

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
 Data File : VV031749.D
 Acq On : 25 Jul 2023 18:25
 Operator : SY/MD
 Sample : 03712-08
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y5

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: VV031749.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	237223	263769	15.59%	1.943%
2	1.532	146	153	169	rVB	210091	254823	15.06%	1.877%
3	2.060	309	317	328	rBV	398368	569570	33.66%	4.196%
4	2.529	460	463	465	rBV4	2601	2011	0.12%	0.015%
5	2.571	467	476	490	rVV	54673	107004	6.32%	0.788%
6	2.976	598	602	603	rBV3	1861	929	0.05%	0.007%
7	2.986	603	605	610	rVB6	2529	1785	0.11%	0.013%
8	3.008	610	612	617	rBV6	1752	1638	0.10%	0.012%
9	3.034	617	620	622	rBV3	1701	1186	0.07%	0.009%
10	3.098	636	640	642	rBV5	1733	1203	0.07%	0.009%
11	3.124	645	648	651	rBV3	1644	1158	0.07%	0.009%
12	3.178	662	665	666	rBV2	1075	617	0.04%	0.005%
13	3.223	675	679	687	rBV10	2225	2859	0.17%	0.021%
14	3.252	687	688	689	rBV	701	165	0.01%	0.001%
15	3.288	696	699	700	rBV3	831	381	0.02%	0.003%
16	3.313	705	707	708	rBV2	857	359	0.02%	0.003%
17	3.387	727	730	731	rBV2	1242	500	0.03%	0.004%
18	3.468	751	755	759	rBV6	1797	1983	0.12%	0.015%
19	3.500	764	765	767	rVV2	786	328	0.02%	0.002%
20	3.522	771	772	775	rVV2	1130	577	0.03%	0.004%
21	3.584	789	791	792	rBV2	1662	648	0.04%	0.005%
22	3.793	844	856	880	rBV	139198	407695	24.10%	3.003%
23	4.256	984	1000	1029	rBV	303160	787855	46.56%	5.804%
24	4.500	1074	1076	1078	rBV2	1561	796	0.05%	0.006%
25	4.767	1157	1159	1162	rBV4	976	532	0.03%	0.004%
26	4.847	1181	1184	1188	rBV5	1280	759	0.04%	0.006%
27	4.866	1188	1190	1194	rVB4	912	687	0.04%	0.005%
28	4.895	1196	1199	1201	rBV4	749	409	0.02%	0.003%
29	4.963	1202	1220	1247	rBV2	628183	1691968	100.00%	12.464%
30	5.381	1347	1350	1352	rBV4	1693	1143	0.07%	0.008%
31	5.423	1361	1363	1366	rVB4	1550	901	0.05%	0.007%
32	5.448	1368	1371	1373	rBV3	954	585	0.03%	0.004%
33	5.481	1377	1381	1384	rBV4	1277	807	0.05%	0.006%
34	5.542	1387	1400	1423	rBV	403026	854542	50.51%	6.295%
35	5.828	1480	1489	1505	rVB2	47518	98798	5.84%	0.728%
36	5.995	1529	1541	1578	rVB	396986	850842	50.29%	6.268%

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

37	6.333	1645	1646	1649	rBV3	1321	636	0.04%	0.005%
38	6.416	1668	1672	1675	rBV5	1568	1296	0.08%	0.010%
39	6.468	1685	1688	1689	rBV2	1568	812	0.05%	0.006%
40	6.513	1690	1702	1720	rVV2	68866	144518	8.54%	1.065%
41	6.699	1758	1760	1763	rBV4	1251	729	0.04%	0.005%
42	6.773	1780	1783	1789	rBV7	1489	1583	0.09%	0.012%
43	6.812	1794	1795	1797	rVB2	914	260	0.02%	0.002%
44	6.837	1801	1803	1804	rVB2	568	145	0.01%	0.001%
45	6.857	1804	1809	1811	rBV5	1303	694	0.04%	0.005%
46	6.918	1818	1828	1845	rBV	179889	330564	19.54%	2.435%
47	7.249	1920	1931	1949	rBV	607326	1077606	63.69%	7.938%
48	7.558	2017	2027	2053	rBV2	133876	250999	14.83%	1.849%
49	7.792	2097	2100	2101	rBV2	1138	575	0.03%	0.004%
50	7.850	2115	2118	2119	rBV3	1328	884	0.05%	0.007%
51	7.972	2153	2156	2161	rBV5	1412	1408	0.08%	0.010%
52	8.030	2164	2174	2215	rBV2	441597	938740	55.48%	6.915%
53	8.628	2356	2360	2361	rBV3	690	406	0.02%	0.003%
54	8.641	2361	2364	2367	rVB5	1406	875	0.05%	0.006%
55	8.712	2384	2386	2387	rBV2	646	262	0.02%	0.002%
56	8.725	2388	2390	2396	rVB6	1629	1247	0.07%	0.009%
57	8.789	2396	2410	2431	rBV	671982	1127528	66.64%	8.306%
58	9.217	2538	2543	2549	rVB9	1302	1044	0.06%	0.008%
59	9.246	2549	2552	2556	rVB5	836	694	0.04%	0.005%
60	9.265	2556	2558	2561	rBV4	1315	905	0.05%	0.007%
61	9.310	2570	2572	2574	rBV3	859	428	0.03%	0.003%
62	9.349	2581	2584	2586	rVB3	1183	702	0.04%	0.005%
63	9.371	2588	2591	2595	rBV5	806	703	0.04%	0.005%
64	9.394	2595	2598	2601	rVV4	1185	665	0.04%	0.005%
65	9.426	2605	2608	2612	rBV4	1290	1142	0.07%	0.008%
66	9.471	2619	2622	2624	rBV3	1520	882	0.05%	0.006%
67	9.673	2684	2685	2686	rBV	870	247	0.01%	0.002%
68	9.898	2746	2755	2759	rBV10	6228	8131	0.48%	0.060%
69	10.024	2791	2794	2795	rBV2	995	599	0.04%	0.004%
70	10.159	2822	2836	2858	rBV	552242	896710	53.00%	6.606%
71	10.513	2943	2946	2952	rVB7	1320	1303	0.08%	0.010%
72	10.538	2952	2954	2955	rBV	1021	401	0.02%	0.003%
73	10.689	2997	3001	3002	rBV3	938	507	0.03%	0.004%
74	10.760	3021	3023	3024	rBV	298	150	0.01%	0.001%
75	10.773	3024	3027	3029	rVV4	1248	685	0.04%	0.005%
76	10.792	3031	3033	3036	rBV3	837	532	0.03%	0.004%

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Title : VOC Analysis

77	10.969	3084	3088	3090	rBV3	1532	1332	0.08%	0.010%
78	11.001	3090	3098	3102	rBV6	3696	5757	0.34%	0.042%
79	11.078	3120	3122	3124	rBV2	598	405	0.02%	0.003%
80	11.133	3131	3139	3146	rBV7	18279	28258	1.67%	0.208%
81	11.191	3147	3157	3174	rVV	690916	1055306	62.37%	7.774%
82	11.432	3231	3232	3234	rBV2	997	503	0.03%	0.004%
83	11.500	3239	3253	3262	rBV8	13788	31710	1.87%	0.234%
84	11.567	3263	3274	3296	rVB	745041	1175174	69.46%	8.657%
85	11.943	3379	3391	3413	rBV2	154418	255617	15.11%	1.883%
86	12.252	3478	3487	3503	rBV2	95104	149085	8.81%	1.098%
87	12.815	3659	3662	3664	rBV4	1259	717	0.04%	0.005%
88	13.516	3878	3880	3883	rBV3	1676	713	0.04%	0.005%
89	13.577	3894	3899	3904	rBV6	1907	2194	0.13%	0.016%
90	13.873	3984	3991	4009	rVB2	104102	157924	9.33%	1.163%

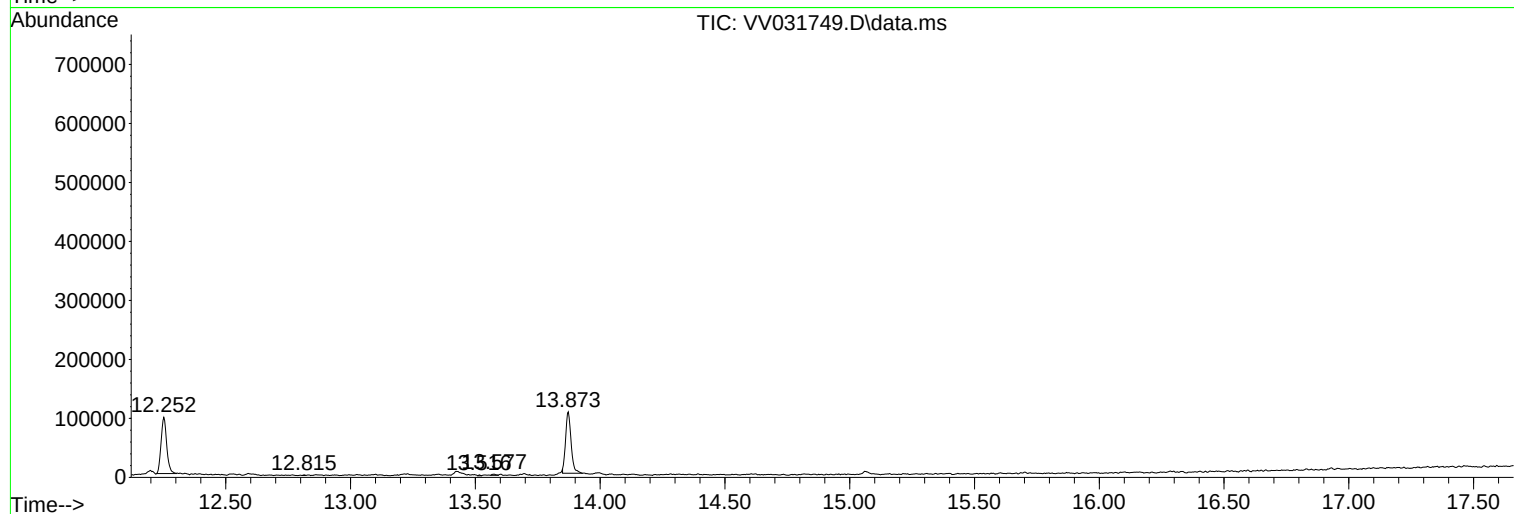
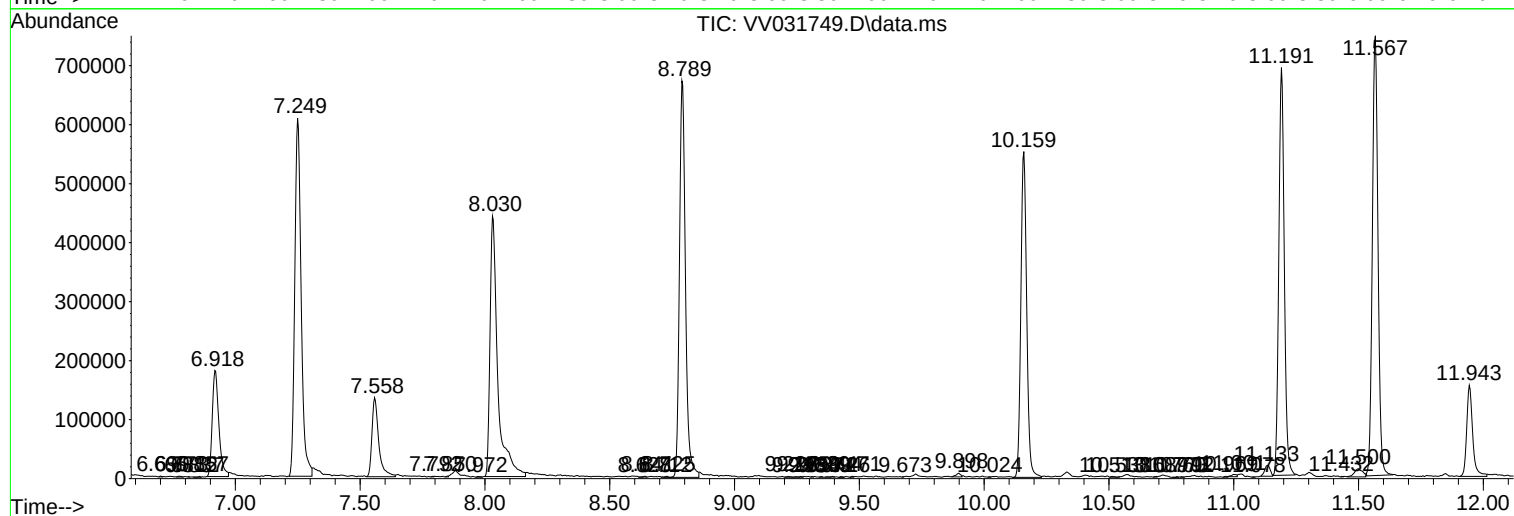
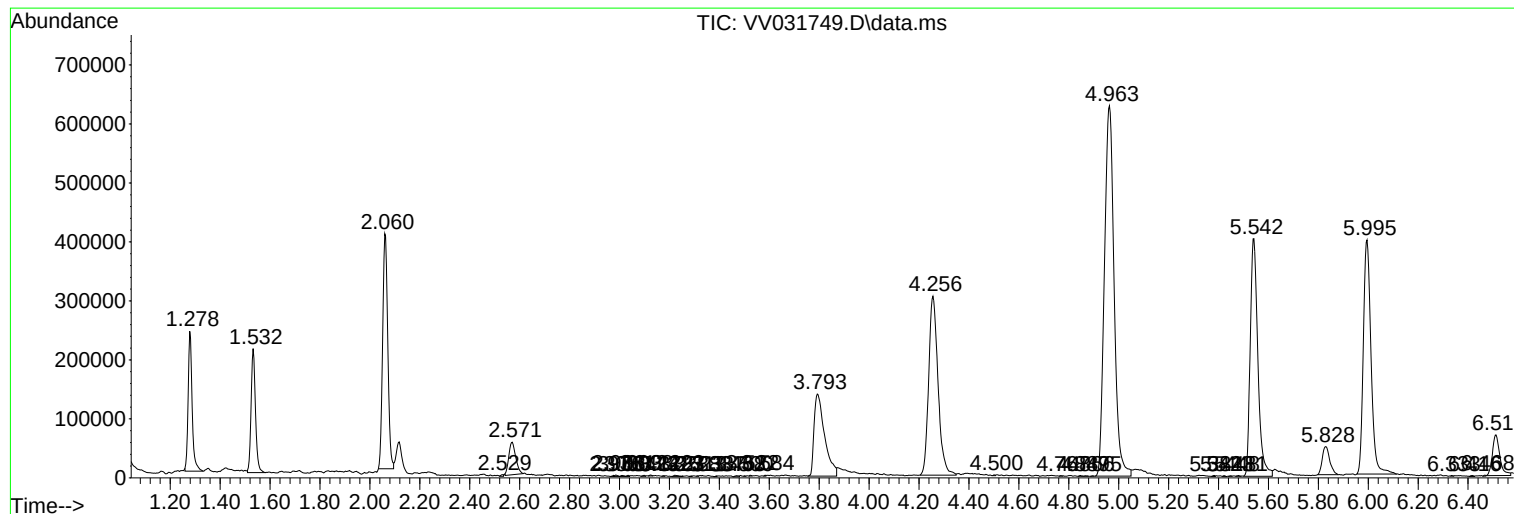
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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



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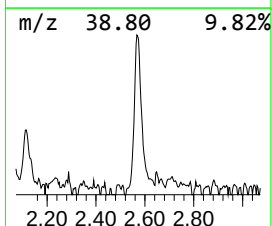
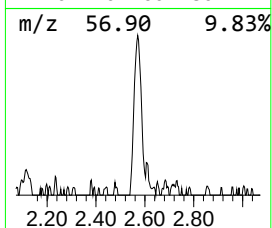
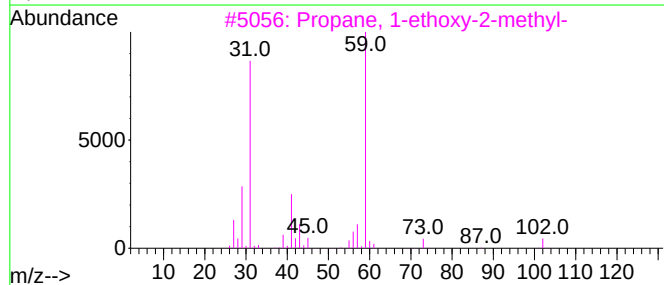
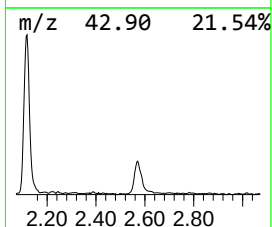
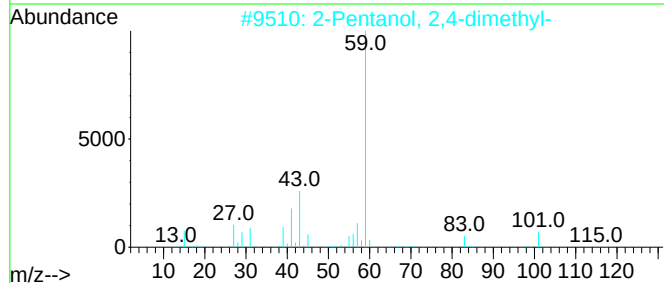
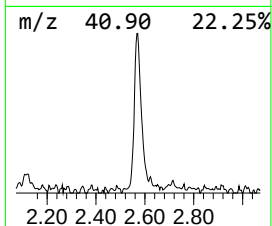
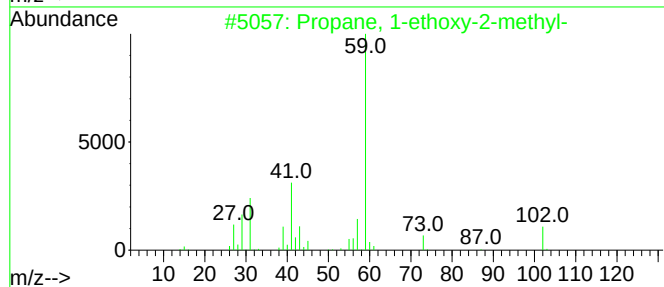
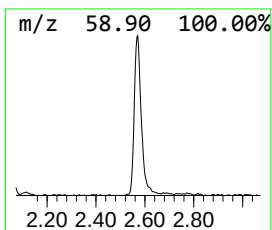
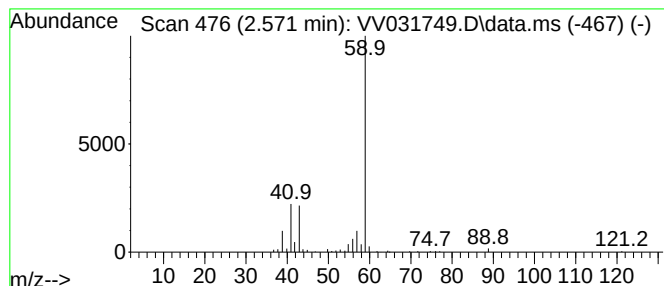
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propane, 1-ethoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.571	6.26 ug/L	107004	1,4-Difluorobenzene	5.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	78
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	64
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	64
4			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	43
5			2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	43



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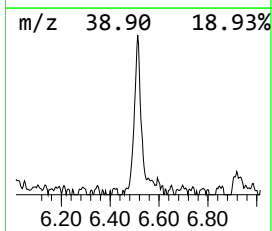
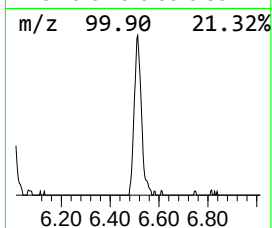
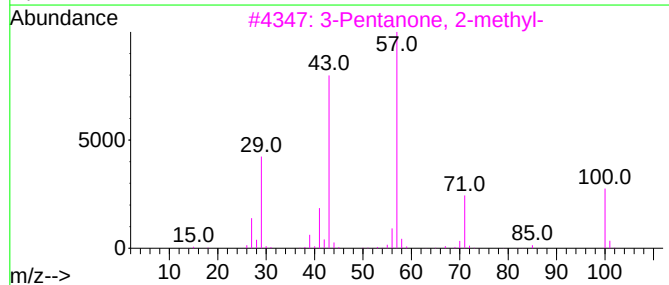
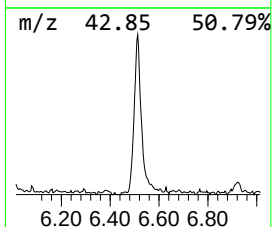
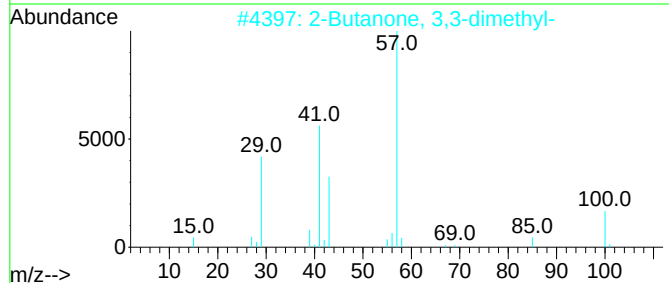
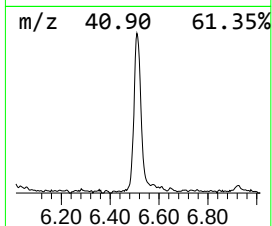
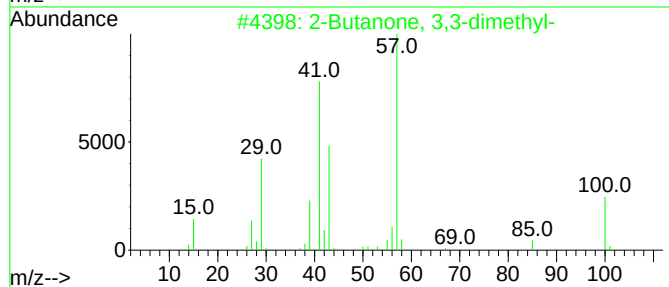
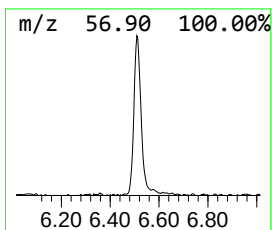
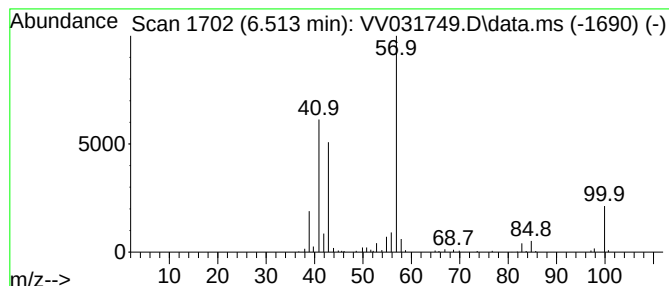
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.513	8.46 ug/L	144518	1,4-Difluorobenzene	5.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	80	
2	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	72	
3	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	64	
4	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	58	
5	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	43	



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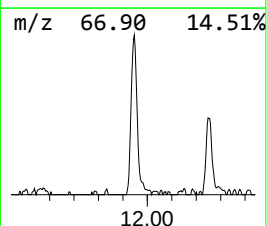
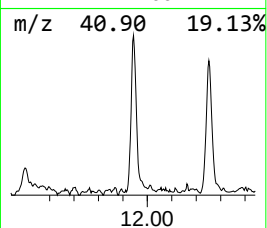
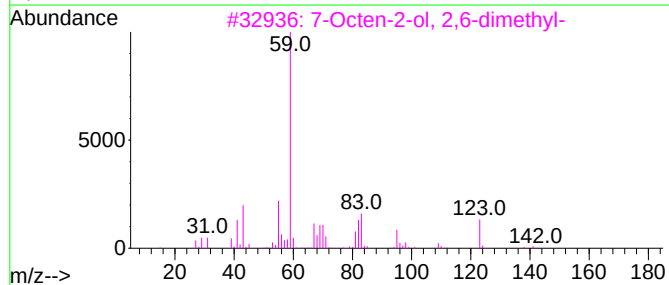
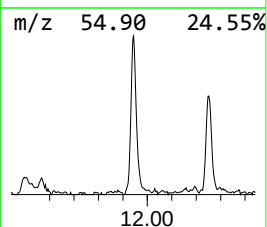
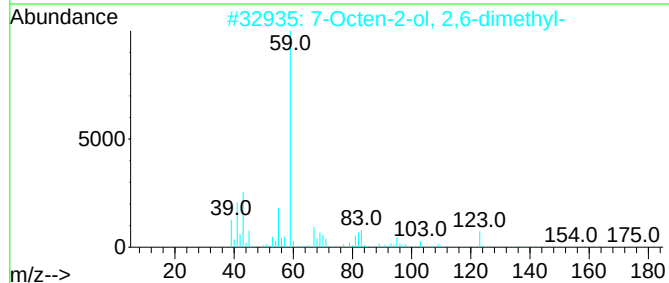
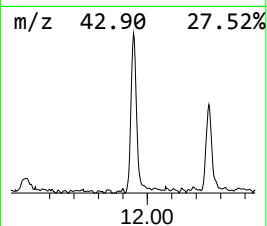
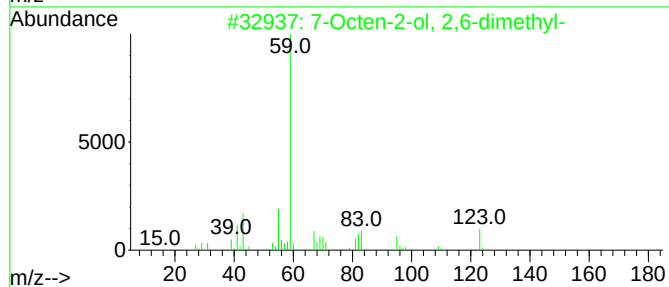
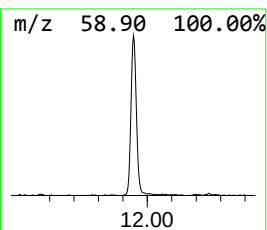
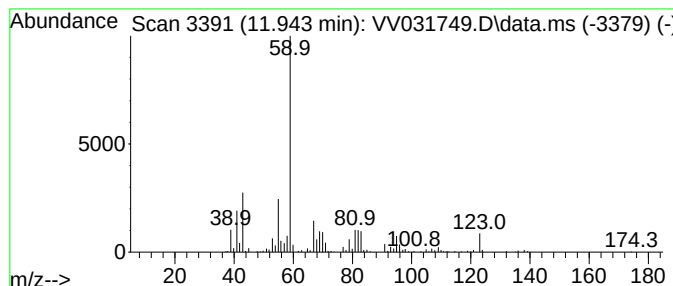
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.943	12.11 ug/L	255617	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	90
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
4			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
5			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	64



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Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

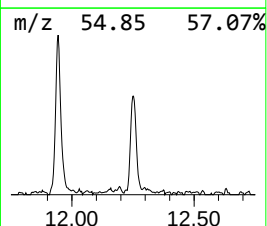
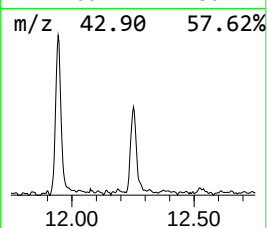
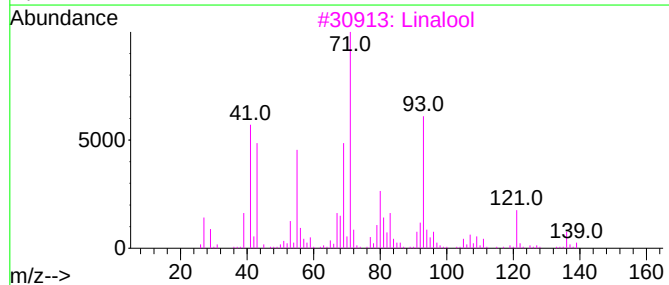
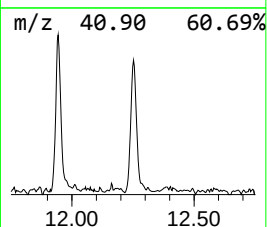
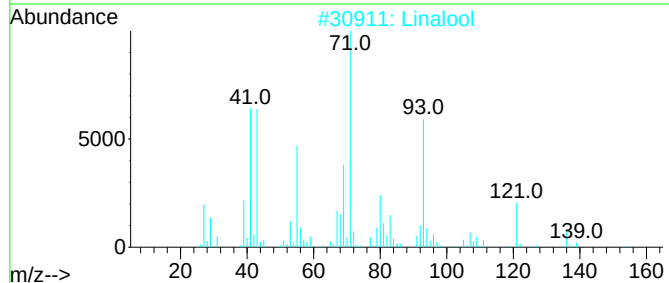
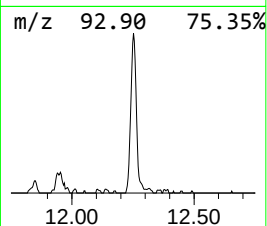
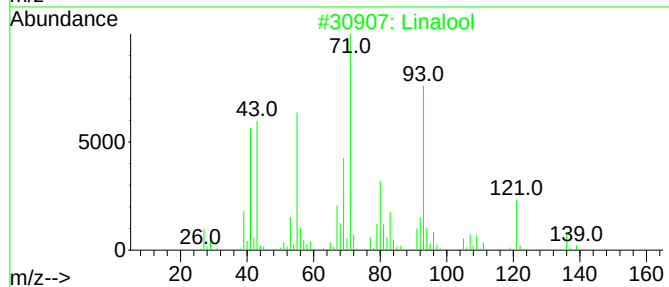
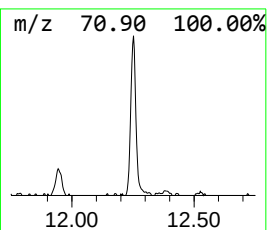
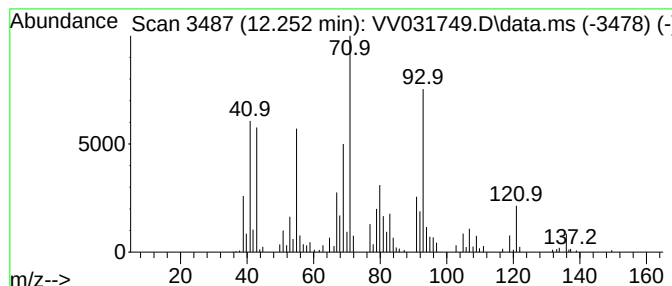
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Quant Title : VOC Analysis

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

Peak Number 6 Linalool Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.252	7.06 ug/L	149085	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linalool	154	C10H18O	000078-70-6	80
2			Linalool	154	C10H18O	000078-70-6	80
3			Linalool	154	C10H18O	000078-70-6	80
4			Linalool	154	C10H18O	000078-70-6	80
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031749.D
Acq On : 25 Jul 2023 18:25
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

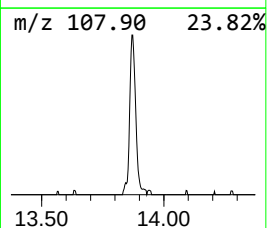
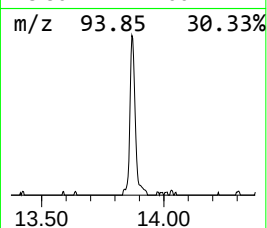
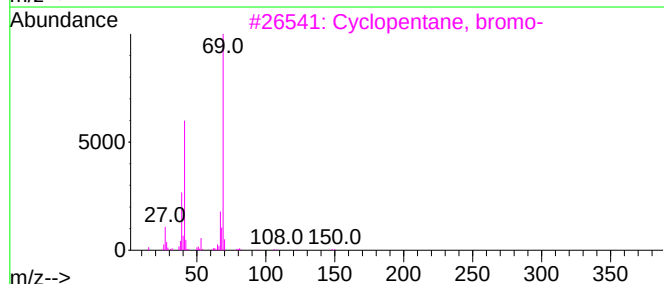
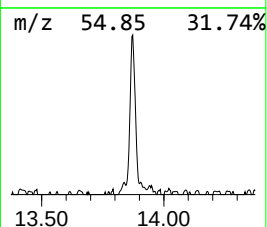
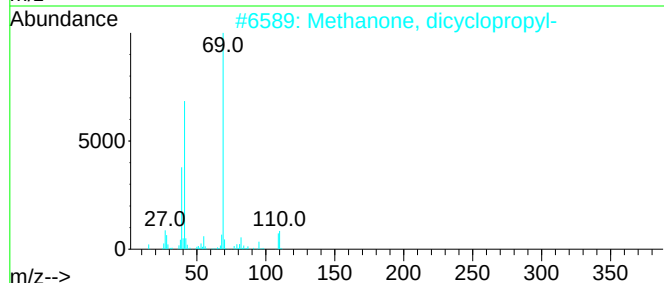
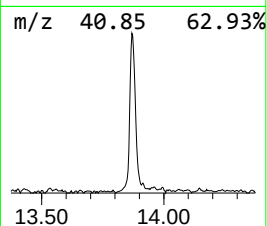
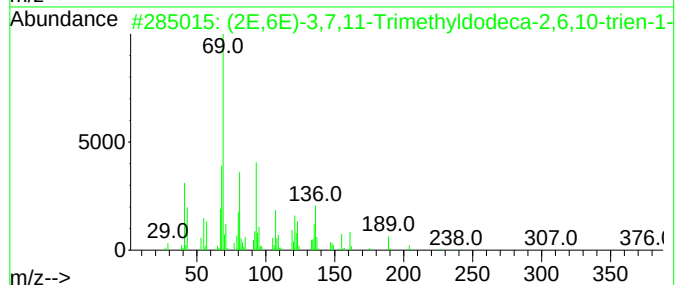
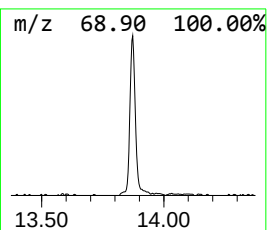
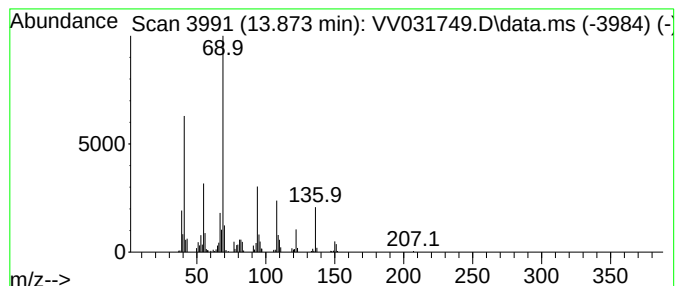
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Quant Title : VOC Analysis

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

Peak Number 7 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	7.48 ug/L	157924	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	40		
2	Methanone, dicyclopentyl-	110	C7H10O	001121-37-5	38		
3	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	38		
4	Methanone, dicyclopentyl-	110	C7H10O	001121-37-5	38		
5	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	38		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031749.D
Acq On : 25 Jul 2023 18:25
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1-etho...	2.571	6.3	ug/L	107004	1	5.542	854542	50.0
2-Butanone, 3,3...	6.513	8.5	ug/L	144518	1	5.542	854542	50.0
7-Octen-2-ol, 2...	11.943	12.1	ug/L	255617	3	11.191	1055310	50.0
Linalool	12.252	7.1	ug/L	149085	3	11.191	1055310	50.0
unknown-01	13.873	7.5	ug/L	157924	3	11.191	1055310	50.0