

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
 Data File : VV031770.D
 Acq On : 26 Jul 2023 15:36
 Operator : SY/MD
 Sample : 03754-17
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Z3

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

Signal : TIC: VV031770.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	68	74	91	rVB	207269	233203	14.87%	1.953%
2	1.532	146	153	167	rVB	200796	239362	15.26%	2.004%
3	2.063	309	318	328	rBV	368286	529244	33.75%	4.432%
4	2.764	533	536	539	rVB5	1052	739	0.05%	0.006%
5	2.780	539	541	542	rBV	1145	457	0.03%	0.004%
6	2.790	542	544	550	rVB6	2394	1624	0.10%	0.014%
7	2.819	550	553	556	rVB5	2153	1276	0.08%	0.011%
8	2.838	556	559	563	rBV5	1862	1438	0.09%	0.012%
9	2.883	569	573	578	rBV7	1735	1766	0.11%	0.015%
10	2.921	582	585	589	rVB5	1548	1158	0.07%	0.010%
11	2.944	589	592	593	rBV2	1131	511	0.03%	0.004%
12	3.015	611	614	616	rBV3	1035	618	0.04%	0.005%
13	3.031	616	619	621	rBV3	1613	888	0.06%	0.007%
14	3.073	629	632	634	rVB2	998	505	0.03%	0.004%
15	3.085	634	636	638	rVB3	944	433	0.03%	0.004%
16	3.105	638	642	645	rBV6	2338	1988	0.13%	0.017%
17	3.188	666	668	671	rBV4	978	674	0.04%	0.006%
18	3.253	685	688	690	rBV4	1201	748	0.05%	0.006%
19	3.294	698	701	702	rBV2	523	203	0.01%	0.002%
20	3.301	702	703	706	rVB3	1166	584	0.04%	0.005%
21	3.317	706	708	710	rBV2	410	242	0.02%	0.002%
22	3.362	720	722	723	rBV2	575	263	0.02%	0.002%
23	3.381	725	728	733	rBV4	1743	991	0.06%	0.008%
24	3.400	733	734	737	rVB3	1804	773	0.05%	0.006%
25	3.423	737	741	744	rBV5	1654	1540	0.10%	0.013%
26	3.452	747	750	751	rBV2	981	587	0.04%	0.005%
27	3.529	772	774	775	rBV2	579	143	0.01%	0.001%
28	3.568	784	786	789	rBV4	1176	724	0.05%	0.006%
29	3.584	789	791	793	rBV3	1239	662	0.04%	0.006%
30	3.793	846	856	886	rBV	136080	402228	25.65%	3.368%
31	4.256	987	1000	1024	rBV	272382	710127	45.29%	5.946%
32	4.552	1089	1092	1095	rBV4	1365	1052	0.07%	0.009%
33	4.661	1124	1126	1129	rBV4	1236	712	0.05%	0.006%
34	4.751	1152	1154	1155	rBV2	1043	383	0.02%	0.003%
35	4.844	1180	1183	1186	rBV3	1362	707	0.05%	0.006%
36	4.860	1186	1188	1191	rBV4	1289	671	0.04%	0.006%

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 Title : VOC Analysis

37	4.876	1191	1193	1194	rBV2	973	440	0.03%	0.004%
38	4.902	1199	1201	1202	rBV2	1022	328	0.02%	0.003%
39	4.963	1203	1220	1246	rBV2	586221	1568068	100.00%	13.130%
40	5.330	1331	1334	1336	rVB4	1871	986	0.06%	0.008%
41	5.352	1339	1341	1345	rVB5	2247	1157	0.07%	0.010%
42	5.371	1345	1347	1349	rBV3	994	706	0.05%	0.006%
43	5.458	1372	1374	1376	rBV3	1395	579	0.04%	0.005%
44	5.542	1388	1400	1425	rBV	392451	824088	52.55%	6.901%
45	5.828	1480	1489	1510	rVB3	59195	122412	7.81%	1.025%
46	5.995	1530	1541	1560	rBV	379464	759915	48.46%	6.363%
47	6.304	1635	1637	1639	rBV3	1228	493	0.03%	0.004%
48	6.407	1666	1669	1671	rBV4	1597	1207	0.08%	0.010%
49	6.796	1788	1790	1792	rBV3	1113	642	0.04%	0.005%
50	6.867	1810	1812	1813	rBV2	643	273	0.02%	0.002%
51	6.918	1818	1828	1844	rBV	158816	299707	19.11%	2.510%
52	7.249	1920	1931	1961	rBV	550898	997447	63.61%	8.352%
53	7.558	2018	2027	2047	rBV2	123337	223076	14.23%	1.868%
54	7.834	2111	2113	2118	rBV6	1004	688	0.04%	0.006%
55	8.031	2164	2174	2189	rBV3	408023	780943	49.80%	6.539%
56	8.500	2318	2320	2324	rBV4	1688	1443	0.09%	0.012%
57	8.590	2345	2348	2351	rBV4	2398	1702	0.11%	0.014%
58	8.661	2366	2370	2377	rBV8	2166	2707	0.17%	0.023%
59	8.728	2389	2391	2393	rBV2	1509	819	0.05%	0.007%
60	8.789	2399	2410	2433	rBV	648182	1085978	69.26%	9.094%
61	9.146	2519	2521	2522	rBV2	911	323	0.02%	0.003%
62	9.156	2522	2524	2527	rVB4	1578	725	0.05%	0.006%
63	9.326	2573	2577	2579	rBV4	1905	1218	0.08%	0.010%
64	9.368	2585	2590	2593	rBV5	1662	1258	0.08%	0.011%
65	9.397	2596	2599	2601	rBV4	2257	1493	0.10%	0.013%
66	9.468	2619	2621	2622	rBV2	947	410	0.03%	0.003%
67	9.696	2691	2692	2693	rBV	1281	388	0.02%	0.003%
68	9.973	2776	2778	2781	rBV4	1546	1122	0.07%	0.009%
69	10.050	2800	2802	2805	rVB4	1195	583	0.04%	0.005%
70	10.159	2824	2836	2855	rBV	497661	795481	50.73%	6.661%
71	10.609	2974	2976	2980	rBV4	1058	668	0.04%	0.006%
72	10.789	3030	3032	3034	rBV3	821	393	0.03%	0.003%
73	10.886	3060	3062	3063	rBV2	961	420	0.03%	0.004%
74	10.969	3085	3088	3091	rVB5	1599	889	0.06%	0.007%
75	11.001	3092	3098	3101	rBV8	3180	4079	0.26%	0.034%
76	11.136	3133	3140	3146	rBV8	11425	16209	1.03%	0.136%

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Title : VOC Analysis

77	11.191	3147	3157	3175	rVV	645186	990858	63.19%	8.297%
78	11.368	3209	3212	3214	rBV4	1800	1100	0.07%	0.009%
79	11.493	3243	3251	3262	rBV7	17925	39565	2.52%	0.331%
80	11.567	3263	3274	3289	rVB	680641	1079106	68.82%	9.036%
81	11.944	3384	3391	3406	rVB2	38637	61189	3.90%	0.512%
82	12.252	3481	3487	3497	rVB7	23436	32871	2.10%	0.275%
83	12.718	3630	3632	3635	rBV4	1362	790	0.05%	0.007%
84	12.735	3635	3637	3639	rBV3	1725	785	0.05%	0.007%
85	12.886	3682	3684	3687	rBV4	1742	933	0.06%	0.008%
86	12.982	3707	3714	3717	rBV8	2132	2587	0.16%	0.022%
87	13.178	3769	3775	3778	rBV7	2901	3574	0.23%	0.030%
88	13.873	3984	3991	4010	rVB2	48044	76505	4.88%	0.641%
89	14.352	4138	4140	4145	rVB5	1818	1045	0.07%	0.009%
90	14.477	4175	4179	4181	rBV4	1908	1465	0.09%	0.012%
91	14.615	4217	4222	4227	rBV9	2805	3824	0.24%	0.032%
92	14.657	4233	4235	4239	rVB4	1360	665	0.04%	0.006%
93	14.943	4320	4324	4326	rBV4	1055	1002	0.06%	0.008%
94	15.136	4383	4384	4386	rBV2	1033	538	0.03%	0.005%
95	15.551	4509	4513	4519	rBV8	2640	3215	0.21%	0.027%

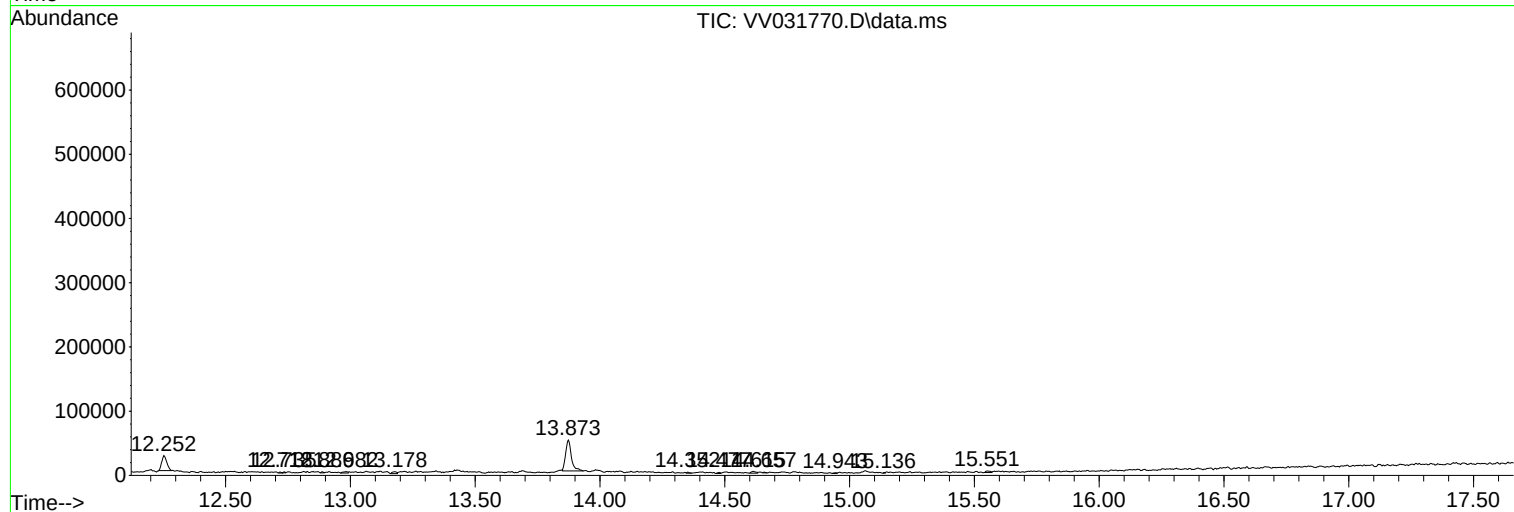
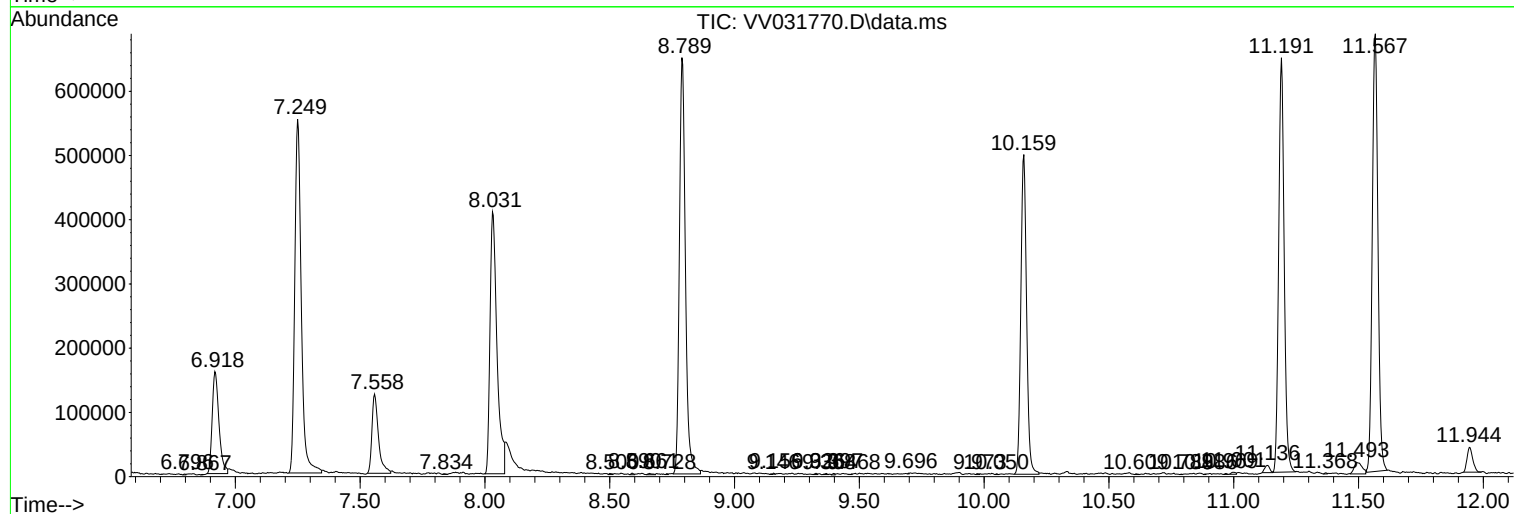
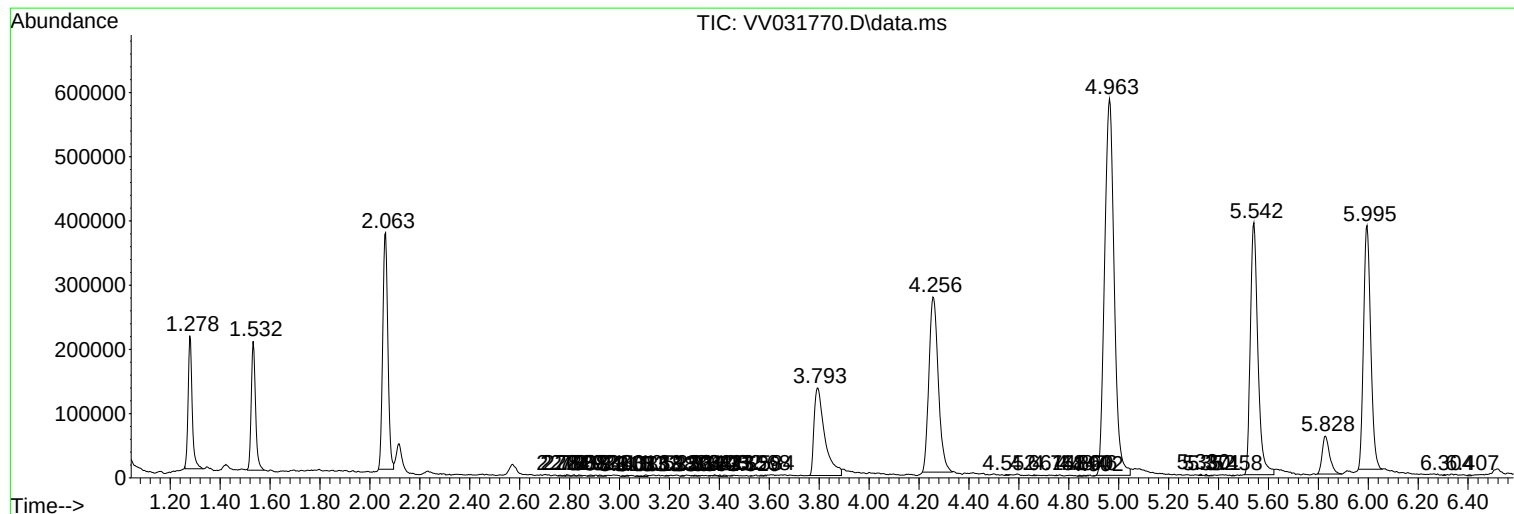
Sum of corrected areas: 11942304

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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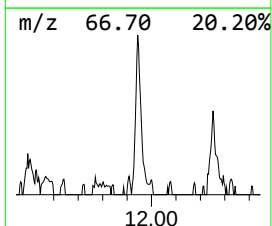
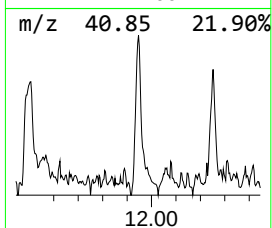
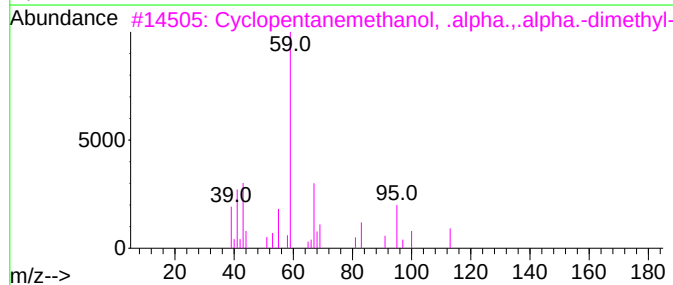
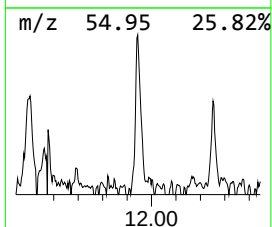
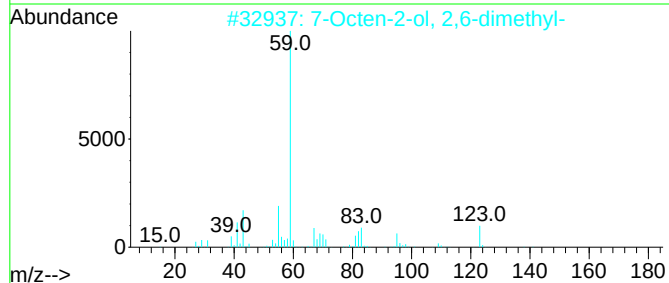
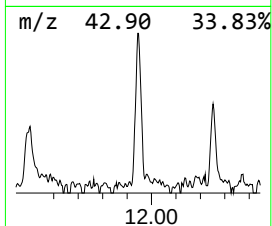
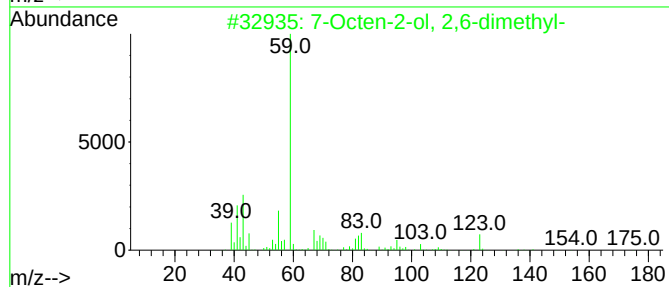
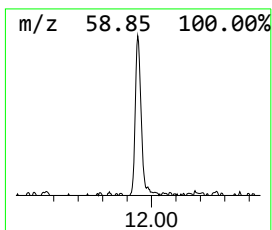
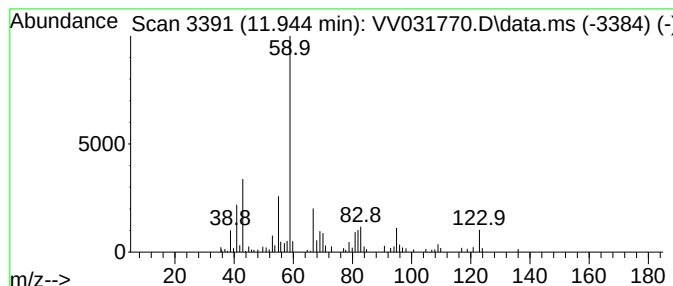
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.944	3.09 ug/L	61189	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
3			Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	59
4			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	56
5			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	45



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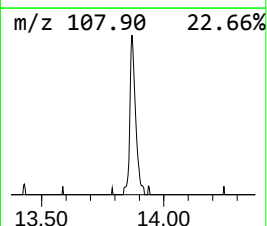
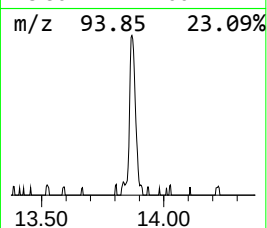
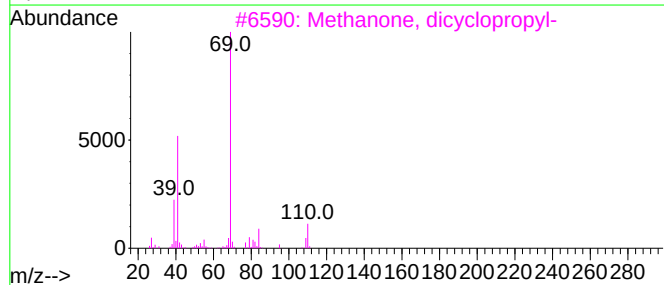
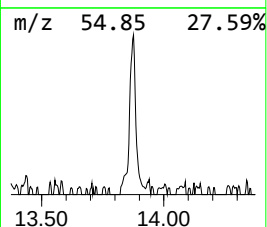
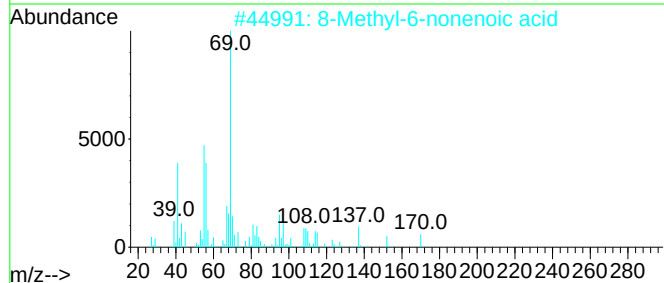
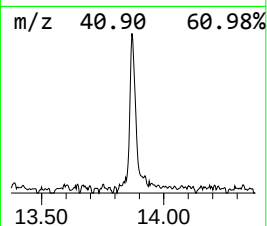
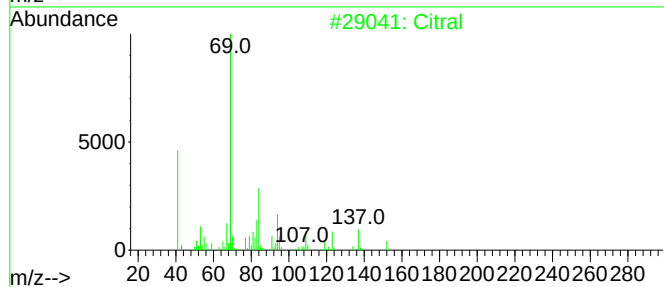
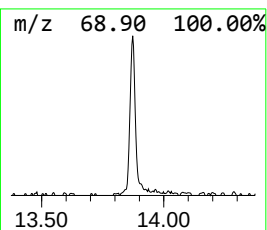
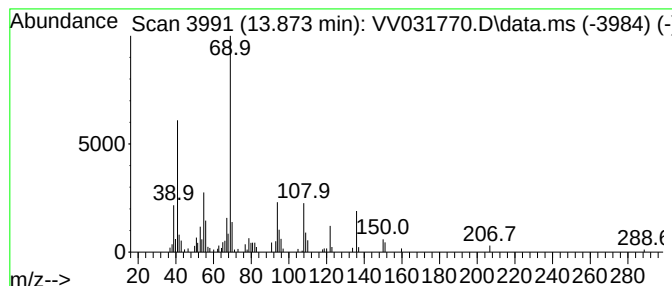
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	3.86 ug/L	76505	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Citral	152	C10H16O	005392-40-5	42
2			8-Methyl-6-nonenic acid	170	C10H18O2	021382-25-2	38
3			Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38
4			Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38
5			Neral	152	C10H16O	000106-26-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
7-Octen-2-ol, 2...	11.944	3.1	ug/L	61189	3	11.191	990858	50.0
unknown-01	13.873	3.9	ug/L	76505	3	11.191	990858	50.0