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Research Article

Determination of Bioactive Chemical Composition of Methanolic Leaves Extract of *Sinapis arvensis* Using GC-MS Technique

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ABSTRACT

Plants play an important role in providing food for humans. Among plants economic significance medicinal and aromatic plants which played a critical where it used as therapeutic agents to a long time. Thirty bioactive phytochemical compounds were identified in the methanolic extract of *Sinapis arvensis*: Erythritol , Nitro-2-propanol , Cyclopentanemethylamine ,2-isopropylidene-N,N,5-trimethyl, Furfural , 3-(1,3-Dihydroxyisopropyl)-1,5,8,11-tetraoxacyclotridecane , 3-Azabutyl-1-ol,4-cyclopropyl-3,3-dimethyl-,bromide , 1-Butene , 4-isothiocyanato- , 2,4-Difluorobenzene , 1-benzyloxy- , Eicosanoic acid , phenylmethyl ester , α-D-Glucopyranoside ,O-α-D-glucopyranosyl-(1.fwdarw.3)-β- , Trigonelline , 4H-Pyran-4-one ,2,3-dihydro-3,5-dihydroxy-6-methyl , Estragole , Pentanenitrile , 5-(methylthio)- , 5-Hydroxymethylfurfural , Eugenol , Maltose , 2H-Thiopyran-3,5-diol ,tetrahydro-4-nitro-,monoacetate (ester) , Tetraacetyl-d-xylonic nitrile , 3,6-Diazahomoadamantan-9-one Hydrazone , 9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol , (3β,5Z,7E)- , 13-Heptadecyn-1-ol , Tributyl acetylcitrate , E)-13-Docosenoic acid , Phthalic acid , decyl oct-3-yl ester , γ-Tocopherol , Desoxo-9x-hydroxy-7-ketoingol 3,8,9,12-tetraacetate , Campesterol , γ-Sitosterol , . The identification of phytochemical compounds is based on the peak area, retention time molecular weight, molecular formula, MS Fragment- ions and Pharmacological actions.

Keywords: Anti-microbial, Chemical composition, *Sinapis arvensis.*

INTRODUCTION

Natural products of higher plants be possible provide a new source of antimicrobial agents with maybe novel mechanisms of activity. In developing countries, *Sinapis arvensis* L. are used as fodder to livestock, food and folklore medicine. Brassicaceae (the mustard family) is a large family comprising 3,700 species spread over 338 genera1[1-4]. *S. arvensis* is native to Europe and grows wildly in western Asia, North Africa and throughout much of North America[5,6]. The difference between family members are in having a pungent flavor and sulfury odor lead to the volatile isothiocyanate derivatives, acquired upon hydrolysis of glucosinolate. Sinapis (mustard), a genus of Brassicaceae, has a long history of use as condiments and as herbal medicines. In many developing countries, Sinapis species are used as food, fodder to livestock, and in folklore medicine[7-13]. This genus comprises six annual species: *Sinapis alba* L. (white mustard), *S. arvensis* L. (wild mustard), *S. flexuosa* Poir., *S. pubescens* L., *S. recurvata* All., and *S. setigera* J. Gay ex Lange[14]. Many microorganisms caused the infectious are resistant to drugs synthetic, therefore, an optional therapy is much required and pull toward the attention of many researchers the worldwide. The family has a worldwide distribution, but mostly in the Northern temperate regions and strikingly diverse around the Mediterranean. Economic importance includes numerous vegetable and flavoring plants that are of major interest for human health and nutrition[15,16]. Members of the family are distinctive in having a pungent flavor and sulfury odor due to the volatile isothiocyanate derivatives, obtained upon hydrolysis of glucosinolates[17].

MATERIALS AND METHODS

Plant material and extraction

The leaves of *Sinapis arvensis* were dried at room temperature for ten days and when properly dried then powdered using clean pestle and mortar, and the powdered plant was size reduced with a sieve. About fifteen grams of the plant sample powdered were soaked in 100 mL methanol individually. The isolated extracts were re-suspended in a minimum required volume of corresponding solvents and placed on the water bath at 60 C° to evaporate the extra solvents for the isolation of pure extracts[18-40]. Then all the extracts were preserved in separate containers at 5 C° for further experimentations.

Gas chromatography – Mass Spectrum analysis

Sinapis arvensis GC–MS analysis were carried out in a GC system (Agilent 7890 Aseries, USA). The flow rate of the carrier gas, helium (He) was set to beat 1 mL min−1, split ratio was 1:50. The injector temperature was adjusted at 250◦C, while the detector temperature was

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fixed to280◦C. The column temperature was kept at 40◦C for 1 min fol-lowed by linear programming to raise the temperature from 40◦to 120◦C (at 4 Cº min−1with 2 min hold time), 120 Cº to 170 Cº (at 6 Cº min−1with 1 min hold time) and 170 Cº to 200 Cº (at10◦C min−1with 1 min hold time). The transfer line was heated at 280 Cº. Two microliter of FAME sample was injected for analysis[41-52]. Mass spectra were acquired in scan mode (70 eV); in the range of 50–550 m/z. Identification of compounds interpretation of mass spectrum was conducted using the database of National Institute of Standards and Technology (NIST, USA). The database consists of more than 62,000 patterns of known compounds. The spectrum of the extract was matched with the spectrum of the known components stored in the NIST library[53-56].

RESULTS AND DISCUSSION

Plants are very important resource due to produce complex molecular. The plant produce structures such as secondary metabolism and their derivatives have antimicrobial properties, such as alkaloids, phenolic compounds, terpens, tannins, cumarins, flavonoids, isoflavonoids and glycosides[57-60]. Gas chromatography and mass spectroscopy analysis of compounds was carried out in methanolic leaves extract of *Sinapis arvensis,* shown in Table 1. The GC-MS chromatogram of the 30 peaks of the compounds detected was shown in Figure 1. Chromatogram GC-MS analysis of the methanol extract of *Sinapis arvensis* showed the presence of thirty major peaks and the components corresponding to the peaks were determined as follows. Erythritol , Nitro-2-propanol , Cyclopentanemethylamine ,2-isopropylidene-N,N,5-trimethyl, Furfural , 3-(1,3-Dihydroxyisopropyl)-1,5,8,11-tetraoxacyclotridecane , 3-Azabutyl-1-ol,4-cyclopropyl-3,3-dimethyl-,bromide , 1-Butene , 4-isothiocyanato- , 2,4-Difluorobenzene , 1-benzyloxy- , Eicosanoic acid , phenylmethyl ester , α-D-Glucopyranoside ,O-α-D-glucopyranosyl-(1.fwdarw.3)-β- , Trigonelline , 4H-Pyran-4-one ,2,3-dihydro-3,5-dihydroxy-6-methyl , Estragole , Pentanenitrile , 5-(methylthio)- , 5-Hydroxymethylfurfural , Eugenol , Maltose , 2H-Thiopyran-3,5-diol ,tetrahydro-4-nitro- ,monoacetate (ester) , Tetraacetyl-d-xylonic nitrile , 3,6-Diazahomoadamantan-9-one Hydrazone , 9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol , (3β,5Z,7E)- , 13-Heptadecyn-1-ol , Tributyl acetylcitrate , E)-13-Docosenoic acid , Phthalic acid , decyl oct-3-yl ester , γ-Tocopherol , Desoxo-9x-hydroxy-7-ketoingol 3,8,9,12-tetraacetate , Campesterol , γ-Sitosterol.

CONCLUSION

Sinapis arvensis is native plant of Iraq. In the present study determined that forty six phytoconstituents were identified from methanol leaves extract of *Sinapis arvensis* by gas chromatogram and mass spectrometry (GC-MS) analysis. *Sinapis arvensis* leaves can be used as a promising multipurpose medicinal source whereas further clinical trial is required to prove its efficacy.

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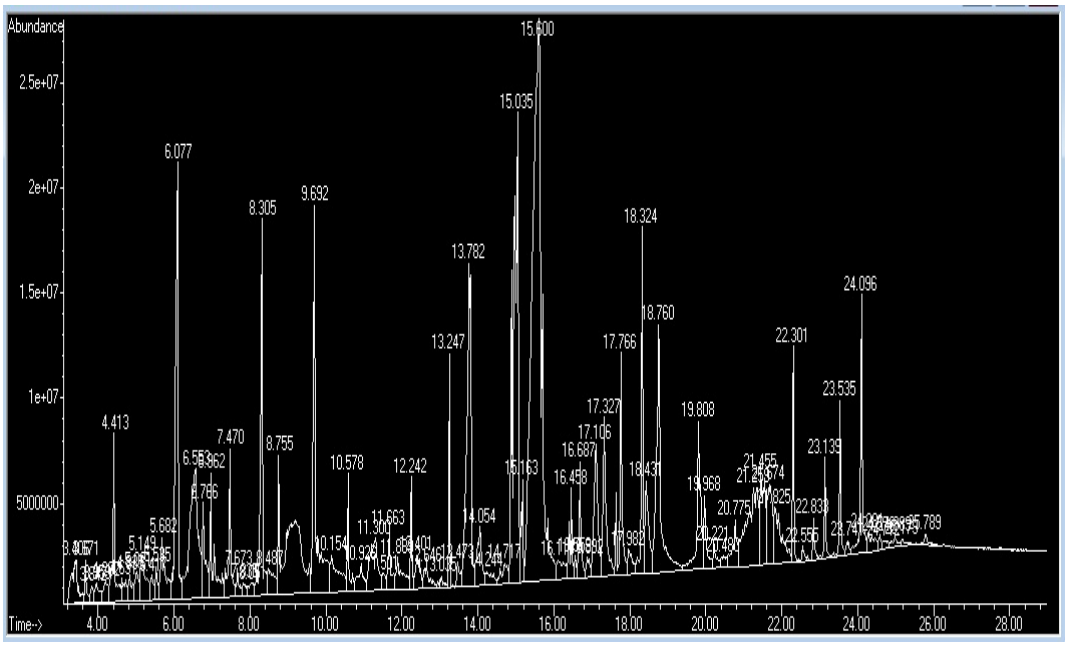


Figure 1: GC-MS chromatogram of methanolic extract of *Sinapis arvensis*.

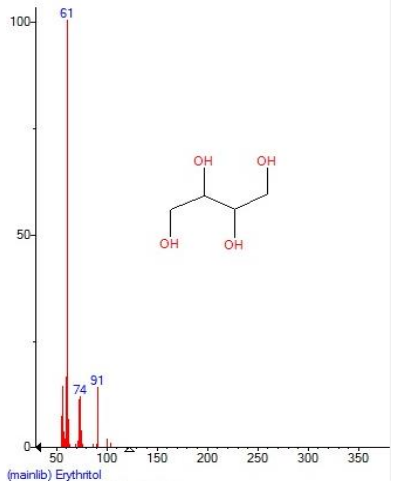


Figure 2: Mass spectrum of Erythritol with Retention Time (RT)= 3.287

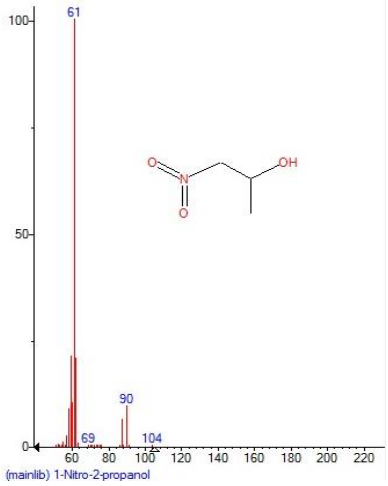


Figure 3: Mass spectrum of 1-Nitro-2-propanol with Retention Time (RT)= 3.424

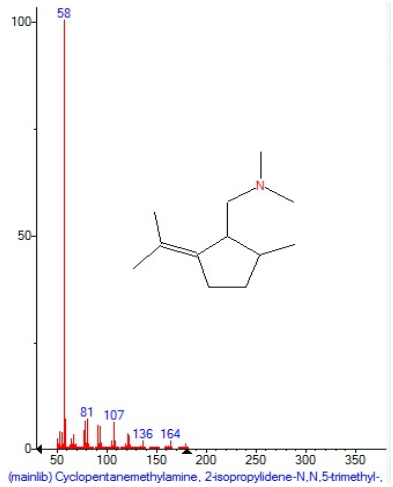


Figure 4: Mass spectrum of Cyclopentanemethylamine ,2-isopropylidene-N,N,5-trimethyl-, with Retention Time (RT)= 3.476

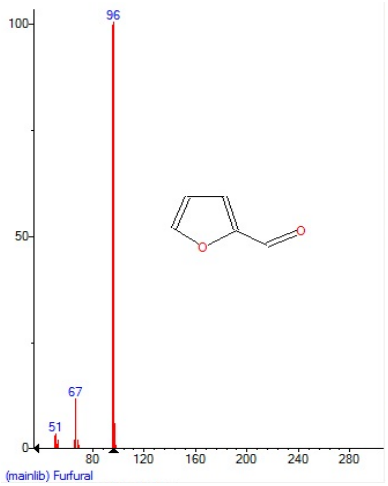


Figure 5: Mass spectrum of Furfural with Retention Time (RT)= 3.665

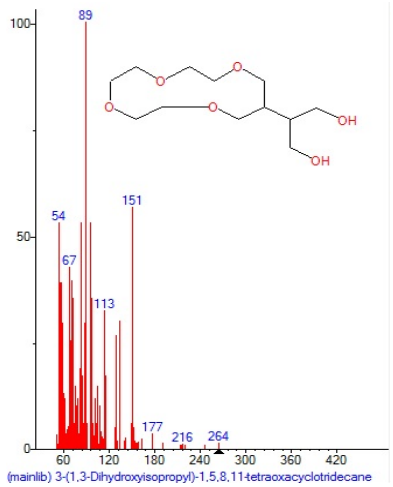


Figure 6: Mass spectrum of 3-(1,3-Dihydroxyisopropyl)-1,5,8,11-tetraoxacyclotridecane with Retention Time (RT)= 3.957

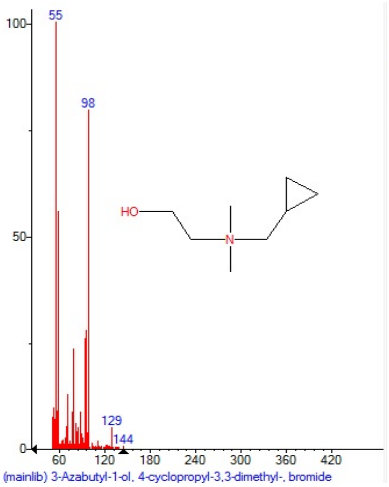


Figure 7: Mass spectrum of 3-Azabutyl-1-ol,4-cyclopropyl-3,3-dimethyl-,bromide with Retention Time (RT)= 4.191

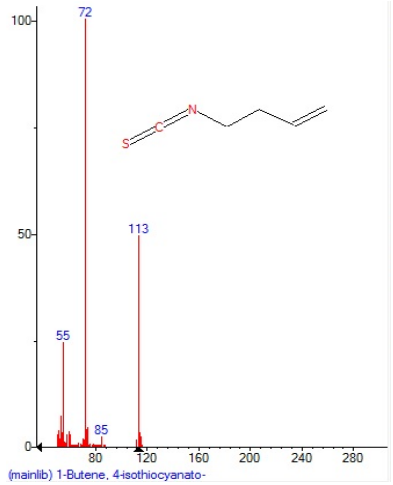


Figure 8: Mass spectrum of 1-Butene , 4-isothiocyanato- with Retention Time (RT)= 4.420

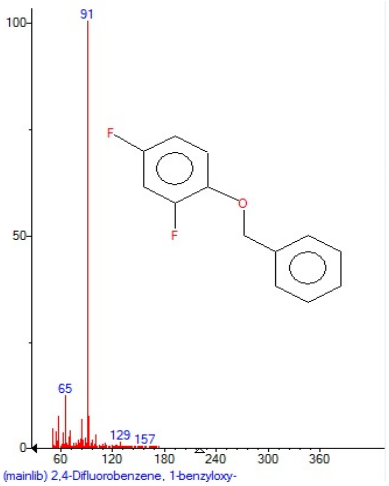


Figure 9: Mass spectrum of 2,4-Difluorobenzene , 1-benzyloxy- with Retention Time (RT)= 4.632

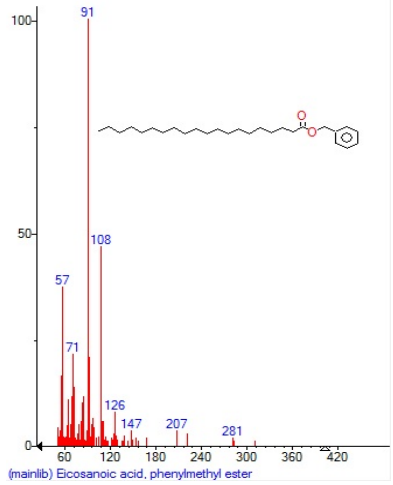


Figure 10: Mass spectrum of Eicosanoic acid , phenylmethyl ester with Retention Time (RT)= 4.832

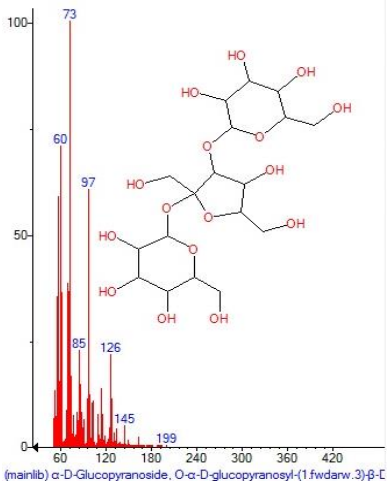


Figure 11 : Mass spectrum of α-D-Glucopyranoside ,O-α-D-glucopyranosyl-(1.fwdarw.3)-β- with Retention Time (RT)= 5.021

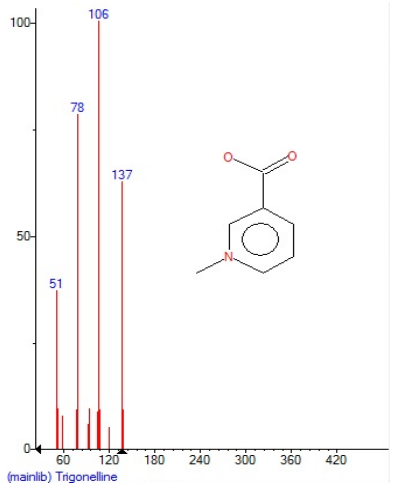


Figure 12: Mass spectrum of Trigonelline with Retention Time (RT)= 5.530

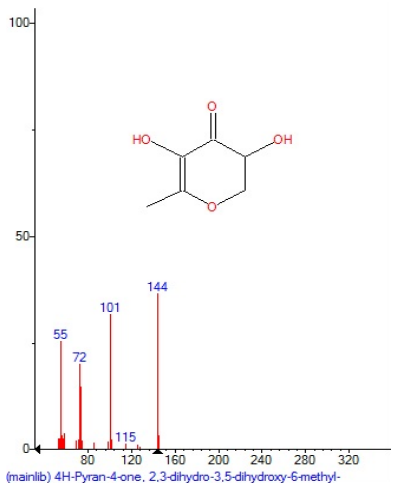


Figure 13: Mass spectrum of 4H-Pyran-4-one ,2,3-dihydro-3,5-dihydroxy-6-methyl- with Retention Time (RT)= 5.673

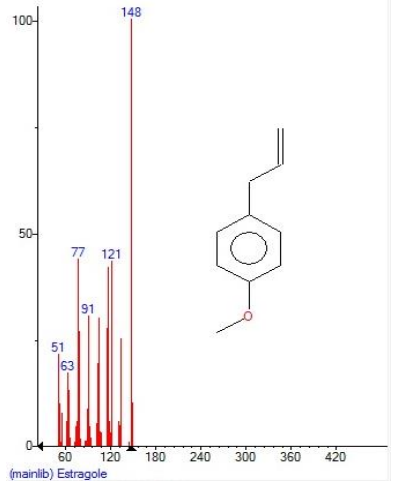


Figure 14: Mass spectrum of Estragole with Retention Time (RT)= 5.965

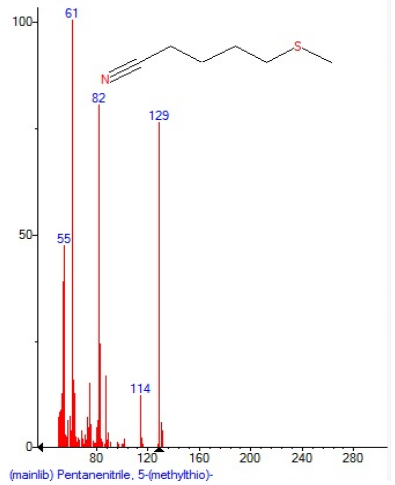


Figure 15: Mass spectrum of Pentanenitrile , 5-(methylthio)- with Retention Time (RT)= 6.034

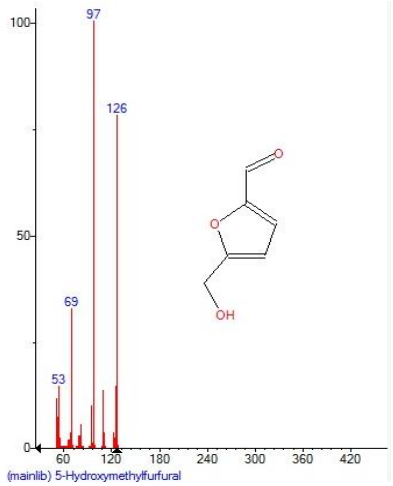


Figure 16: Mass spectrum of 5-Hydroxymethylfurfural with Retention Time (RT)= 6.434

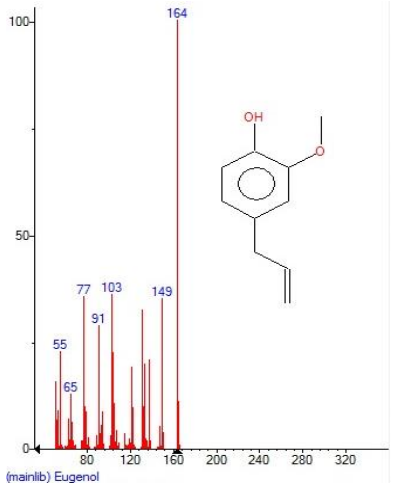


Figure 17: Mass spectrum of Eugenol with Retention Time (RT)= 7.470

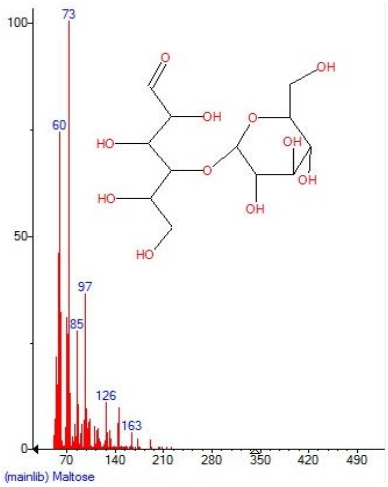


Figure 18: Mass spectrum of Maltose with Retention Time (RT)= 7.750

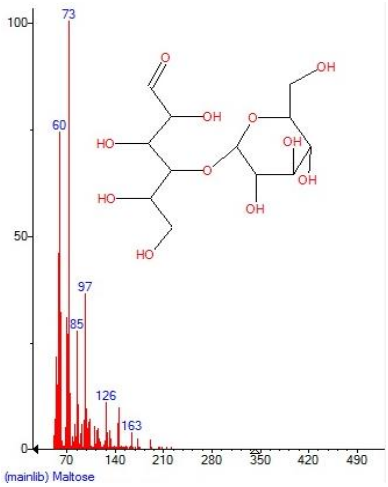


Figure 19: Mass spectrum of 2H-Thiopyran-3,5-diol ,tetrahydro-4-nitro-,monoacetate (ester) with Retention Time (RT)= 8.305

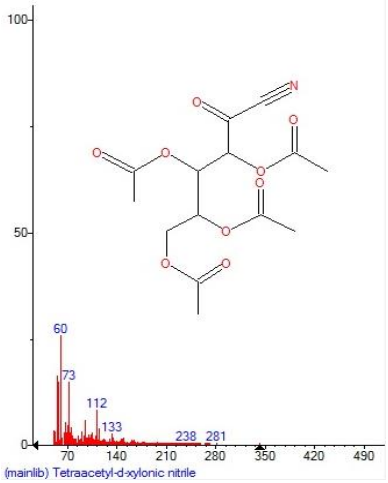


Figure 20: Mass spectrum of Tetraacetyl-d-xylonic nitrile with Retention Time (RT)= 9.558

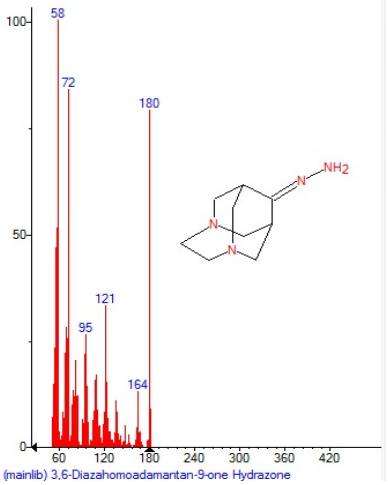


Figure 21: Mass spectrum of 3,6-Diazahomoadamantan-9-one Hydrazone with Retention Time (RT)= 9.753

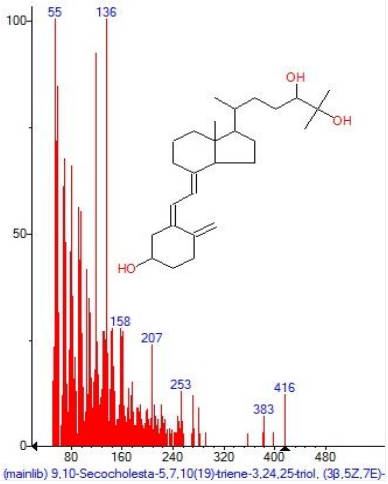


Figure 22: Mass spectrum of 9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol , (3β,5Z,7E)- with Retention Time (RT)= 13.478

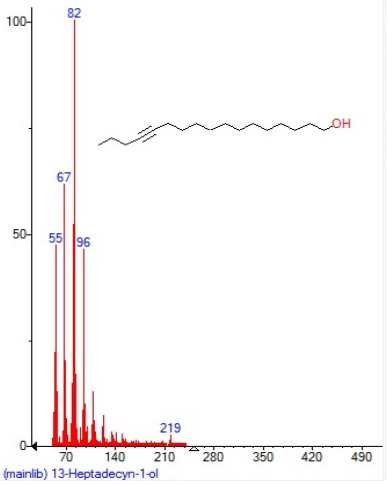


Figure 23: Mass spectrum of 13-Heptadecyn-1-ol with Retention Time (RT)= 14.720

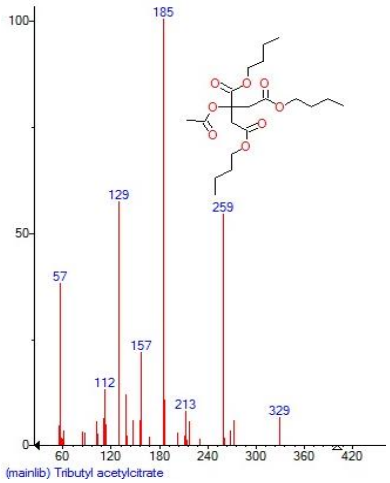


Figure 24: Mass spectrum of Tributyl acetylcitrate with Retention Time (RT)= 16.390

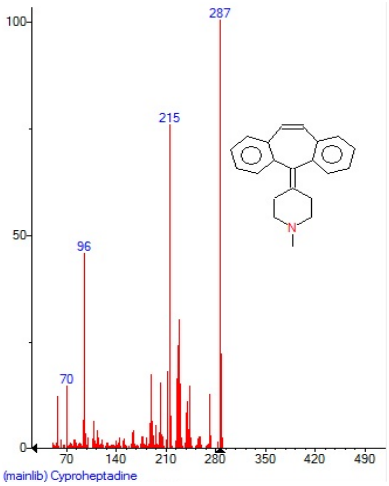


Figure 25: Mass spectrum of Cyproheptadine with Retention Time (RT)= 17.804

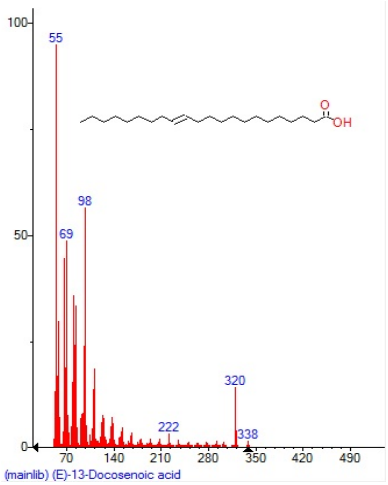


Figure 26: Mass spectrum of (E)-13-Docosenoic acid with Retention Time (RT)= 18.799

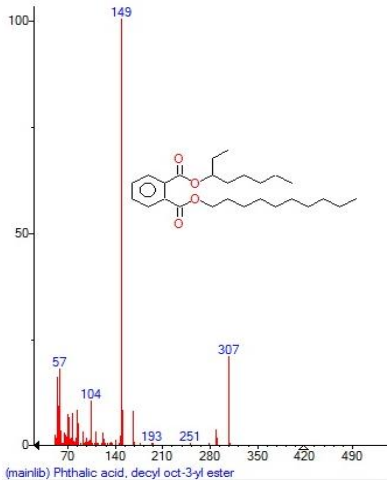


Figure 27: Mass spectrum of Phthalic acid , decyl oct-3-yl ester with Retention Time (RT)= 21.924

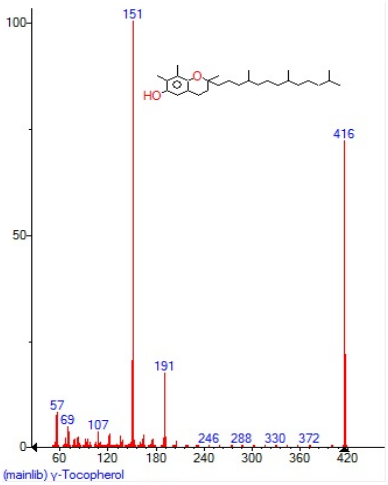


Figure 28: Mass spectrum of γ-Tocopherol with Retention Time (RT)= 22.307

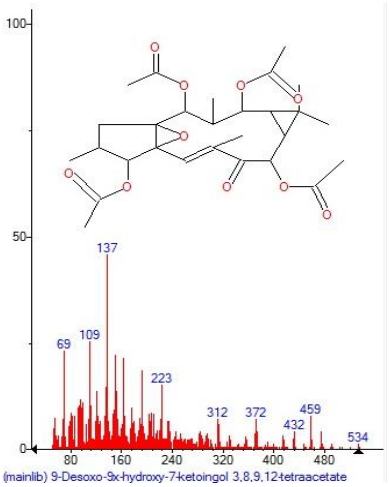
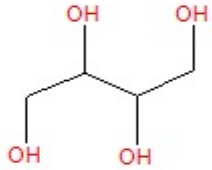
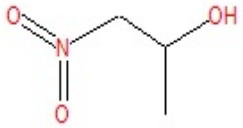
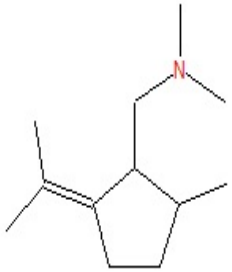
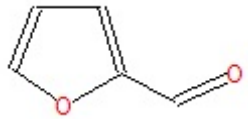
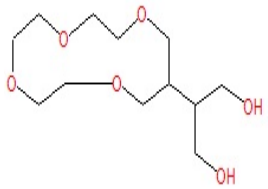
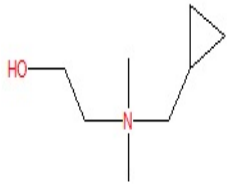
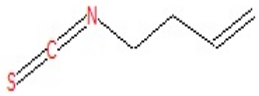
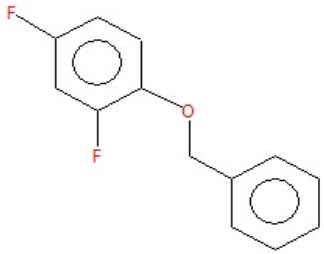
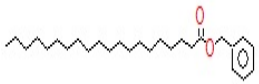
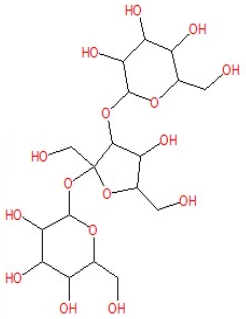
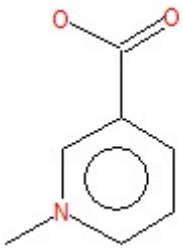
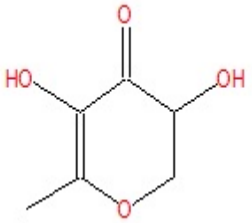
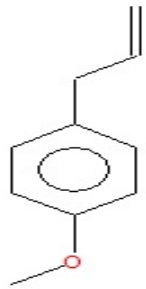
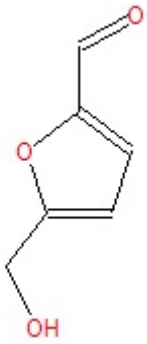


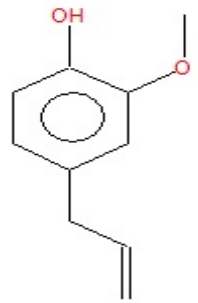
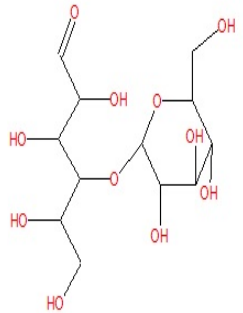
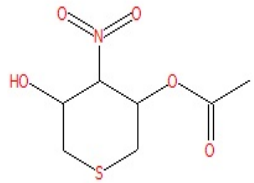
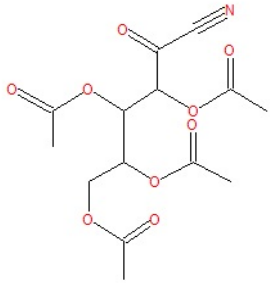
Figure 29: Mass spectrum of 9-Desoxo-9x-hydroxy-7-ketoingol 3,8,9,12-tetraacetate with Retention Time (RT)= 22.850

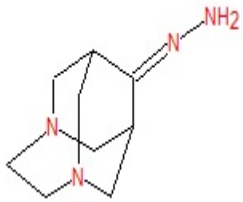
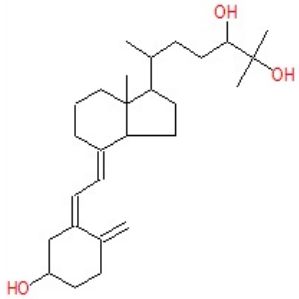
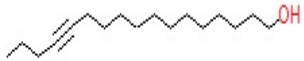
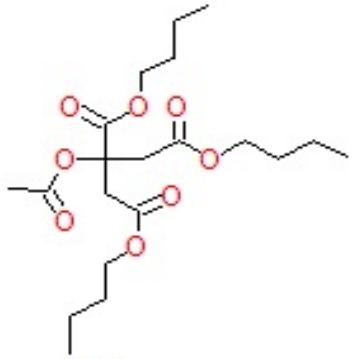
Table 1. Major phytochemical compounds identified in methanolic extract of *Sinapis arvensis*.

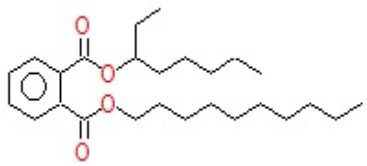
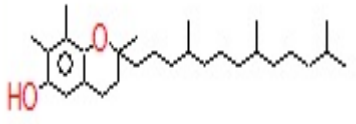
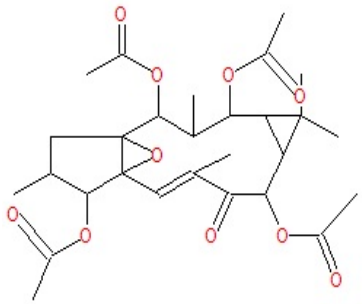
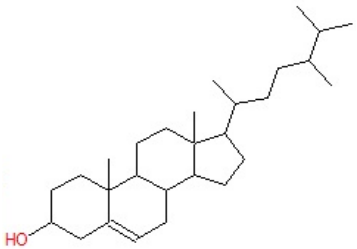
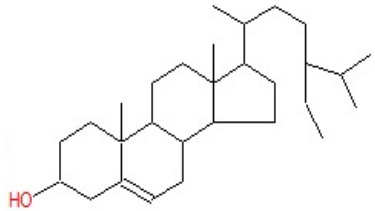
Serial No.	Phytochemical compound	RT (min)	Molecular Weight	Exact Mass	Chemical structure	MS Fragment-ions	Pharmacological actions
1.	Erythritol	3.287	122	122.057909		61,74,91	Anti-Bacterial Agents
2.	1-Nitro-2-propanol	3.424	105	105.042593		61,69,90,104	Anti-Bacterial Agents
3.	Cyclopentanemethylamine ,2-isopropylidene-N,N,5-trimethyl-,	3.476	181	181.18305		58,81,107,136, 164	anti-inflammatory
4.	Furfural	3.665	96	96.021129		51,67,96	anti-tyrosinase activity
5.	3-(1,3-Dihydroxyisopropyl)-1,5,8,11-tetraoxacyclotridecane	3.957	264	264.157288		54,67,89,113,1 51,177,216,264	anti-cancer activity

6.	3-Azabutyl-1-ol,4-cyclopropyl-3,3-dimethyl-,bromide	4.191	144	144.138839		55,98,129,144	New chemical compound
7.	1-Butene , 4-isothiocyanato-	4.420	113	113.02992		55,72,85,113	Antioxidant Activities
8.	2,4-Difluorobenzene , 1-benzyloxy-	4.632	220	220.069971		65,91,129,157	antitumor, anti-inflammatory
9.	Eicosanoic acid , phenylmethyl ester	4.832	402	402.349781		57,71,91,108,126,147,207,281	Anti-inflammatory
10.	α-D-Glucopyranoside ,O-α-D-glucopyranosyl-(1.fwdarw.3)-β-	5.021	504	504.169035		60,73,85,97,126,145,199	anti-inflammatory, antistress

11.	Trigonelline	5.530	137	137.047678		51,78,106,137	antibacterial, antiviral, and anti-tumor activities
12	4H-Pyran-4-one ,2,3-dihydro-3,5-dihydroxy-6-methyl-	5.673	144	144.042258		55,72,101,115, 144	antibacterial activities and antioxidant
13	Estragole	5.965	148	148.088815		51,63,77,91,12 1,148	anti-inflammatory activity
14	Pentanenitrile , 5-(methylthio)-	6.034	129	129.06122		55,61,82,114,1 29	anti-inflammatory and antitumor activities
15	5-Hydroxymethylfurfural	6.434	126	126.031694		53,69,97,126	antioxidant and anti-proliferative activities

16	Eugenol	7.470	164	164.08373		55,65,77,91,103,149,164	antioxidant, anti-inflammatory
17	Maltose	7.750	342	342.11621		60,73,85,97,126,163	anti-inflammatory and analgesic effect
18	2H-Thiopyran-3,5-diol ,tetrahydro-4-nitro- ,monoacetate (ester)	8.305	221	221.035793		57,85,115,161,221	anti-inflammatory
19	Tetraacetyl-d-xylonic nitrile	9.558	343	343.090332		60,73,112,133,238,281	antimicrobial, antioxidant

20	3,6-Diazahomoadamantan-9-one Hydrazone	9.753	180	180.137497		58,72,95,121,164,180	antiviral effect
21	9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol , (3β,5Z,7E)-	13.478	416	416.329044		55,136,158,207,253,383,416	Unknown
22	13-Heptadecyn-1-ol	14.720	252	252.245316		55,67,82,96,219	anti-inflammatory, antifungal
23	Tributyl acetylcitrate	16.390	402	402.225368		57,112,129,157,185,213,259,329	antioxidant and anti-inflammatory
25	(E)-13-Docosenoic acid	18.799	338	338.318481		55,69,98,222,320,338	antimicrobial activity

26	Phthalic acid , decyl oct-3-yl ester	21.924	418	418.30831		57,104,149,193,251,307	anti-bacterial activity
27	γ-Tocopherol	22.307	416	416.36543		57,69,107,151,191,246,288,330,372,416	Anti-inflammatory
28	9-Desoxo-9x-hydroxy-7-ketoingol 3,8,9,12-tetraacetate	22.850	534	534.2465		69,109,137,223,312,372,432,459,534	New chemical compound
29	Campesterol	23.531	400	400.370516		55,81,145,213,255,289,315,400	anti-inflammatory activity
30	γ-Sitosterol	24.121	414	414.386166		55,81,145,213,255,273,303,329,396,414	anti-inflammatory *activity*

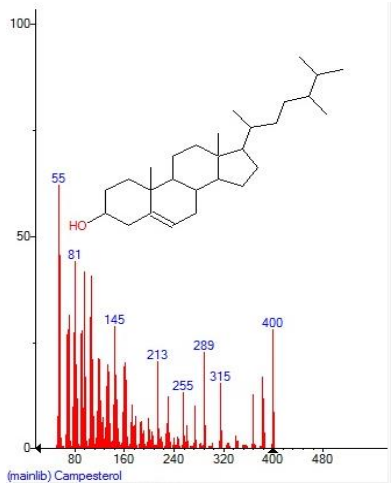


Figure 30: Mass spectrum of Campesterol with Retention Time (RT)= 23.531

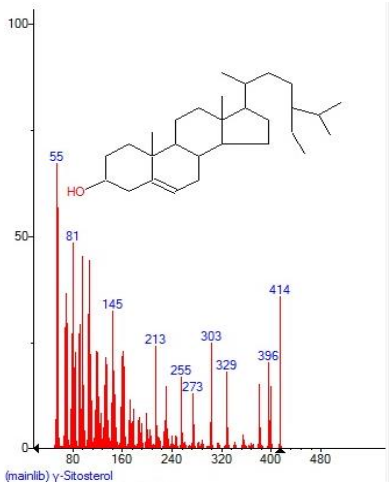


Figure 31: Mass spectrum of γ-Sitosterol with Retention Time (RT)= 24.121

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