

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW072623\
 Data File : VW031766.D
 Acq On : 26 Jul 2023 14:02
 Operator : SY/MD
 Sample : 03712-19
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y6

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs : 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 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: VW031766.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	67	74	91	rVV	212557	243356	14.66%	1.802%
2	1.349	93	96	106	rVB	15969	14993	0.90%	0.111%
3	1.532	146	153	169	rVB	208584	252554	15.22%	1.870%
4	2.060	308	317	328	rBV	377280	557105	33.57%	4.126%
5	2.114	328	334	352	rVB	72351	121128	7.30%	0.897%
6	2.449	436	438	445	rVB8	2237	2151	0.13%	0.016%
7	2.497	450	453	456	rVB3	1110	837	0.05%	0.006%
8	2.513	456	458	461	rBV3	1278	957	0.06%	0.007%
9	2.568	461	475	493	rBV	61756	127089	7.66%	0.941%
10	2.674	506	508	513	rBV4	957	583	0.04%	0.004%
11	2.706	513	518	519	rBV3	2167	1636	0.10%	0.012%
12	2.751	530	532	538	rVB7	1488	1105	0.07%	0.008%
13	2.780	539	541	547	rVB3	859	664	0.04%	0.005%
14	2.883	571	573	577	rBV3	1039	570	0.03%	0.004%
15	2.950	592	594	600	rVB4	1179	672	0.04%	0.005%
16	2.976	600	602	607	rVB5	1122	793	0.05%	0.006%
17	3.002	607	610	612	rBV3	1594	937	0.06%	0.007%
18	3.098	636	640	643	rBV4	865	869	0.05%	0.006%
19	3.111	643	644	648	rBV3	791	584	0.04%	0.004%
20	3.265	690	692	696	rVB3	927	649	0.04%	0.005%
21	3.330	709	712	716	rVB4	1039	848	0.05%	0.006%
22	3.378	722	727	730	rBV3	1084	974	0.06%	0.007%
23	3.433	740	744	746	rBV3	842	574	0.03%	0.004%
24	3.474	753	757	760	rBV4	956	874	0.05%	0.006%
25	3.552	777	781	783	rBV3	999	740	0.04%	0.005%
26	3.581	787	790	791	rBV2	1885	1078	0.06%	0.008%
27	3.609	793	799	800	rBV5	1849	1910	0.12%	0.014%
28	3.793	846	856	884	rBV	141420	424101	25.55%	3.141%
29	4.179	972	976	981	rBV8	2091	2333	0.14%	0.017%
30	4.256	985	1000	1025	rVV	294513	765288	46.11%	5.667%
31	4.442	1056	1058	1062	rVB4	1488	644	0.04%	0.005%
32	4.545	1088	1090	1093	rVB4	1169	578	0.03%	0.004%
33	4.590	1101	1104	1107	rVB5	1108	738	0.04%	0.005%
34	4.671	1127	1129	1132	rBV3	1124	821	0.05%	0.006%
35	4.802	1167	1170	1175	rBB4	1486	959	0.06%	0.007%
36	4.867	1185	1190	1192	rBV4	1080	836	0.05%	0.006%

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Integration Parameters: LSCINT.P

Integrator: RTE
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 Title : VOC Analysis

37	4.886	1195	1196	1201	rVB5	765	557	0.03%	0.004%
38	4.963	1201	1220	1245	rBV3	616163	1659689	100.00%	12.291%
39	5.352	1337	1341	1344	rVB6	1288	842	0.05%	0.006%
40	5.433	1363	1366	1368	rBV3	932	574	0.03%	0.004%
41	5.539	1387	1399	1426	rBV	419685	887457	53.47%	6.572%
42	5.828	1477	1489	1505	rBV2	66202	144091	8.68%	1.067%
43	5.995	1528	1541	1562	rBV	400917	822137	49.54%	6.088%
44	6.510	1689	1701	1714	rBV	64825	137295	8.27%	1.017%
45	6.757	1776	1778	1783	rVB5	1454	871	0.05%	0.006%
46	6.799	1789	1791	1794	rBV3	1242	730	0.04%	0.005%
47	6.867	1808	1812	1817	rBV7	1551	1774	0.11%	0.013%
48	6.918	1817	1828	1848	rBV2	173206	325906	19.64%	2.413%
49	7.121	1888	1891	1893	rBV4	2074	1215	0.07%	0.009%
50	7.249	1919	1931	1954	rBV	580568	1038134	62.55%	7.688%
51	7.558	2017	2027	2052	rBV	128728	236975	14.28%	1.755%
52	7.879	2118	2127	2134	rBV	6136	11646	0.70%	0.086%
53	7.966	2151	2154	2156	rBV4	1625	868	0.05%	0.006%
54	8.031	2164	2174	2188	rBV2	424076	789485	47.57%	5.846%
55	8.449	2301	2304	2305	rVB3	1277	576	0.03%	0.004%
56	8.461	2305	2308	2310	rBV4	1801	1109	0.07%	0.008%
57	8.500	2317	2320	2323	rVB5	2454	1264	0.08%	0.009%
58	8.789	2396	2410	2436	rBV	663388	1122464	67.63%	8.312%
59	8.953	2459	2461	2464	rBV3	1855	1340	0.08%	0.010%
60	9.037	2485	2487	2491	rVB5	1635	1030	0.06%	0.008%
61	9.059	2491	2494	2495	rBV3	1563	905	0.05%	0.007%
62	9.317	2571	2574	2576	rBV3	1224	682	0.04%	0.005%
63	9.471	2620	2622	2624	rBV3	1263	668	0.04%	0.005%
64	9.484	2624	2626	2631	rVV5	1926	1774	0.11%	0.013%
65	9.516	2634	2636	2638	rBV3	1551	740	0.04%	0.005%
66	9.619	2665	2668	2670	rBV5	1671	1199	0.07%	0.009%
67	9.664	2680	2682	2687	rBV5	1436	1070	0.06%	0.008%
68	9.686	2687	2689	2692	rBV3	1280	622	0.04%	0.005%
69	9.719	2695	2699	2700	rBV3	3153	2297	0.14%	0.017%
70	9.818	2727	2730	2733	rBV3	1673	1233	0.07%	0.009%
71	9.883	2748	2750	2751	rBV2	2693	1229	0.07%	0.009%
72	9.976	2776	2779	2781	rBV4	1195	770	0.05%	0.006%
73	10.034	2795	2797	2799	rBV3	1170	539	0.03%	0.004%
74	10.159	2824	2836	2853	rBV	491911	778809	46.92%	5.767%
75	10.329	2884	2889	2897	rVB10	4748	6662	0.40%	0.049%
76	10.567	2958	2963	2971	rVB8	4697	7445	0.45%	0.055%

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Integration Parameters: LSCINT.P

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 Title : VOC Analysis

77	10.680	2995	2998	3001	rBV4	1195	988	0.06%	0.007%
78	10.715	3001	3009	3014	rBV9	4338	6462	0.39%	0.048%
79	10.834	3043	3046	3048	rBV4	2611	1910	0.12%	0.014%
80	10.899	3064	3066	3068	rBV3	1299	760	0.05%	0.006%
81	11.001	3090	3098	3099	rBV8	6389	7572	0.46%	0.056%
82	11.133	3128	3139	3146	rBV5	22136	36490	2.20%	0.270%
83	11.191	3147	3157	3179	rVB	657350	1046151	63.03%	7.747%
84	11.448	3234	3237	3239	rBV3	1601	1121	0.07%	0.008%
85	11.497	3244	3252	3262	rVV5	11155	22477	1.35%	0.166%
86	11.567	3262	3274	3291	rVV	704049	1118632	67.40%	8.284%
87	11.844	3355	3360	3370	rBV10	6473	9739	0.59%	0.072%
88	11.944	3381	3391	3405	rBV	167093	267053	16.09%	1.978%
89	12.252	3477	3487	3500	rBV2	116113	183325	11.05%	1.358%
90	12.593	3590	3593	3594	rBV3	1682	947	0.06%	0.007%
91	12.670	3615	3617	3619	rBV4	1714	690	0.04%	0.005%
92	12.825	3663	3665	3667	rVB3	1773	567	0.03%	0.004%
93	13.185	3775	3777	3779	rBV3	1369	762	0.05%	0.006%
94	13.426	3844	3852	3861	rBV3	10244	19359	1.17%	0.143%
95	13.513	3877	3879	3881	rBV3	1539	935	0.06%	0.007%
96	13.558	3889	3893	3898	rBV7	2132	2719	0.16%	0.020%
97	13.693	3931	3935	3940	rBV7	2084	2167	0.13%	0.016%
98	13.744	3949	3951	3954	rBV4	1678	1316	0.08%	0.010%
99	13.805	3966	3970	3971	rBV4	1707	1105	0.07%	0.008%
100	13.873	3975	3991	4009	rVV	138681	243222	14.65%	1.801%

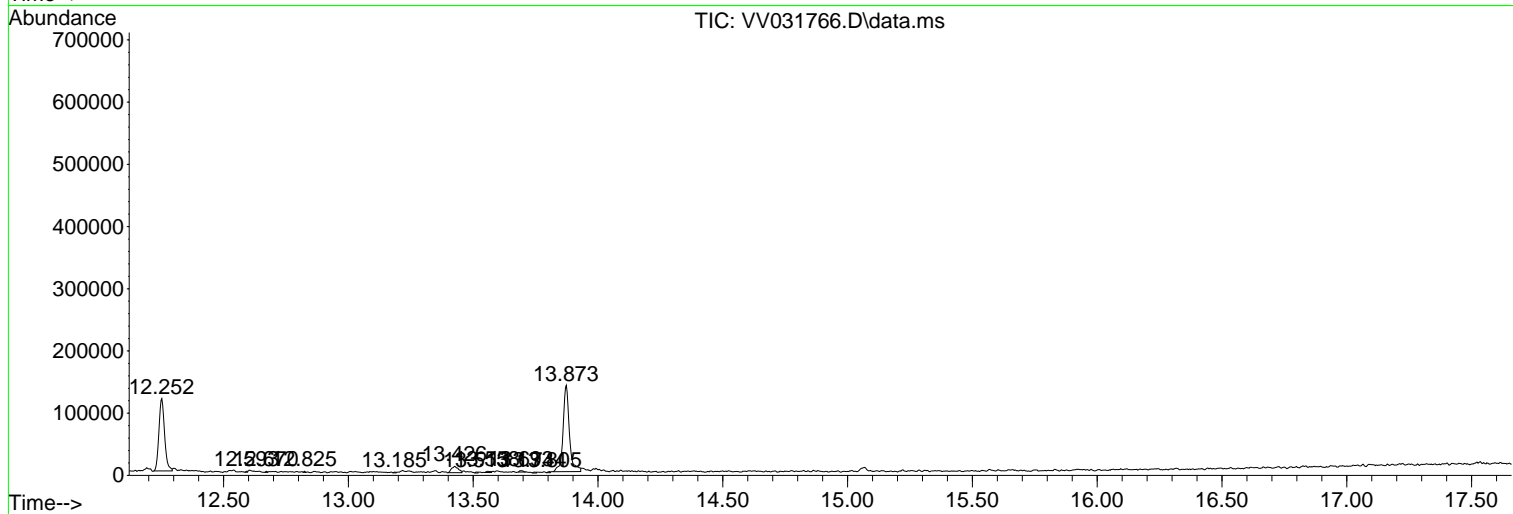
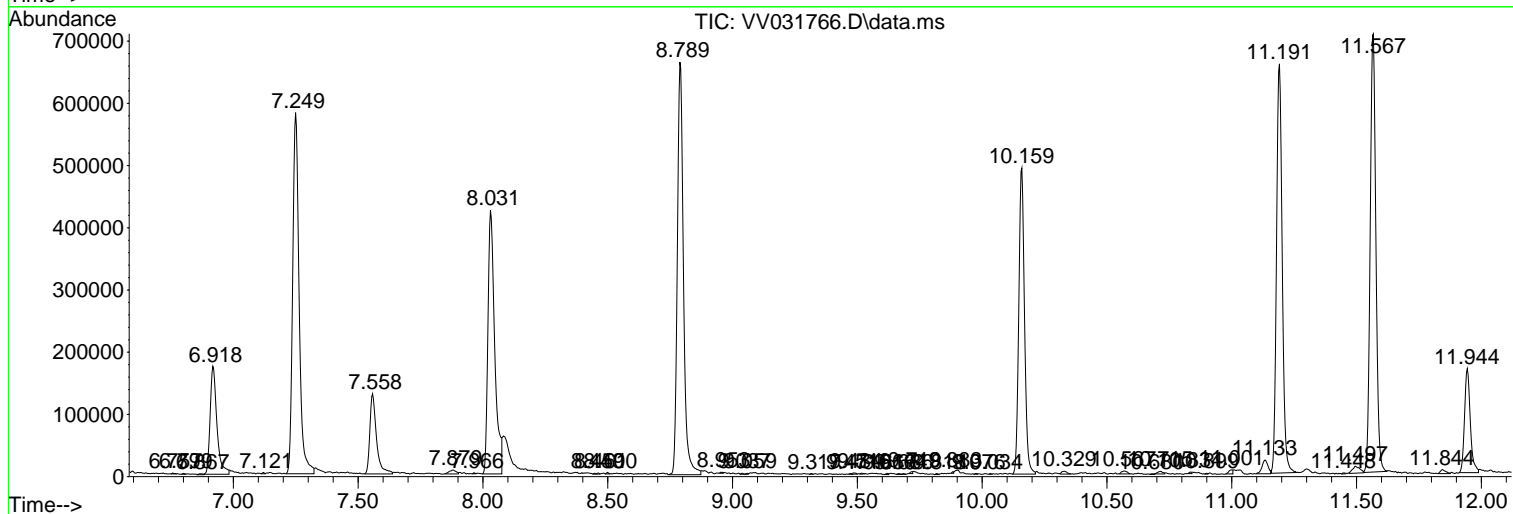
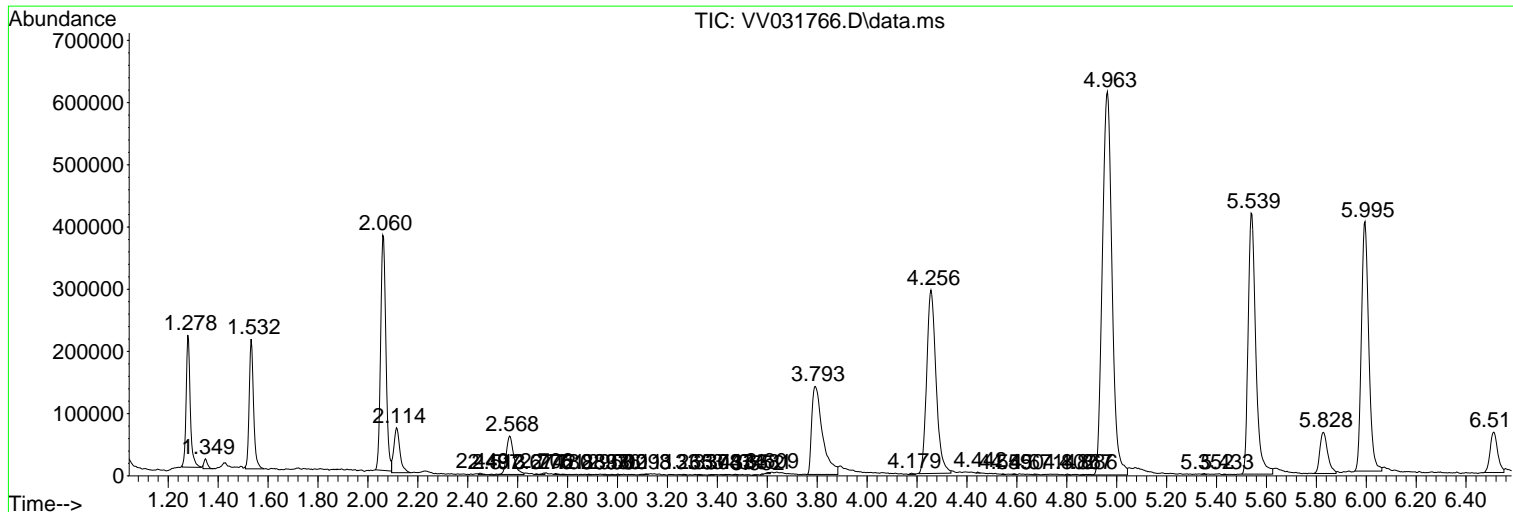
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
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 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y6

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

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P



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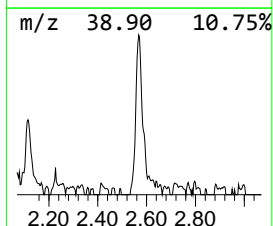
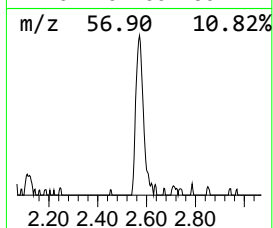
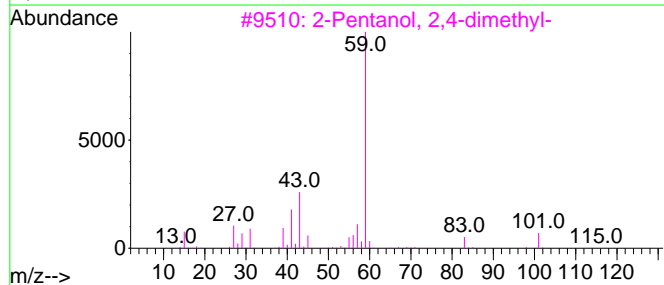
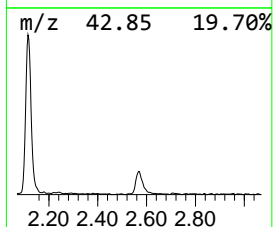
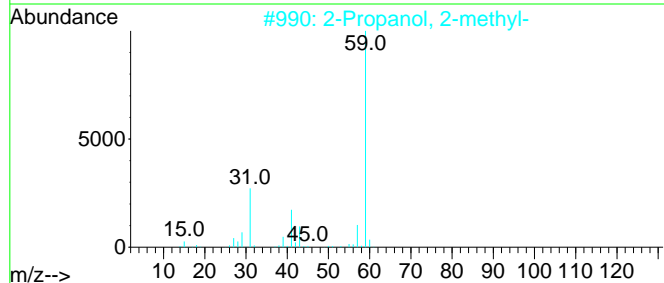
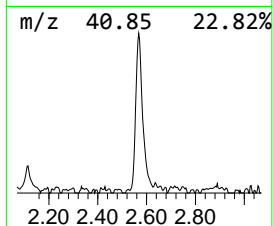
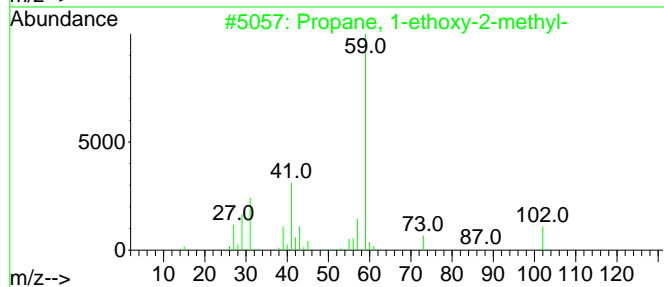
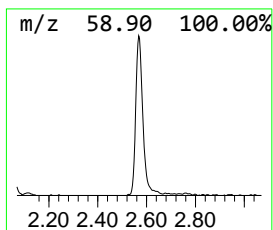
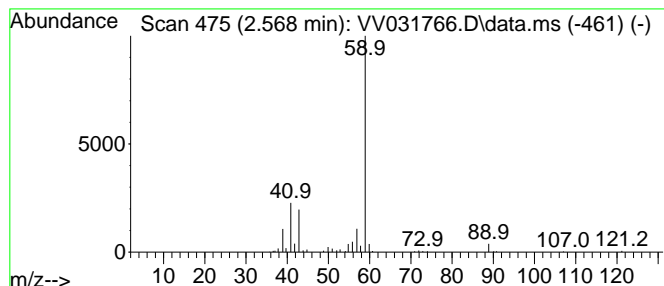
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 1 Propane, 1-ethoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.568	7.16 ug/L	127089	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	78
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
3			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	56
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50



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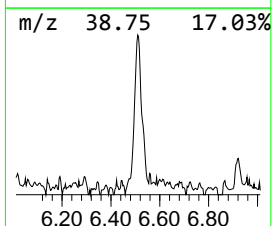
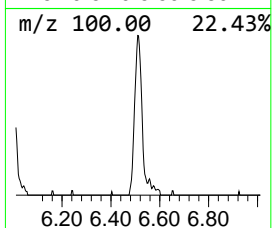
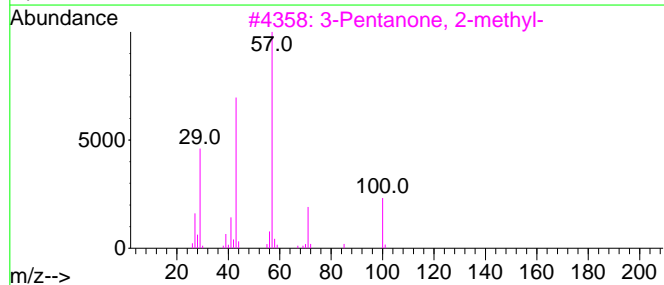
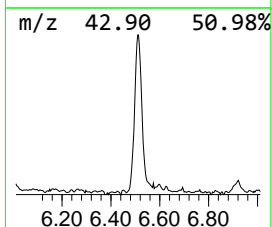
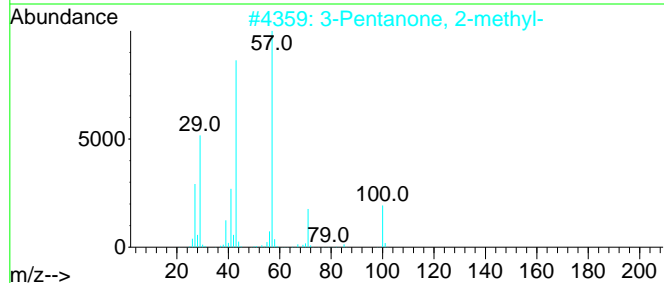
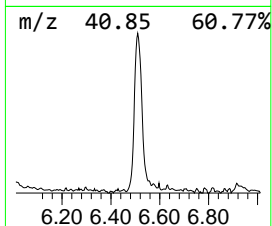
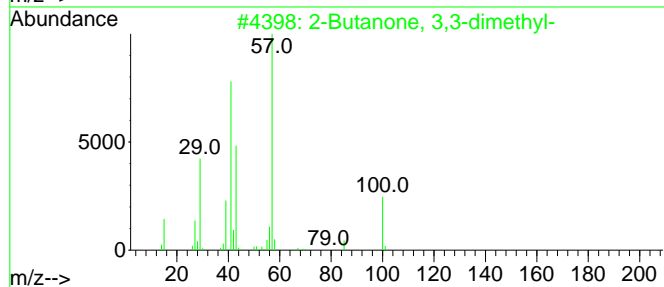
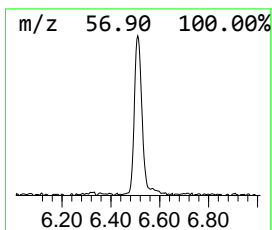
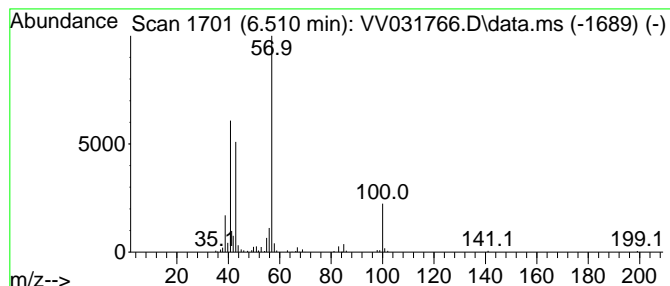
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.510	7.74 ug/L	137295	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	90
2			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
3			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
4			3-Hexanone	100	C6H12O	000589-38-8	59
5			cis-1-Ethoxy-1-butene	100	C6H12O	1000139-43-8	53



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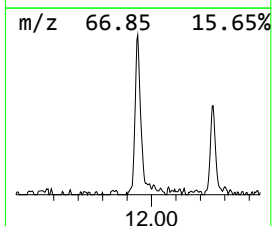
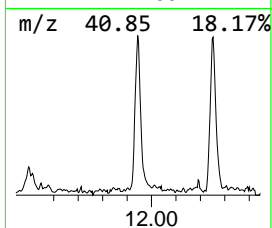
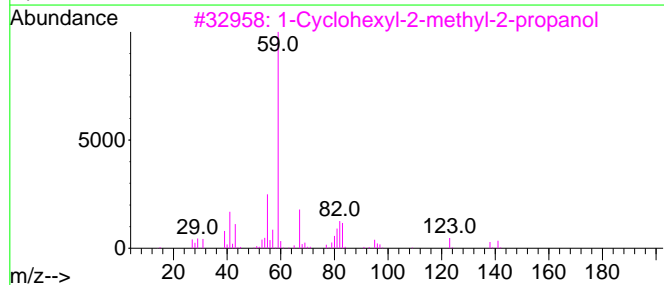
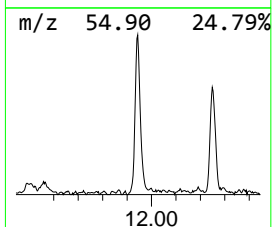
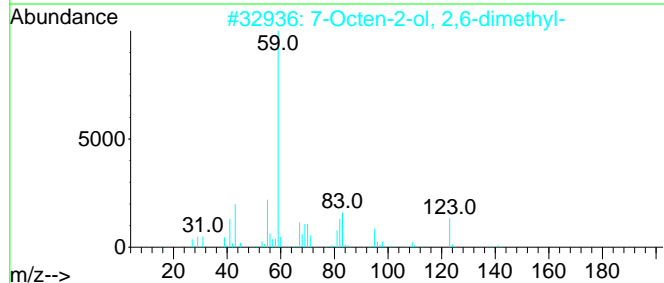
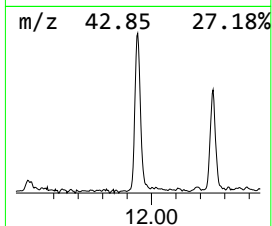
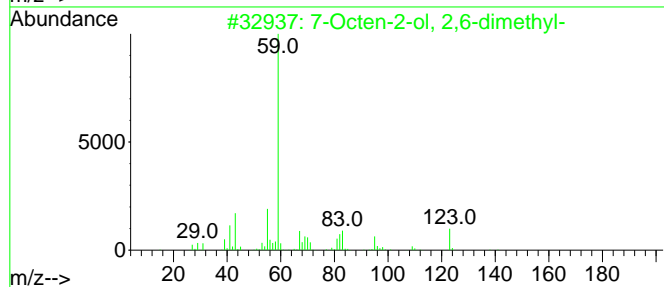
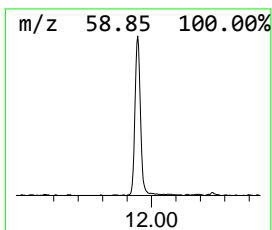
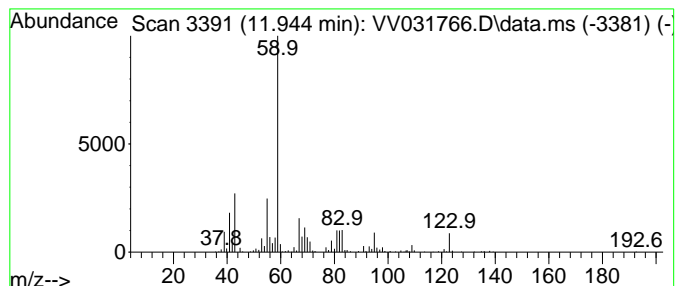
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
 Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.944	12.76 ug/L	267053	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	83		
2	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78		
3	1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	72		
4	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72		
5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
 Data File : VV031766.D
 Acq On : 26 Jul 2023 14:02
 Operator : SY/MD
 Sample : 03712-19
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y6

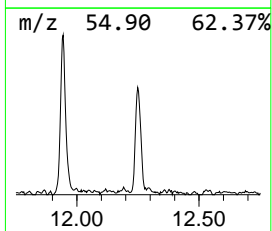
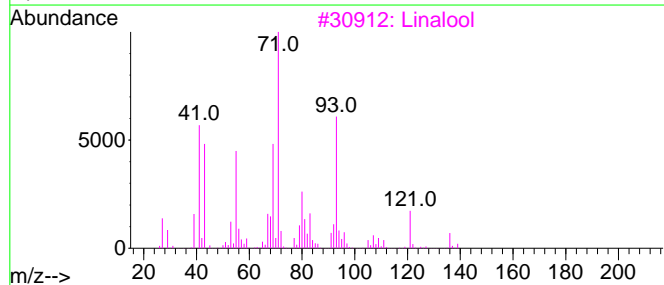
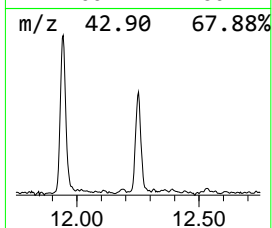
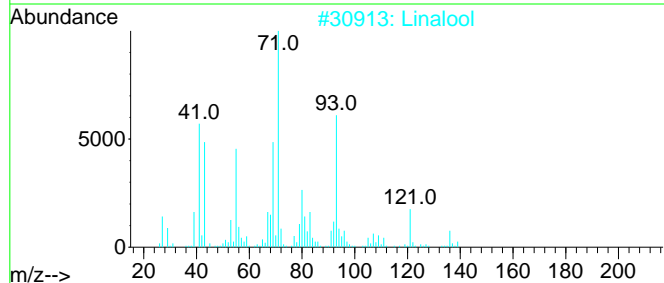
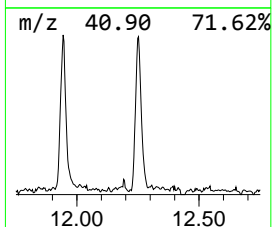
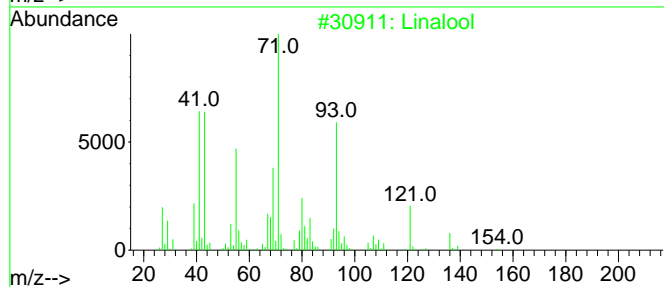
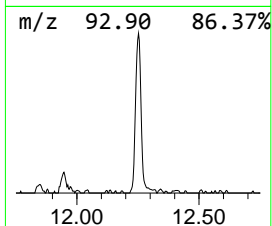
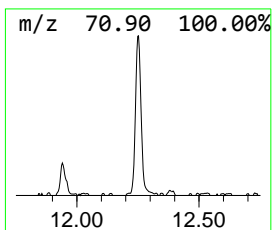
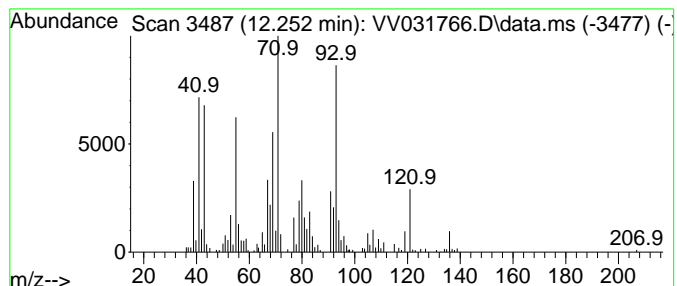
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 Quant Title : VOC Analysis

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

 Peak Number 6 Linalool Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.252	8.76 ug/L	183325	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linalool	154	C10H18O	000078-70-6	64
2			Linalool	154	C10H18O	000078-70-6	64
3			Linalool	154	C10H18O	000078-70-6	64
4			3-Carene	136	C10H16	013466-78-9	53
5			Hexanoic acid, 1-ethenyl-1,5-dim...	252	C16H28O2	007779-23-9	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
 Data File : VV031766.D
 Acq On : 26 Jul 2023 14:02
 Operator : SY/MD
 Sample : 03712-19
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y6

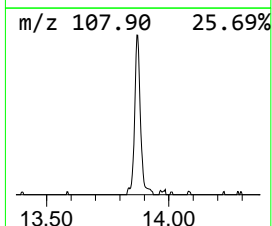
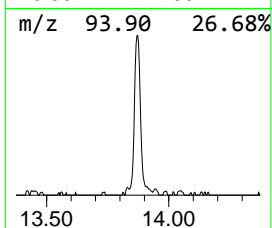
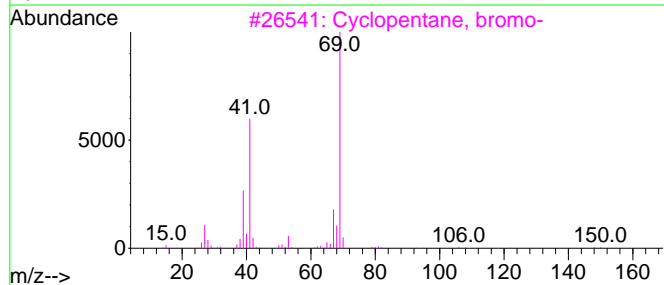
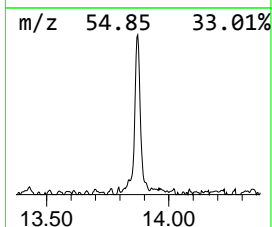
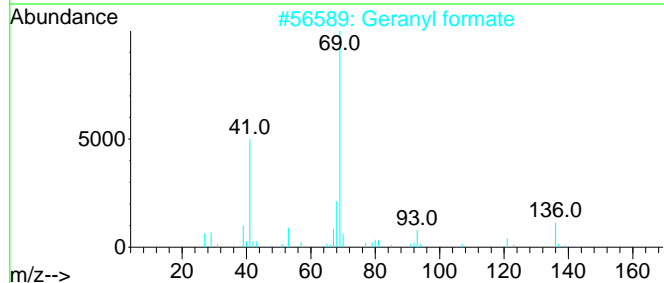
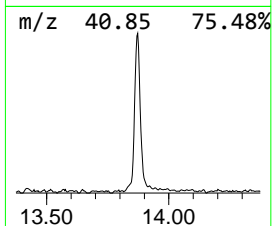
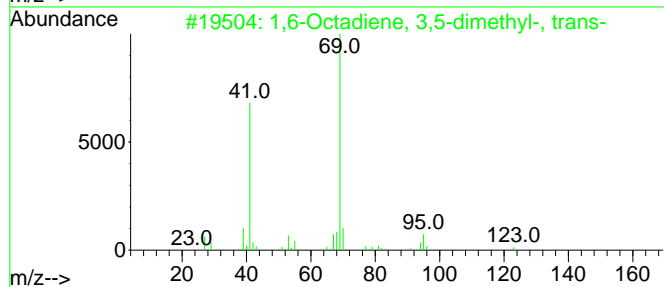
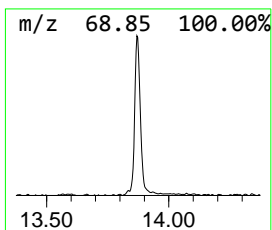
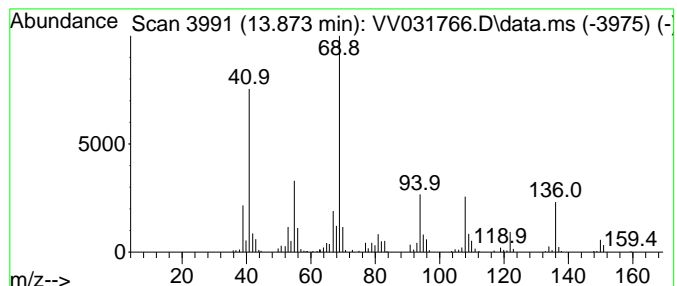
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 Quant Title : VOC Analysis

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

 Peak Number 7 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	11.62 ug/L	243222	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	43
2			Geranyl formate	182	C11H18O2	000105-86-2	43
3			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	41
4			Neral	152	C10H16O	000106-26-3	40
5			Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031766.D
Acq On : 26 Jul 2023 14:02
Operator : SY/MD
Sample : 03712-19
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y6

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1-etho...	2.568	7.2	ug/L	127089	1	5.539	887457	50.0
2-Butanone, 3,3...	6.510	7.7	ug/L	137295	1	5.539	887457	50.0
7-Octen-2-ol, 2...	11.944	12.8	ug/L	267053	3	11.191	1046150	50.0
Linalool	12.252	8.8	ug/L	183325	3	11.191	1046150	50.0
unknown-01	13.873	11.6	ug/L	243222	3	11.191	1046150	50.0