Supplementary Informations

Differences in Phytochemical Profiles and Antifungal Activities against Cutaneous Pathogenic Fungi of Volatile Oils Extracted from Peels of Fresh and Grilled *Citrus hystrix* DC. Fruits

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Chemical compositions of F-ChVO and G-ChVO by GC-MS analysis.

The phytochemical constituents of F-ChVO were analyzed using GC-MS. A total of **33** compounds was identified in F-ChVO.

Figure S1. GC-MS analysis was performed to identify the phytochemical constituents in the F-ChVO

Qualitative Compound Report

Data File	F-01.D	**Sample Name**	F-01
Sample Type		**Position**	1
Instrument Name	GCMS	**User Name**	
Acq Method	NA2-671003.M	**Acquired Time**	8/2/2024 2:03:58 PM
IRM Calibration Status	Not Applicable	**DA Method**	default.m
Comment			
Expected Barcode		**Sample Amount**	
Dual Inj Vol	1	**TuneName**	20240802_atune.u
TunePath	D:\MassHunter\GCMS\1\5977\	**MSFirmwareVersion**	6.00.21
Acquisition Time #2	2024-08-02 07:03:58Z	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.02.1938 08-Sep-2014 Copyright © 1989-2014 Agilent Technologies, Inc.

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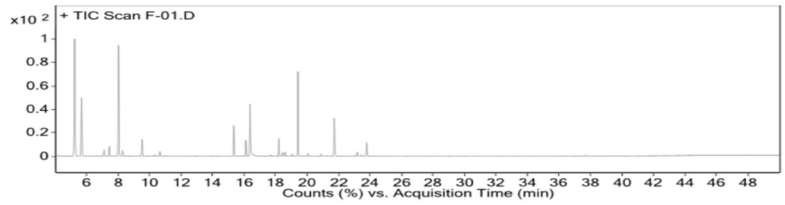
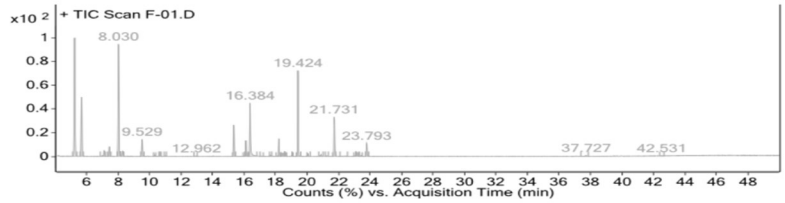


Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** Unspecified



User Chromatogram Peak List

RT	Height	Normalized Height	Height %	Area	Area %	Area Sum %	Base Peak m/z	Width
5.246	1518873	99.76	100	5898833	100	22.02	93.1	0.255
5.681	758260	49.8	49.92	2761369	46.81	10.31	93.1	0.244
7.116	73707	4.84	4.85	294154	4.99	1.1	93.1	0.372
7.446	124892	8.2	8.22	421353	7.14	1.57	121.1	0.191
8.03	1436939	94.38	94.61	4879311	82.72	18.22	68.1	0.213
8.296	66325	4.36	4.37	232135	3.94	0.87	93.1	0.234
9.529	217745	14.3	14.34	708156	12.01	2.64	93.1	0.244
10.326	18826	1.24	1.24	59777	1.01	0.22	119	0.17
10.656	56010	3.68	3.69	179216	3.04	0.67	93	0.159
10.996	7978	0.52	0.53	25148	0.43	0.09	44	0.138

12.962	5439	0.36	0.36	22846	0.39	0.09	56	0.223
15.354	401959	26.4	26.46	1153620	19.56	4.31	59	0.213
15.991	6644	0.44	0.44	17844	0.3	0.07	44	0.138
16.129	202276	13.29	13.32	573435	9.72	2.14	59.1	0.213
16.384	682086	44.8	44.91	2466277	41.81	9.21	69.1	0.489
17.107	4608	0.3	0.3	19109	0.32	0.07	44	0.202
17.692	16927	1.11	1.11	45302	0.77	0.17	161.1	0.106
18.213	227937	14.97	15.01	626870	10.63	2.34	71.1	0.319
18.468	46324	3.04	3.05	194989	3.31	0.73	93	0.191
18.627	49066	3.22	3.23	143599	2.43	0.54	81.1	0.159
19.084	22215	1.46	1.46	56971	0.97	0.21	93	0.106
19.424	1100345	72.27	72.44	3092032	52.42	11.54	71.1	0.223
20.073	32076	2.11	2.11	89705	1.52	0.33	93.1	0.191
20.902	26813	1.76	1.77	103945	1.76	0.39	69.1	0.266
21.252	8361	0.55	0.55	21966	0.37	0.08	84	0.191
21.731	502636	33.01	33.09	1648594	27.95	6.15	59	0.191
22.454	6002	0.39	0.4	54901	0.93	0.2	44	0.478
23.059	10649	0.7	0.7	30616	0.52	0.11	84	0.159
23.198	48763	3.2	3.21	191463	3.25	0.71	161.1	0.191
23.453	13812	0.91	0.91	54617	0.93	0.2	69	0.213
23.793	165292	10.86	10.88	628383	10.65	2.35	69.1	0.213
37.727	10434	0.69	0.69	71617	1.21	0.27	44	0.478
42.531	2363	0.16	0.16	18068	0.31	0.07	43.9	0.266

Compound Table

Compound Label	RT	Name	DB Formula	Hits (DB)
Cpd 1: 2(10)-Pinene, (1S,5S)-(-)-	5.246	2(10)-Pinene, (1S,5S)-(-)-	C10H16	10
Cpd 2: 4(10)-Thujene	5.681	4(10)-Thujene	C10H16	10
Cpd 3: 1,6-Octadiene, 7-methyl-3-methylene-	7.116	1,6-Octadiene, 7-methyl-3-methylene-	C10H16	10
Cpd 4: .ALPHA. TERPINENE	7.446	.ALPHA. TERPINENE	C10H16	10
Cpd 5: D-Limonene	8.03	D-Limonene	C10H16	10
Cpd 6: 4(10)-Thujene	8.296	4(10)-Thujene	C10H16	10
Cpd 7: .gamma.-Terpinene	9.529	.gamma.-Terpinene	C10H16	10
Cpd 8: Benzene, methyl(1-methylethyl)-	10.326	Benzene, methyl(1-methylethyl)-	C10H14	10
Cpd 9: Cyclohexene, 1-methyl 4-(1-methylethylidene)-	10.656	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	C10H16	10
Cpd 10: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	10.996	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 11: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	12.962	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 12: 2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-, cis-	15.354	2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-, cis-	C10H18O2	10
Cpd 13: Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(Z),4-pentadienyl]acetoacetate	15.991	Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(Z),4-pentadienyl]acetoacetate	C23H30O4	10
Cpd 14: TRANS-LINALOOL OXIDE	16.129	TRANS-LINALOOL OXIDE	C10H18O2	10
Cpd 15: Citronellal	16.384	Citronellal	C10H18O	10

Cpd 16: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	17.107	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 17: 1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, 2,3,3a.alpha.,3b.alpha.,4,5,6,7-octahydro-4.alpha.-isopropyl-7.beta.-methyl-3-methylene-	17.692	1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, 2,3,3a.alpha.,3b.alpha.,4,5,6,7-octahydro-4.alpha.-isopropyl-7.beta.-methyl-3-methylene-	C15H24	10
Cpd 18: Linalool	18.213	Linalool	C10H18O	10
Cpd 19: TRANS-PINENE HYDRATE	18.468	TRANS-PINENE HYDRATE	C10H18O	10
Cpd 20: Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	18.627	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	C10H18O	10
Cpd 21: Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (E)-(1R,9S)-(-)-	19.084	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (E)-(1R,9S)-(-)-	C15H24	10
Cpd 22: 3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	19.424	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	C10H18O	10
Cpd 23: p-menth-2-en-1-ol	20.073	p-menth-2-en-1-ol	C10H18O	10
Cpd 24: 6-Octen-1-ol, 3,7-dimethyl-, acetate	20.902	6-Octen-1-ol, 3,7-dimethyl-, acetate	C12H22O2	10
Cpd 25: Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(E),4-pentadienyl]acetoacetate	21.252	Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(E),4-pentadienyl]acetoacetate	C23H30O4	7
Cpd 26: 2-(4-METHYL-3-CYCLOHEXEN-1-YL)-2-PROPANOL	21.731	2-(4-METHYL-3-CYCLOHEXEN-1-YL)-2-PROPANOL	C10H18O	10
Cpd 27: Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(Z),4-pentadienyl]acetoacetate	22.454	Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(Z),4-pentadienyl]acetoacetate	C23H30O4	10
Cpd 28: 2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, trans-	23.059	2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, trans-	C10H18O	10
Cpd 29: 1-ISOPROPYL-4,7-DIMETHYL-1,2,4A,5,8,8A-HEXAHYDRONAPHTHALENE	23.198	1-ISOPROPYL-4,7-DIMETHYL-1,2,4A,5,8,8A-HEXAHYDRONAPHTHALENE	C15H24	10
Cpd 30: 4-Hexen-1-ol, 2-isopropenyl-5-methyl-, acetate	23.453	4-Hexen-1-ol, 2-isopropenyl-5-methyl-, acetate	C12H20O2	10
Cpd 31: 6-Octen-1-ol, 3,7-dimethyl-	23.793	6-Octen-1-ol, 3,7-dimethyl-	C10H20O	10
Cpd 32: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	37.727	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 33: 1,3-Dioxolane	42.531	1,3-Dioxolane	C3H6O2	10

Compound Label	Name	RT	Algorithm
Cpd 1: 2(10)-Pinene, (1S,5S)-(-)-	**2(10)-Pinene, (1S,5S)-(-)-**	5.246	Find by Integration

Figure S2 GC-MS analysis was performed to identify the phytochemical constituents in the G-ChVO

The phytochemical constituents of G-ChVO were analyzed using GC-MS. A total of 91 compounds was identified in G-ChVO.

Qualitative Compound Report

Data File	G01.D	**Sample Name**	G01
Sample Type		**Position**	1
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IRM Calibration Status	Not Applicable	**DA Method**	default.m
Comment			

Expected Barcode		**Sample Amount**	
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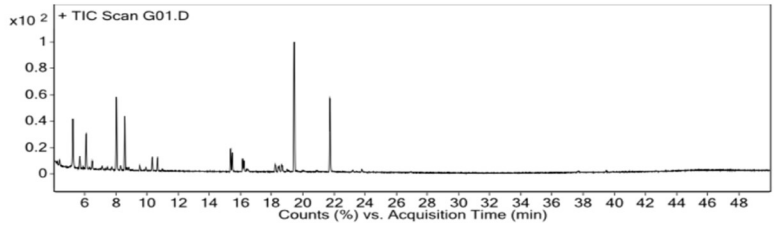
TunePath	D:\MassHunter\GCMS\1\5977\	**MSFirmwareVersion**	6.00.21
Acquisition Time #2	2024-07-09 06:39:48Z	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.02.1938 08-Sep-2014 Copyright © 1989-2014 Agilent Technologies, Inc.

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** Unspecified



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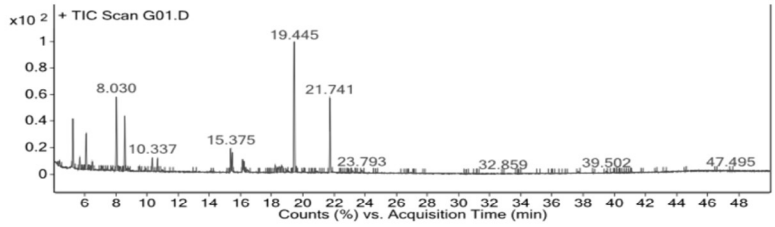


User Chromatogram Peak List

RT	Height	Normalized Height	Height %	Area	Area %	Area Sum %	Base Peak m/z	Width
4.384	20767	4.08	4.14	69753	3.22	0.77	93.1	0.159
5.235	187293	36.76	37.36	692645	32.01	7.66	93.1	0.213
5.681	45125	8.86	9	171922	7.95	1.9	93.1	0.17
5.904	8775	1.72	1.75	24771	1.14	0.27	43.9	0.159
6.085	137284	26.94	27.38	487355	22.52	5.39	93.1	0.223
6.308	8003	1.57	1.6	28109	1.3	0.31	44	0.149
6.478	32093	6.3	6.4	119234	5.51	1.32	93.1	0.191
6.988	3537	0.69	0.71	9167	0.42	0.1	44	0.074
7.116	12457	2.44	2.48	43222	2	0.48	93.1	0.117
7.446	10476	2.06	2.09	35984	1.66	0.4	44.1	0.149

7.732	9533	1.87	1.9	26024	1.2	0.29	44	0.159
8.03	283856	55.71	56.62	982337	45.4	10.86	68.1	0.223
8.306	16963	3.33	3.38	71380	3.3	0.79	93	0.191
8.455	2291	0.45	0.46	7161	0.33	0.08	44	0.096
8.572	210676	41.35	42.02	646175	29.86	7.15	68.1	0.159
8.71	8019	1.57	1.6	20490	0.95	0.23	44	0.096
8.817	11205	2.2	2.23	37556	1.74	0.42	93	0.128
9.529	19354	3.8	3.86	65778	3.04	0.73	93.1	0.138
9.933	12064	2.37	2.41	37495	1.73	0.41	44	0.159
10.337	53406	10.48	10.65	176271	8.15	1.95	119.1	0.181
10.677	49282	9.67	9.83	156849	7.25	1.73	119.1	0.191
10.985	8319	1.63	1.66	35964	1.66	0.4	44	0.223
11.527	2243	0.44	0.45	10018	0.46	0.11	44	0.223
13.079	2055	0.4	0.41	8732	0.4	0.1	44	0.159
14.184	3249	0.64	0.65	11012	0.51	0.12	44	0.096
15.226	1896	0.37	0.38	7388	0.34	0.08	44	0.128
15.375	86468	16.97	17.25	255467	11.81	2.82	59	0.128
15.47	71496	14.03	14.26	205310	9.49	2.27	59.1	0.138
16.14	41757	8.2	8.33	114543	5.29	1.27	59.1	0.106
16.214	32166	6.31	6.42	76532	3.54	0.85	59.1	0.106
16.448	10043	1.97	2	76220	3.52	0.84	44	0.255
17.192	1672	0.33	0.33	10131	0.47	0.11	44	0.096
17.713	3558	0.7	0.71	16098	0.74	0.18	44	0.128
17.809	2666	0.52	0.53	10567	0.49	0.12	44	0.138
17.989	1924	0.38	0.38	7892	0.36	0.09	44	0.128
18.223	28377	5.57	5.66	125826	5.81	1.39	71	0.159
18.478	20994	4.12	4.19	118247	5.46	1.31	44	0.213
18.638	26884	5.28	5.36	135100	6.24	1.49	44	0.223
18.999	8182	1.61	1.63	31202	1.44	0.35	43.9	0.117
19.286	2916	0.57	0.58	8426	0.39	0.09	44	0.096
19.445	501354	98.4	100	2163891	100	23.93	71.1	0.223
19.626	3057	0.6	0.61	8473	0.39	0.09	44	0.128
19.977	5428	1.07	1.08	19611	0.91	0.22	44	0.138
20.094	4758	0.93	0.95	15039	0.69	0.17	44	0.096
20.455	3013	0.59	0.6	8017	0.37	0.09	44	0.128
20.678	3002	0.59	0.6	11110	0.51	0.12	44	0.159
20.902	6279	1.23	1.25	36511	1.69	0.4	44	0.255
21.252	2964	0.58	0.59	16896	0.78	0.19	44	0.181
21.741	286570	56.24	57.16	1066023	49.26	11.79	59.1	0.255
22.4	2194	0.43	0.44	7291	0.34	0.08	44	0.096
22.655	2667	0.52	0.53	7166	0.33	0.08	44	0.085
22.91	2092	0.41	0.42	6641	0.31	0.07	44	0.096
23.059	2390	0.47	0.48	11642	0.54	0.13	44	0.138
23.208	8102	1.59	1.62	41689	1.93	0.46	44	0.255
23.463	4409	0.87	0.88	14954	0.69	0.17	44	0.138
23.793	10536	2.07	2.1	45389	2.1	0.5	44	0.202
24.59	1999	0.39	0.4	7411	0.34	0.08	44	0.128
24.739	2219	0.44	0.44	8523	0.39	0.09	44	0.128
26.354	1806	0.35	0.36	6641	0.31	0.07	44	0.159
26.684	1665	0.33	0.33	8093	0.37	0.09	44	0.191
26.928	3909	0.77	0.78	25029	1.16	0.28	44	0.319
27.204	1515	0.3	0.3	6495	0.3	0.07	44	0.128
27.789	1386	0.27	0.28	6671	0.31	0.07	44	0.159
30.457	2757	0.54	0.55	12107	0.56	0.13	44	0.128
30.51	2034	0.4	0.41	9410	0.43	0.1	43.9	0.128
31.041	2063	0.4	0.41	11862	0.55	0.13	44	0.223
31.222	1324	0.26	0.26	7134	0.33	0.08	44	0.159
32.859	2230	0.44	0.44	8112	0.37	0.09	44	0.159
33.699	1641	0.32	0.33	6856	0.32	0.08	44	0.128
33.911	1719	0.34	0.34	8186	0.38	0.09	44	0.191
35.091	1804	0.35	0.36	7822	0.36	0.09	44	0.191

35.909	1678	0.33	0.33	9130	0.42	0.1	44	0.159
36.09	1709	0.34	0.34	6922	0.32	0.08	44	0.191
36.558	1824	0.36	0.36	16650	0.77	0.18	44	0.223
36.94	2052	0.4	0.41	7834	0.36	0.09	43.9	0.128
37.695	6107	1.2	1.22	44268	2.05	0.49	44	0.223
38.683	2180	0.43	0.43	7439	0.34	0.08	44	0.128
39.502	6910	1.36	1.38	34821	1.61	0.39	44	0.223
39.895	1983	0.39	0.4	9497	0.44	0.11	43.9	0.159
40.14	2652	0.52	0.53	6958	0.32	0.08	44	0.159
40.288	1842	0.36	0.37	7116	0.33	0.08	44	0.128
40.469	2277	0.45	0.45	8732	0.4	0.1	44	0.117
40.714	3003	0.59	0.6	10553	0.49	0.12	44.1	0.128
40.958	3085	0.61	0.62	7450	0.34	0.08	44	0.128
41.086	2393	0.47	0.48	8301	0.38	0.09	44	0.117
41.787	2540	0.5	0.51	7322	0.34	0.08	44	0.128
42.68	2978	0.58	0.59	10508	0.49	0.12	44	0.138
43.307	3945	0.77	0.79	15842	0.73	0.18	44	0.159
44.593	2048	0.4	0.41	6834	0.32	0.08	44	0.096
46.559	2301	0.45	0.46	12393	0.57	0.14	44	0.159
47.495	2971	0.58	0.59	9753	0.45	0.11	44	0.159

Compound Table

Compound Label	RT	Name	DB Formula	Hits (DB)
Cpd 1: Octadecanoic acid	4.384	Octadecanoic acid	C18H36O2	10
Cpd 2: 2(10)-Pinene, (1S,5S)-(-)-	5.235	2(10)-Pinene, (1S,5S)-(-)-	C10H16	10
Cpd 3: Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)-	5.681	Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)-	C10H16	10
Cpd 4: Heneicosanoic acid	5.904	Heneicosanoic acid	C21H42O2	7
Cpd 5: 2(10)-Pinene, (1S,5S)-(-)-	6.085	2(10)-Pinene, (1S,5S)-(-)-	C10H16	10
Cpd 6: Heneicosanoic acid	6.308	Heneicosanoic acid	C21H42O2	1
Cpd 7: 4(10)-Thujene	6.478	4(10)-Thujene	C10H16	10
Cpd 8: Ethyl 4-Benzyloxy-2-[2 methyl-2(E)-butenyl]-2-[2(E),4-pentadienyl]acetoacetate	6.988	Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(E),4-pentadienyl]acetoacetate	C23H30O4	3
Cpd 9: 7.116	7.116			0
Cpd 10: 7.446	7.446			0
Cpd 11: Heneicosanoic acid	7.732	Heneicosanoic acid	C21H42O2	1
Cpd 12: D-Limonene	8.03	D-Limonene	C10H16	10
Cpd 13: Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(E),4-pentadienyl]acetoacetate	8.306	Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(E),4-pentadienyl]acetoacetate	C23H30O4	2
Cpd 14: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	8.455	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	5
Cpd 15: D-Limonene	8.572	D-Limonene	C10H16	10
Cpd 16: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	8.71	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	1
Cpd 17: 8.817	8.817			0
Cpd 18: 1,6-Octadien-3-ol, 3,7-dimethyl-, acetate	9.529	1,6-Octadien-3-ol, 3,7-dimethyl-, acetate	C12H20O2	10
Cpd 19: p-Cyanophenyl p-(2-propoxyethoxy)benzoate	9.933	p-Cyanophenyl p-(2-propoxyethoxy)benzoate	C19H19NO4	2

Cpd 20: Benzene, methyl(1-methylethyl)-	10.337	Benzene, methyl(1-methylethyl)-	C10H14	10
Cpd 21: Benzene, methyl(1-methylethyl)-	10.677	Benzene, methyl(1-methylethyl)-	C10H14	10
Cpd 22: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	10.985	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	9
Cpd 23: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	11.527	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 24: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	13.079	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	10
Cpd 25: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	14.184	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	10
Cpd 26: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	15.226	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 27: TRANS-LINALOOL OXIDE	15.375	TRANS-LINALOOL OXIDE	C10H18O2	10
Cpd 28: 2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-,	15.47	2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-,	C10H18O2	10
Cpd 29: 2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-,	16.14	2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-,	C10H18O2	10
Cpd 30: 2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-,	16.214	2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-,	C10H18O2	10
Cpd 31: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	16.448	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	8
Cpd 32: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	17.192	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 33: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	17.713	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	10
Cpd 34: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	17.809	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	10
Cpd 35: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	17.989	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 36: Cyclohexene, 1-methyl-4-(1-methylethylidene)-	18.223	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	C10H16	10
Cpd 37: Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	18.478	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	C10H18O	10
Cpd 38: Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	18.638	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	C10H18O	10
Cpd 39: Fenchol, exo-	18.999	Fenchol, exo-	C10H18O	10
Cpd 40: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	19.286	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10

Cpd 41: 3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	19.445	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	C10H18O	10
Cpd 42: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	19.626	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 43: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	19.977	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 44: Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(E),4-pentadienyl]acetoacetate	20.094	Ethyl 4-Benzyloxy-2-[2-methyl-2(E)-butenyl]-2-[2(E),4-pentadienyl]acetoacetate	C23H30O4	10
Cpd 45: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	20.455	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	10
Cpd 46: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	20.678	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 47: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	20.902	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	5
Cpd 48: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	21.252	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	10
Cpd 49: .alpha.-Terpineol	21.741	.alpha.-Terpineol	C10H18O	10
Cpd 50: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	22.4	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 51: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	22.655	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 52: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	22.91	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 53: (S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	23.059	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3	10
Cpd 54: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	23.208	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 55: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	23.463	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 56: Dodecanal	23.793	Dodecanal	C12H24O	10
Cpd 57: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	24.59	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 58: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	24.739	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 59: 6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	26.354	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2	10

Cpd 60: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	26.684	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 61: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	26.928	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 62: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	27.204	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 63: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	27.789	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 64: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	30.457	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 65: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	30.51	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 66: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	31.041	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 67: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	31.222	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 68: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	32.859	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 69: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	33.699	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 70: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	33.911	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 71: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	35.091	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 72: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	35.909	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 73: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	36.09	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 74: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	36.558	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 75: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	36.94	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10

Cpd 76: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	37.695	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	8
Cpd 77: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	38.683	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 78: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	39.502	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 79: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	39.895	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 80: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	40.14	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 81: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	40.288	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 82: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	40.469	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 83: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	40.714	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 84: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	40.958	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 85: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	41.086	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 86: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	41.787	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 87: Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	42.68	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pent-2-enopyranoside	C21H26O6	10
Cpd 88: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	43.307	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 89: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	44.593	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 90: 2-Methoxy-N-methylethylamine	46.559	2-Methoxy-N-methylethylamine	C4H11NO	10
Cpd 91: 2-Methoxy-N-methylethylamine	47.495	2-Methoxy-N-methylethylamine	C4H11NO	10

Compound Label	Name	RT	Algorithm
Cpd 1: Octadecanoic acid	**Octadecanoic acid**	4.384	Find by Integration

Figure S3. GC-MS analysis for the identification and retention time confirmation of *β*-pinene

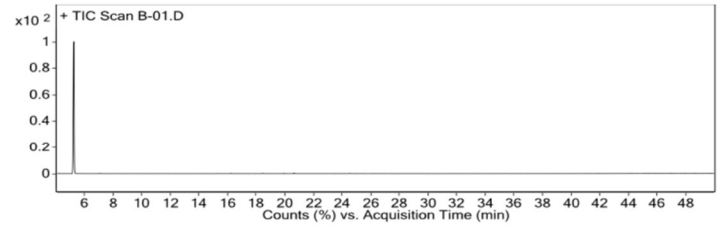
In this study, (−)-*β*-pinene (purity 99%, Sigma-Aldrich, China) was analyzed using GC-MS to confirm its retention time. Due to the structural similarity between *β*-pinene and α-pinene, there is a potential for misidentification.

Qualitative Compound Report

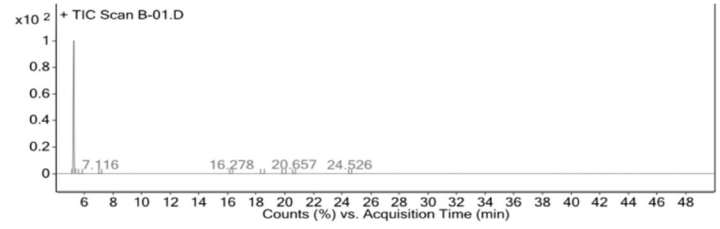
Data File	B-01.D	**Sample Name**	B-01
Sample Type		**Position**	2
Instrument Name	GCMS	**User Name**	
Acq Method	NA2-671003.M	**Acquired Time**	8/2/2024 3:01:32 PM
IRM Calibration Status	Not Applicable	**DA Method**	default.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol	1	**TuneName**	20240802_atune.u
TunePath	D:\MassHunter\GCMS\1\5977\	**MSFirmwareVersion**	6.00.21
Acquisition Time #2	2024-08-02 08:01:32Z	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.02.1938 08-Sep-2014 Copyright © 1989-2014 Agilent Technologies, Inc.

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** Unspecified



Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** Unspecified



User Chromatogram Peak List

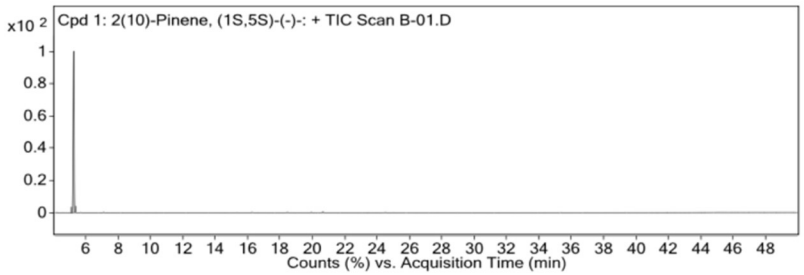
RT	Height	Normalized Height	Height %	Area	Area %	Area Sum %	Base Peak m/z	Width
5.267	6855061	99.87	100	28422470	100	98.58	93.1	0.244
5.681	8928	0.13	0.13	34493	0.12	0.12	93	0.266
7.116	20167	0.29	0.29	68606	0.24	0.24	93.1	0.255
16.278	17453	0.25	0.25	52532	0.18	0.18	43.9	0.159
18.468	18223	0.27	0.27	60074	0.21	0.21	81	0.266
19.945	18269	0.27	0.27	49654	0.17	0.17	79	0.213
20.657	33963	0.49	0.5	93046	0.33	0.32	92	0.213
24.526	13157	0.19	0.19	50980	0.18	0.18	79	0.213

Compound Table

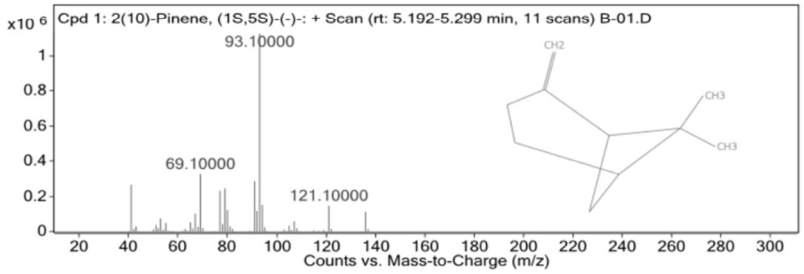
Qualitative Compound Report

Compound Label	RT	Name	DB Formula	Hits (DB)
Cpd 1: 2(10)-Pinene, (1S,5S)-(-)-	5.267	2(10)-Pinene, (1S,5S)-(-)-	C10H16	10
Cpd 2: 3-(Bistrifluoromethylamino-	5.681	3-(Bistrifluoromethylamino-oxy)nortricylene	C9H9F6NO	10
Cpd 3: 1,6-Octadiene, 7-methyl-3-methylene-	7.116	1,6-Octadiene, 7-methyl-3-methylene-	C10H16	10
Cpd 4: Spiro[bicyclo[3.1.1]heptane-2,2'-oxirane], 6,6-dimethyl-	16.278	Spiro[bicyclo[3.1.1]heptane-2,2'-oxirane], 6,6-dimethyl-	C10H16O	10
Cpd 5: 2(10)-Pinen-3-one, (1S,5S)-(-)-	18.468	2(10)-Pinen-3-one, (1S,5S)-(-)-	C10H14O	10
Cpd 6: .alpha.-Thujenal	19.945	.alpha.-Thujenal	C10H14O	10
Cpd 7: 2(10)-Pinen-3-ol, (1S,3R,5S)-(-)-	20.657	2(10)-Pinen-3-ol, (1S,3R,5S)-(-)-	C10H16O	10
Cpd 8: 2-Pinen-10-ol	24.526	2-Pinen-10-ol	C10H16O	10

Compound Label	Name	RT	Algorithm
Cpd 1: 2(10)-Pinene, (1S,5S)-(-)-	**2(10)-Pinene, (1S,5S)-(-)-**	5.267	Find by Integration



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Abund
41	266040
69.1	325909.81
77	231301.09
79.09	244587.64
80.05	120655.27
91.1	285944.72
92.03	115849.45
93.1	1125486.5
94.1	150281.45
121.1	145119.27

Library Spectrum

Figure S4. GC-MS Analysis for the Identification and Retention Time Confirmation of D-limonene

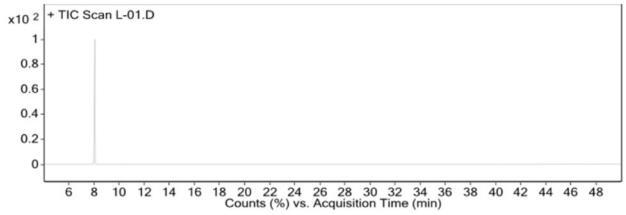
In this study, (R)-(+)-limonene (purity 97%, Sigma-Aldrich, Mexico) was analyzed using GC-MS to confirm its retention time. As D-limonene and L-limonene are enantiomers with similar retention times, there is a potential for misidentification.

Qualitative Compound Report

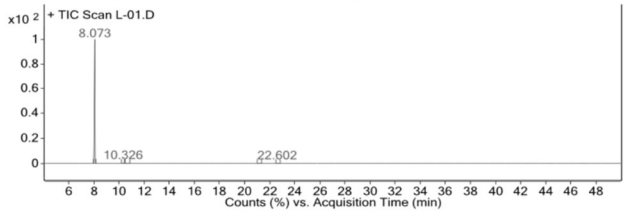
Data File	L-01.D	**Sample Name**	L-01
Sample Type		**Position**	3
Instrument Name	GCMS	**User Name**	
Acq Method	NA2-671003.M	**Acquired Time**	8/2/2024 3:59:09 PM
IRM Calibration Status	Not Applicable	**DA Method**	default.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol	1	**TuneName**	20240802_atune.u
TunePath	D:\MassHunter\GCMS\1\5977\	**MSFirmwareVersion**	6.00.21
Acquisition Time #2	2024-08-02 08:59:09Z	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.02.1938 08-Sep-2014 Copyright © 1989-2014 Agilent Technologies, Inc.

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** Unspecified



Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** Unspecified



User Chromatogram Peak List

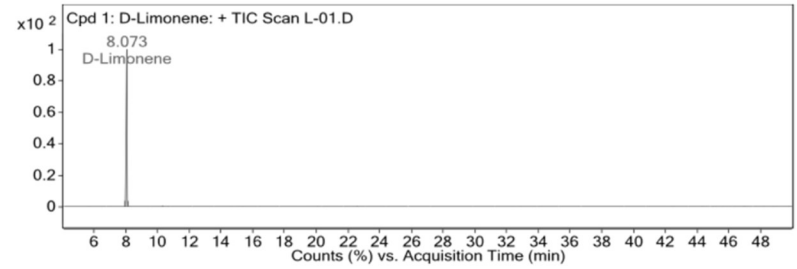
RT	Height	Normalized Height	Height %	Area	Area %	Area Sum %	Base Peak m/z	Width
8.073	8914183	99.97	100	34725794	100	99.31	68.1	0.255
10.326	34391	0.39	0.39	109028	0.31	0.31	119	0.244
10.656	11666	0.13	0.13	44658	0.13	0.13	93.1	0.361
21.093	7358	0.08	0.08	34859	0.1	0.1	44	0.372
22.602	13328	0.15	0.15	51027	0.15	0.15	82.1	0.361

Compound Table

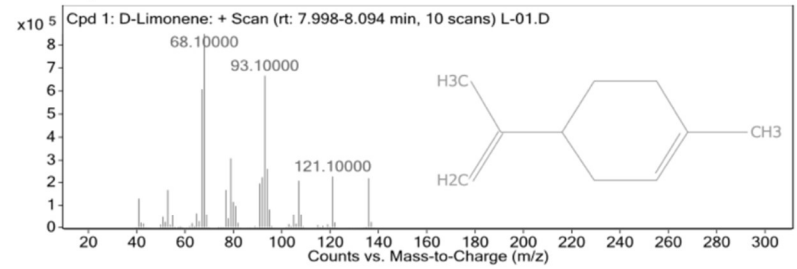
Compound Label	RT	Name	DB Formula	Hits (DB)
Cpd 1: D-Limonene	8.073	D-Limonene	C10H16	10

Cpd 2: Benzene, methyl(1-methylethyl)-	10.326	Benzene, methyl(1-methylethyl)-	C10H14	10
Cpd 3: Cyclohexene, 1-methyl-4-(1-methylethylidene)-	10.656	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	C10H16	10
Cpd 4: Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	21.093	Pyrano[3,4-b]indol-3(9H)-one, 1-(4-pentynyl)-	C16H13NO2	10
Cpd 5: 2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)-	22.602	2-Cyclohexen-1-one, 2-methyl-5-(1-methylethenyl)-	C10H14O	10

Compound Label	Name	RT	Algorithm
Cpd 1: D-Limonene	**D-Limonene**	8.073	Find by Integration



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Abund
67.08	608505.63
68.1	850035.19
79.08	306002.41
91.05	196488
92.08	224139.2
93.1	667654.38
94.1	260020.8
107.1	208248.8
121.1	227388
136.1	219400

Library Spectrum

Figure S5. GC-MS Analysis for the Identification and Retention Time Confirmation of Terpinen-4-ol

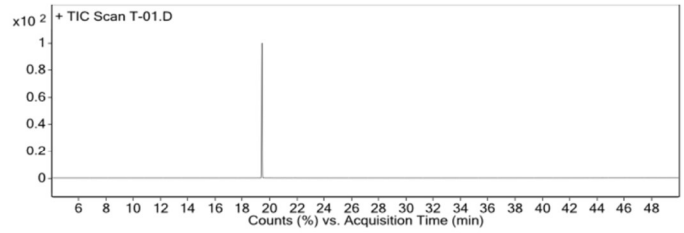
In this study, (-)-Terpinen-4-al (purity ≥ 99%, Sigma-Aldrich, Spain) was analyzed using GC-MS to confirm its retention time.

Qualitative Compound Report

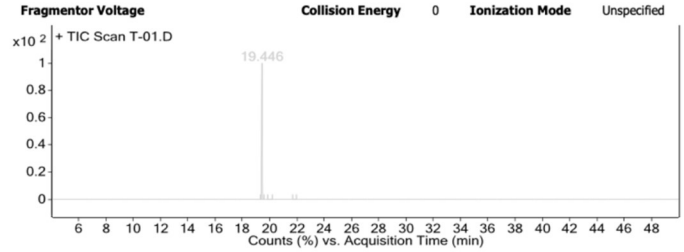
Data File	T-01.D	**Sample Name**	T-01
Sample Type		**Position**	4
Instrument Name	GCMS	**User Name**	
Acq Method	NA2-671003.M	**Acquired Time**	8/2/2024 4:56:43 PM
IRM Calibration Status	Not Applicable	**DA Method**	default.m
Comment			

Expected Barcode		**Sample Amount**	
Dual Inj Vol	1	**TuneName**	20240802_atune.u
TunePath	D:\MassHunter\GCMS\1\5977\	**MSFirmwareVersion**	6.00.21
Acquisition Time #2	2024-08-02 09:56:43Z	**OperatorName**	
RunCompletedFlag	True	**Acquisition SW Version**	MassHunter GC/MS Acquisition B.07.02.1938 08-Sep-2014 Copyright © 1989-2014 Agilent Technologies, Inc.

Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** Unspecified



Fragmentor Voltage **Collision Energy** 0 **Ionization Mode** Unspecified



User Chromatogram Peak List

RT	Height	Normalized Height	Height %	Area	Area %	Area Sum %	Base Peak m/z	Width
19.446	9266591	99.96	100	28078113	100	99.73	71.1	0.276
20.062	7859	0.08	0.08	41076	0.15	0.15	44	0.319
21.773	6300	0.07	0.07	35430	0.13	0.13	95.1	0.276

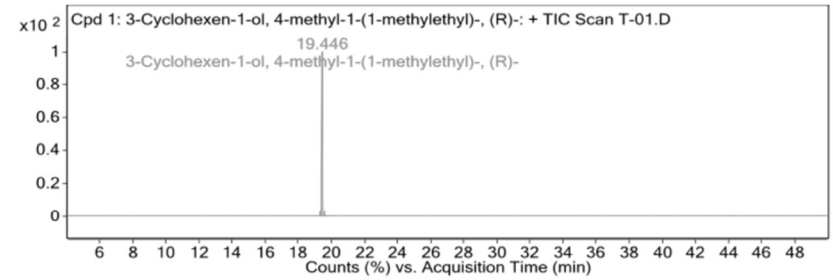
Compound Table

Compound Label	RT	Name	DB Formula	Hits (DB)
Cpd 1: 3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	19.446	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	C10H18O	10

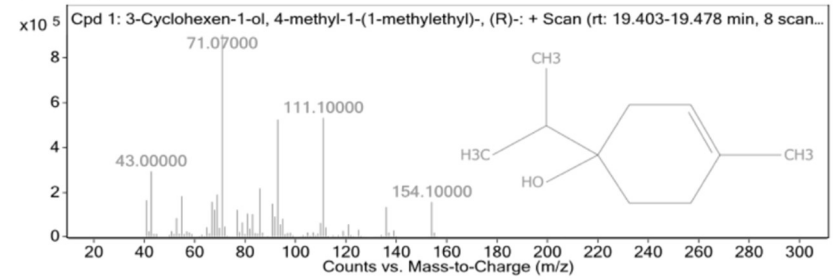
Qualitative Compound Report

Cpd 2: 3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	20.062	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS	10
Cpd 3: 3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-ylidene)-2-propanone oxime	21.773	3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-ylidene)-2-propanone oxime	C13H21NO	10

Compound Label	Name	RT	Algorithm
Cpd 1: 3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	**3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-**	19.446	Find by Integration



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Abund
41	165673
43	293822
55	183716
67.03	158497
69.1	190982
71.07	900856
86.1	218267
93.07	524166
111.1	531474
154.1	157745

Library Spectrum