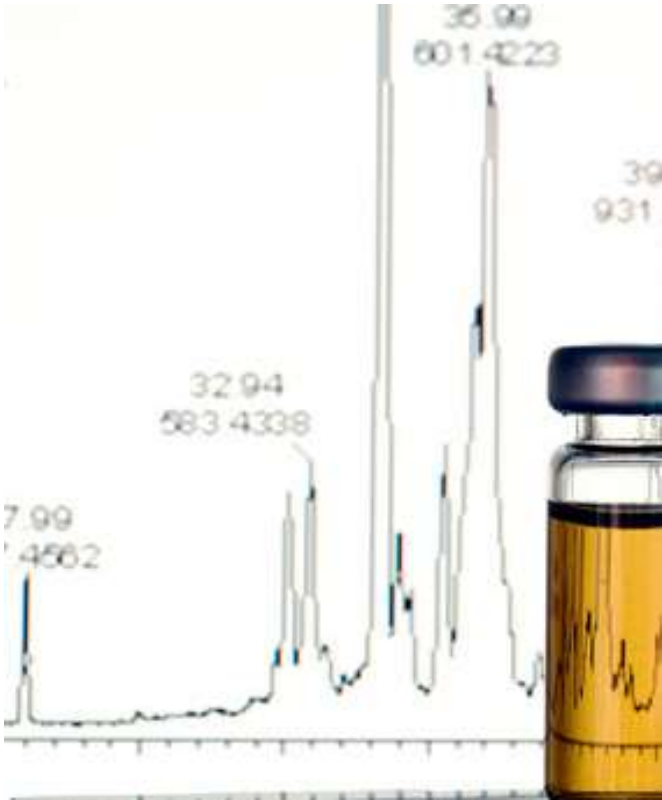


GC-MS uses to Detection and Identification the ANTIMICROBIAL Compounds

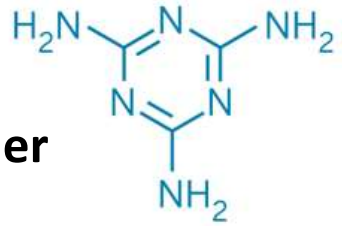
- SCREENING OF ACTIVE PHYTOCOMPOUNDS BY GC – MS STUDY AND ANTIMICROBIAL
- EVALUATION OF ANTIMICROBIAL METABOLITES FROM MARINE MICROALGAE TETRASELMIS SUECICA USING GAS CHROMATOGRAPHY – MASS SPECTROMETRY (GC – MS) ANALYSIS
- GC/MS analysis and antimicrobial activity of the essential oil of fresh leaves of Eucalytus globulus







- **GC/MS Analysis of Melamine in Milk Powder**



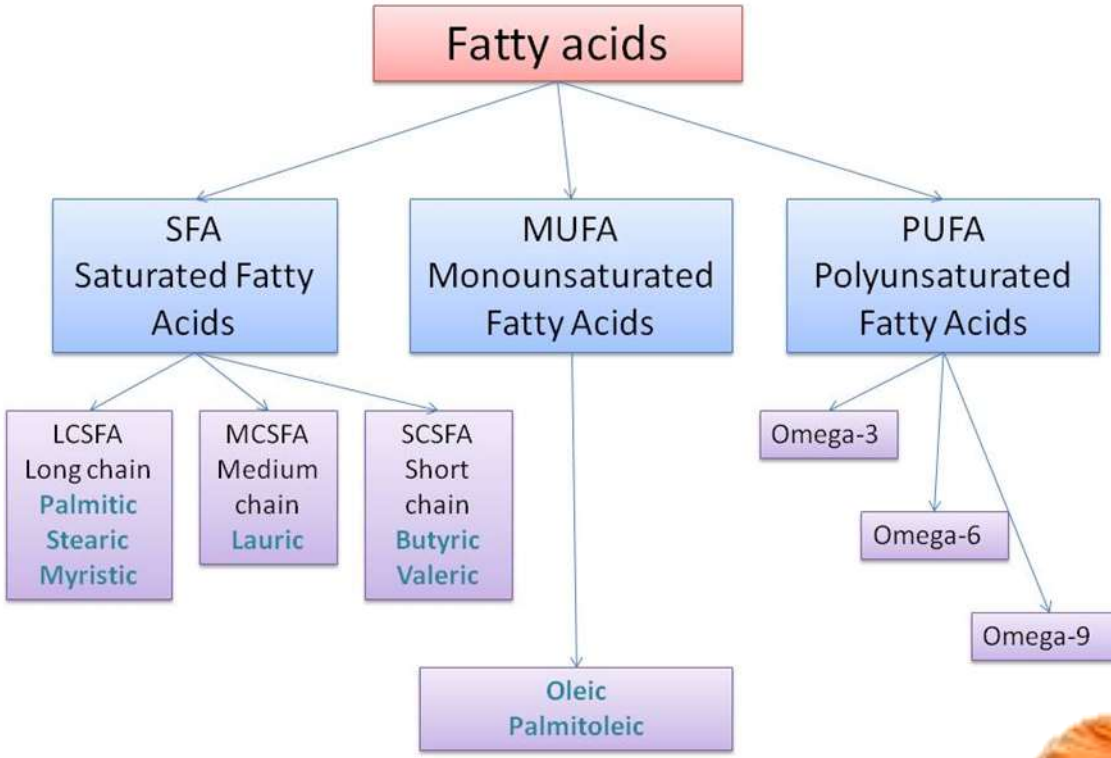
Melamine

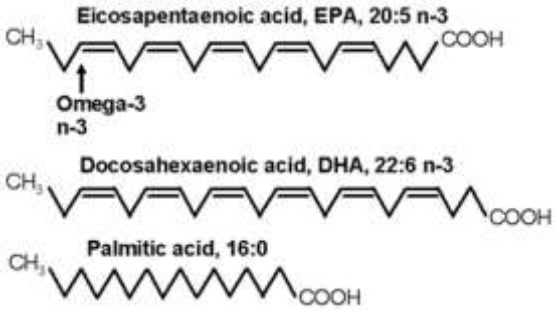
- **determination of volatile compounds in cows' milk using headspace GC-MS**.

Forty-one compounds in milk were isolated and identified from GC-MS headspace analysis.

- **Determination of Veterinary Drug Residues in Milk by GC/MS**

GC-MS analysis of Fatty acids

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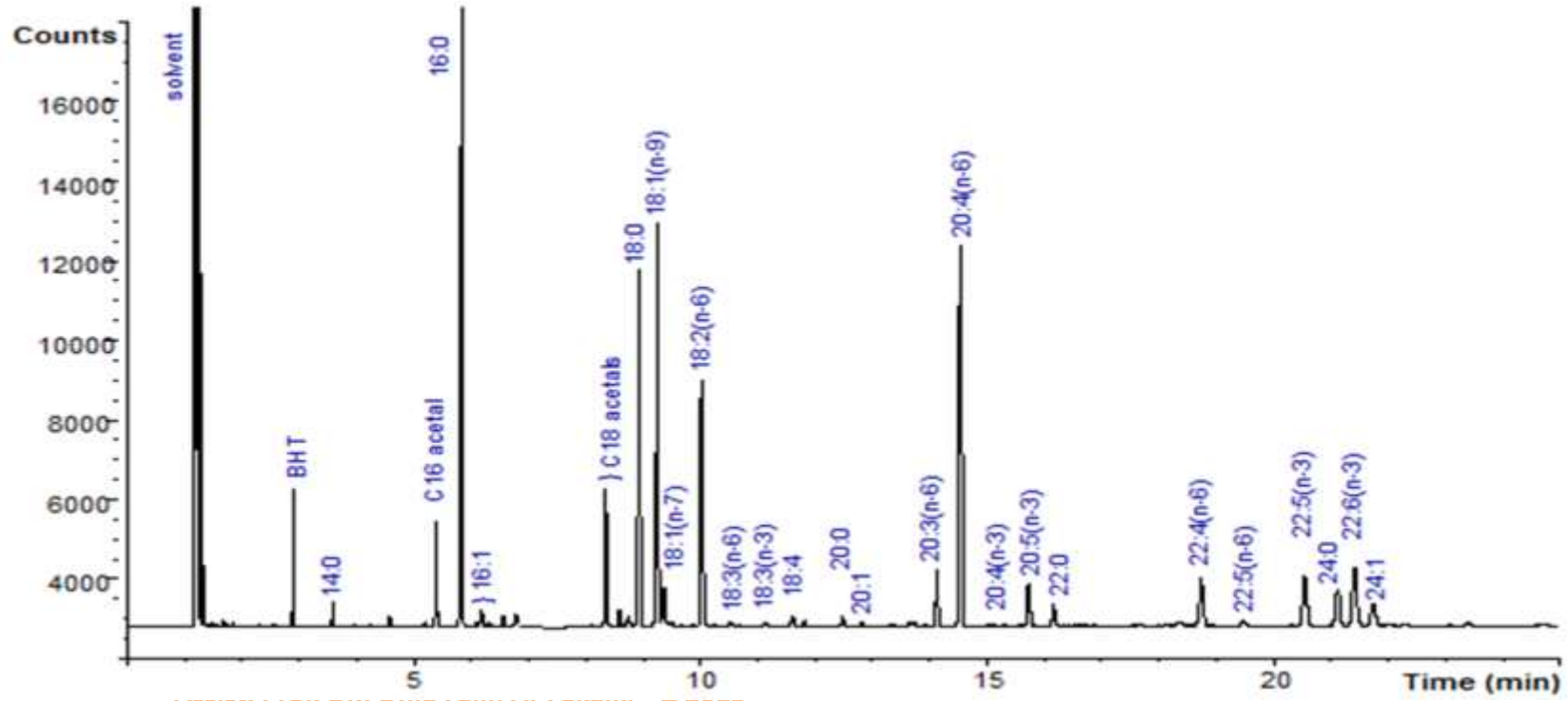
CH3
COOH
Omega-3
n-3
Docosahexaenoic acid, DHA, 22:6 n-3
CH3
COOH
Palmitic acid, 16:0
CH3
COOH


Counts
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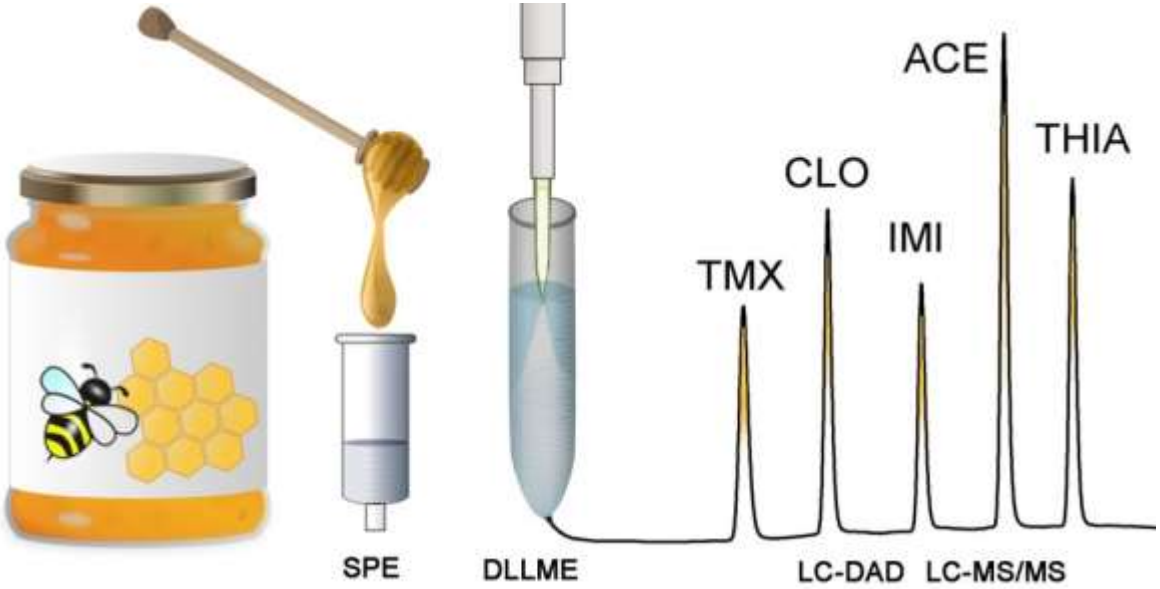
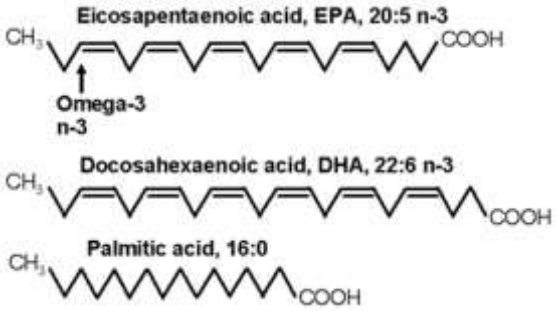
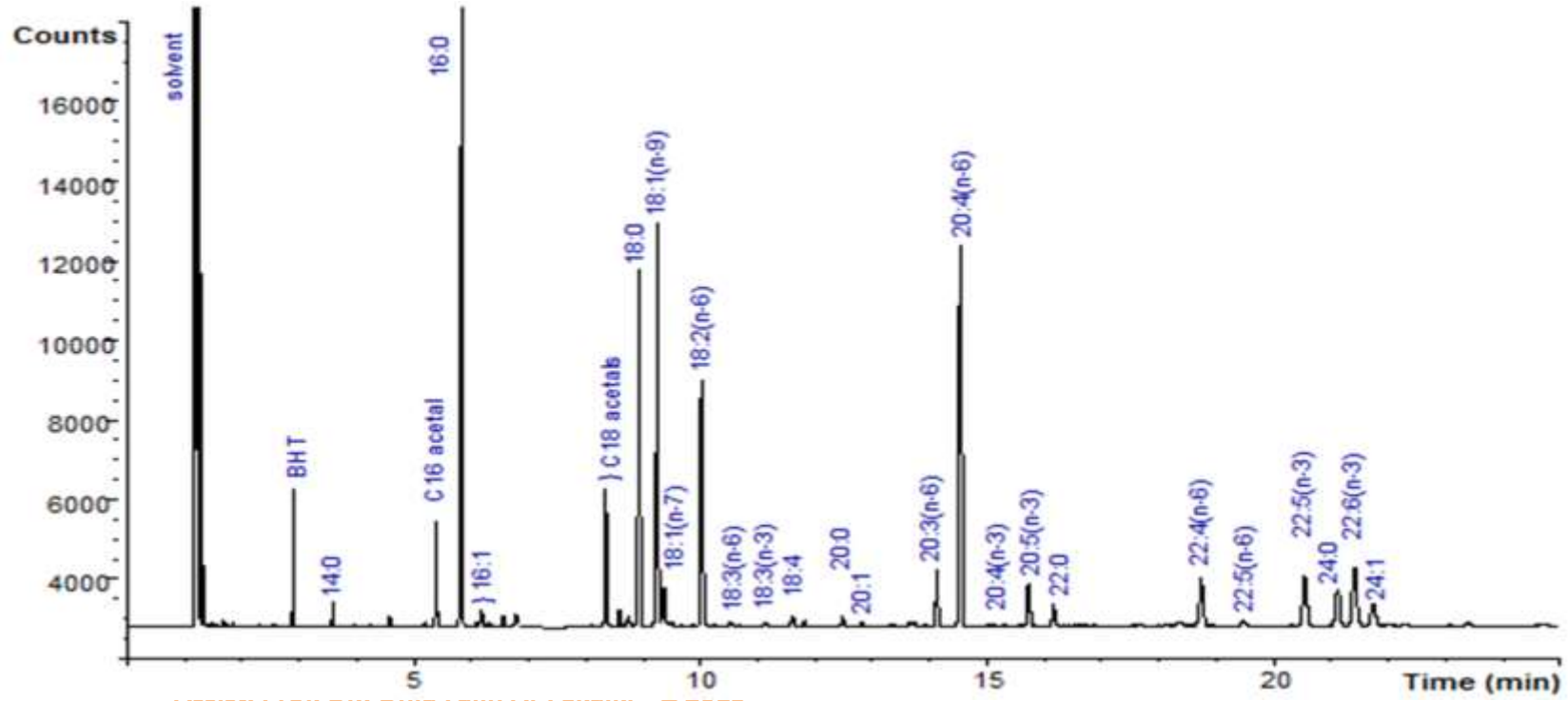
14000
12000
10000
8000
6000
4000
solvent
BHT
14:0
C16 acetal
16:0
16:1
C18 acetals
18:0
18:1(n-9)
18:1(n-7)
18:2(n-6)
18:3(n-6)
18:3(n-3)
18:4
20:0
20:1
20:3(n-6)
20:4(n-6)
20:4(n-3)
20:5(n-3)
22:0
22:4(n-6)
22:5(n-6)
22:5(n-3)
24:0
22:6(n-3)
24:1
5
10
15
20
Time (min)

Volatile Compounds in Honey

A new methodology based on GC-MS to detect honey adulteration with commercial syrups.




Eicosapentaenoic acid, EPA, 20:5 n-3
CH3
COOH
Omega-3
n-3
Docosahexaenoic acid, DHA, 22:6 n-3
CH3
COOH
Palmitic acid, 16:0
CH3
COOH


Counts
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14000
12000
10000
8000
6000
4000
solvent
BHT
14:0
C16 acetal
16:0
16:1
C18 acetals
18:0
18:1(n-9)
18:1(n-7)
18:2(n-6)
18:3(n-6)
18:3(n-3)
18:4
20:0
20:1
20:3(n-6)
20:4(n-6)
20:4(n-3)
20:5(n-3)
22:0
22:4(n-6)
22:5(n-6)
22:5(n-3)
24:0
22:6(n-3)
24:1
5
10
15
20
Time (min)

GC-MS analysis of t-BDMS derivatives of amino acids

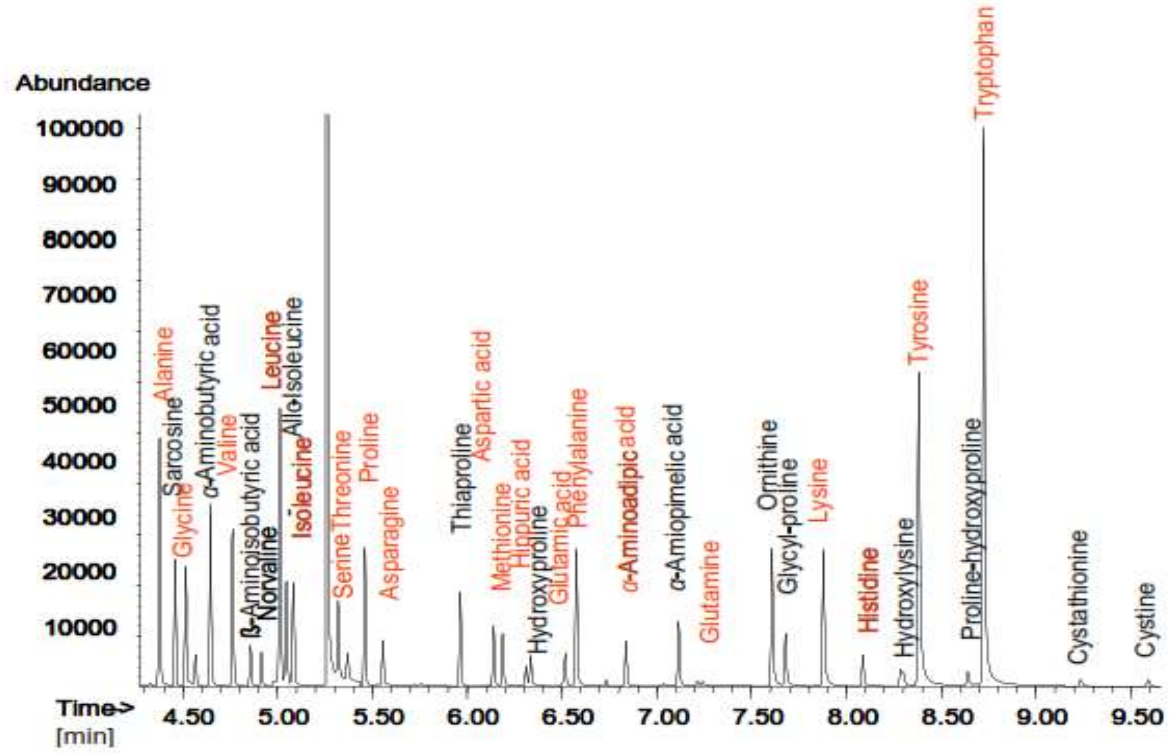


Figure 18: Typical GC-MS chromatogram for the analysis of an amino acid standard on a 15 m x 0.25 mm ID ZB-AAA column after derivatization with propyl chloroformate. Amino acids printed in red were quantified using the corresponding stable-isotope-labeled amino acid as internal standards for quantification.

Analysis of Pesticides in Food Matrix by GC/MS/MS

Inspection results for 138 pesticides using GC/MS/MS and LC/MS/MS have been reported by the EURL (European Union Reference Laboratory). Of the 138 substances, it was recommended that 66 of those substances be analyzed using the triple quadrupole GC/MS/MS, and that the remaining 72 substances be analyzed by the triple quadrupole LC/MS/MS. Thus, the pesticides were analyzed using the GCMSTQ8030 and LCMS-8040 as recommended. The combined use of GC/MS/MS and LC/MS/MS permits high-sensitivity comprehensive analysis of residual pesticides in foods.

Pesticides Recommended for GC/MS/MS Analysis (66 Compounds)

Acrinathrin	Endosulfan	Myclobutanil	Tebufenpyrad
Bifenthrin	Ethion	Oxadixyl	Tefluthrin
Bromopropylate	Etofenprox	Parathion	Tetraconazole
Bupirimate	Etoprofos	Parathion-methyl	Tetradifon
Buprofezin	Fenarimol	Pendimethalin	Tolclofos-methyl
Captan	Fenazaquin	Permethrin	Tolyfluanid
Chlorfenvinphos	Fenitrothion	Phenthoate	Triazophos
Chlorotalonil	Fenpropathrin	Phosalone	Trifluralin
Chlorpropham	Fenthion	Pirimicarb	Vinclozolin
Chlorpyriphos	Fenvalerate	Pirimiphos-methyl	
Clorpyriphos-methyl	Fipronil	Procymidone	
Cyfluthrin	Flusilazole	Profenofos	
Cypermethrin	Folpet	Propiconazole	
Cyprodinil	Iprodione	Propyzamide	
Deltamethrin	λ-Cyhalothrin	Pyridaben	
Diazinon	Malathion	Pyrimethanyl	
Dichlofluanid	Mepanipyrim	Pyriproxyfen	
Dichloran	Metalaxyl	Taufluvalinate	
Diphenylamine	Methidathion	Tebuconazole	

Fig. 2 Compounds Recommended for GC/MS/MS

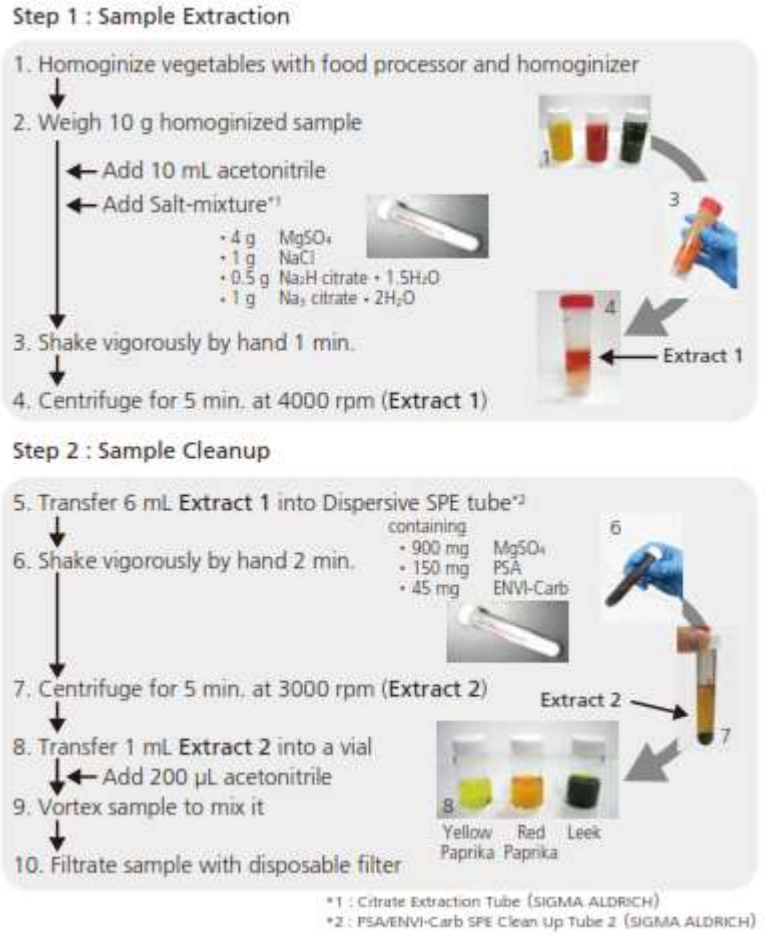


Fig. 1 Preparation of Actual Sample (QuEChERS Method Used in EU)

The Application of GC/MS to the Analysis of Pesticides in Foodstuffs

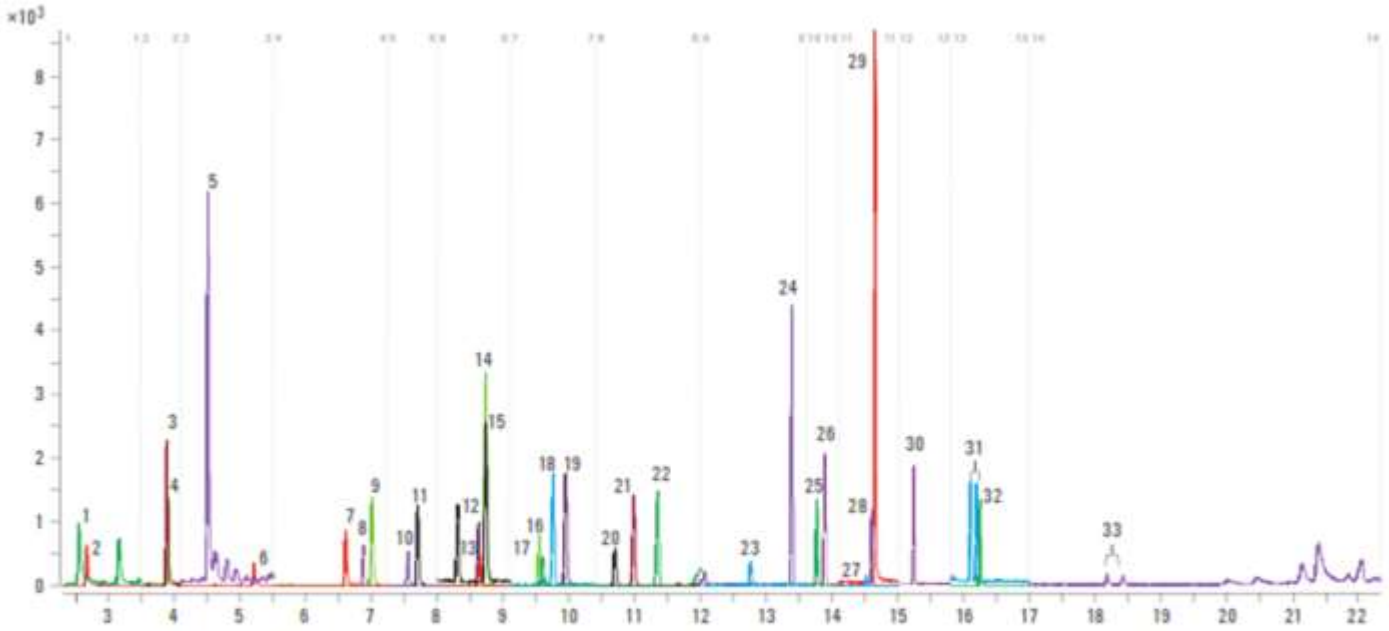


Figure 1. GC/MS/MS chromatogram (MRM) for 10 ppb spiked QuEChERS sample using Ultra Inert liner with wool (p/n 5190-2293). Peak identification: 1. Methamidophos, 2. Dichlorvos, 3. Mevinphos, 4. Acephate, 5. σ-Phenylphenol, 6. Omenthoate, 7. Dimenthoate, 8. Altrazine, 9. Lindane, 10. Diazinon, 11. Chlorothalonil, 12. Chloropyrifos methyl, 13. Vinclozolin, 14. Carbaryl, 15. Tolclofos methyl, 16. Dichlorfluanid, 17. Aldrin, 18. Malathion, 19. Dichlorobenzophenone, 20. Pirimiphos ethyl, 21. Tolyfluanid, 22 Procymidone, 23. Endrin, 24. Ethion, 25. Endosulfan sulfate, 26. DDT, 27. Endrin ketone, 28. Iprodione, 29. Phosmet, 30. Phosalone, 31. Permethrin isomers, 32. Coumaphos, 33. Deltamethrin isomers.

Determination of Quinolone Residues in Bovine Liver

A method for the determination of 11 Quinolone antibiotics in bovine liver has been established:

Analysis of Dithiocarbamate Pesticides by GC-MS

The class of dithiocarbamate fungicides (DTCs) is widely used in agriculture. They are non-systemic and both the formulation and their break-down products typically remain at the site of application. DTCs are characterized by a broad spectrum of activity against various plant pathogens, low acute mammal toxicity, and low production costs The dithiocarbamate moiety is highly reactive: it readily chelates most heavy metals, reacts with sulfhydryl groups of proteins, rendering itself neurotoxic, teratogenic, and cytotoxic.

GC/MS Analysis of Phthalates in Children's Products

Plastic is a well suited material for the manufacture of a wide range of products. Children's products, from plates and cups to mattress liners and diapers and toys, are made of plastic,as a result of its low cost and durability. The manufacture of plastic products often includes additives which are intended to modify the physical properties of the polymer. Common additives are plasticizers, antioxidants and flame retardants. There are a num- ber of different compounds classified as plasticizers – the most common are

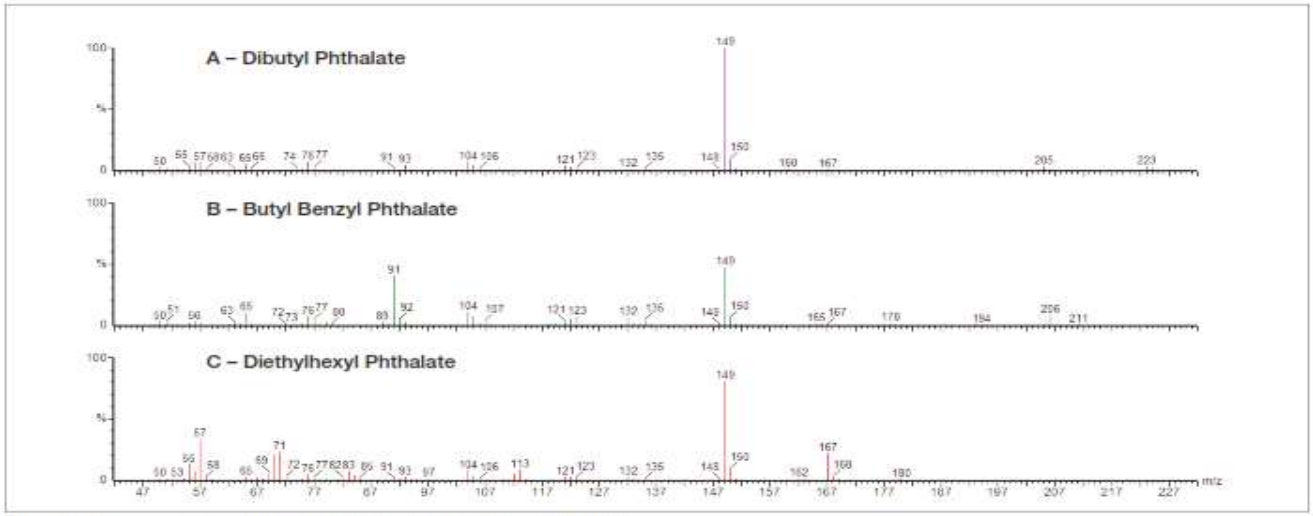
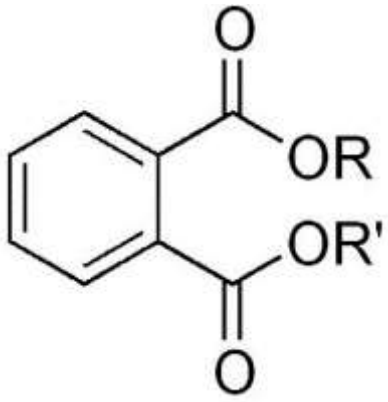
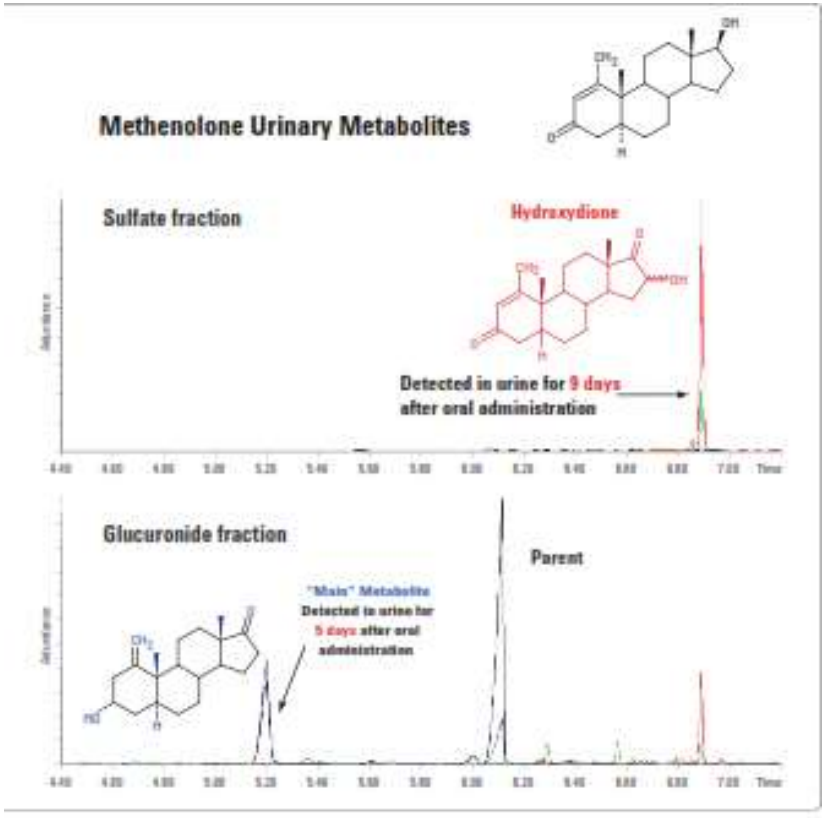


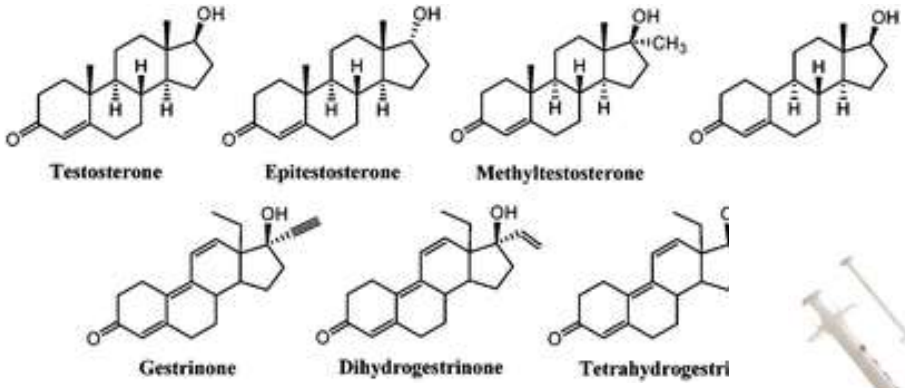
Figure 4. The comparison of the spectral data of three different phthalates.



Detection of Anabolic Steroid Metabolites in Urine by GC/MS

A gas chromatography-mass spectrometry (GC-MS) method to determine eight anabolic steroids (diethylstilbestrol, methyltestosterone, norethindrone, 17α-ethynylestradiol, estradiol, 6α-methyl-17α-hydroxy-progesterone, estradiol benzoate, and chlormadinone acetate) was developed..





Multi-Residue Pesticides Analysis in Herbal Tea Products by GC-MS/MS

The residue analysis of pesticides has developed in recent years into a comprehensive methodology for the detection of many hundreds of potentially food contaminating compounds. A multi-residue method for teas and herbal products in general is faced with particular challenges with the high number of pesticides due to a worldwide origin of the products and the complex matrix of the dried plant materials.
In the due quality control of raw materials, the unknown or undeclared local plant protection treatment has to be taken into account with a wide variety of potential pesticide contaminations. The dried leaves, fruits or seeds and other medical products deliver highly complex extracts from the sample preparation due to the rich content in active ingredients, essential oils and the typical high boiling natural polymer compounds from broken cells, leaves or fruit skins.

Application of Gas chromatography Mass Spectrometry (GC MS) in Food Science and Biotechnology

Dhia Falih Al-fekaiki

Food sciences- Biochemistry /enzymes

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