

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
 Data File : VV031751.D
 Acq On : 25 Jul 2023 19:12
 Operator : SY/MD
 Sample : 03712-19
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y6

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: VV031751.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	66	74	90	rBV	212992	242477	15.06%	1.847%
2	1.349	93	96	107	rVB	17971	19730	1.23%	0.150%
3	1.532	146	153	167	rVB	209040	247246	15.36%	1.884%
4	2.060	308	317	327	rBV	379292	553695	34.40%	4.218%
5	2.114	328	334	349	rVB	72316	111416	6.92%	0.849%
6	2.445	435	437	442	rVB5	2100	1573	0.10%	0.012%
7	2.571	465	476	491	rVV	63020	125561	7.80%	0.957%
8	2.709	516	519	523	rBV6	2316	2304	0.14%	0.018%
9	2.889	572	575	580	rVB7	2110	1544	0.10%	0.012%
10	2.966	596	599	604	rVB5	1330	1065	0.07%	0.008%
11	2.995	604	608	610	rBV5	1548	1101	0.07%	0.008%
12	3.082	631	635	637	rBV5	1600	1059	0.07%	0.008%
13	3.121	641	647	652	rBV7	2181	2826	0.18%	0.022%
14	3.333	710	713	718	rBV6	1015	1102	0.07%	0.008%
15	3.468	751	755	758	rVB6	1543	1150	0.07%	0.009%
16	3.587	788	792	793	rBV3	3281	1970	0.12%	0.015%
17	3.793	846	856	884	rBV2	146023	420646	26.13%	3.204%
18	4.256	984	1000	1028	rBV	285958	742410	46.12%	5.656%
19	4.555	1090	1093	1099	rVB7	1709	1513	0.09%	0.012%
20	4.584	1099	1102	1104	rBV3	2202	1570	0.10%	0.012%
21	4.651	1121	1123	1129	rBV6	1440	1147	0.07%	0.009%
22	4.741	1148	1151	1155	rBV5	1768	1696	0.11%	0.013%
23	4.783	1161	1164	1167	rVB4	1417	950	0.06%	0.007%
24	4.960	1202	1219	1248	rBV2	596028	1609750	100.00%	12.263%
25	5.394	1350	1354	1357	rVB6	1296	1049	0.07%	0.008%
26	5.416	1358	1361	1365	rBV5	1637	1137	0.07%	0.009%
27	5.542	1387	1400	1420	rBV	389226	826833	51.36%	6.299%
28	5.828	1478	1489	1507	rBV2	52734	114097	7.09%	0.869%
29	5.918	1513	1517	1522	rBV7	3832	4562	0.28%	0.035%
30	5.995	1528	1541	1562	rBV	371599	769715	47.82%	5.864%
31	6.510	1690	1701	1719	rBV	64179	132712	8.24%	1.011%
32	6.828	1794	1800	1802	rVB6	1720	1593	0.10%	0.012%
33	6.841	1802	1804	1807	rBV3	1345	1124	0.07%	0.009%
34	6.918	1817	1828	1861	rBV	160963	313191	19.46%	2.386%
35	7.056	1868	1871	1878	rVB7	1426	1288	0.08%	0.010%
36	7.249	1919	1931	1957	rBV	536018	976990	60.69%	7.443%

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Stop Thrs : 0

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

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

37	7.558	2017	2027	2046	rBV	120524	218986	13.60%	1.668%
38	7.764	2088	2091	2097	rVB4	1227	950	0.06%	0.007%
39	7.879	2116	2127	2134	rBV6	9304	16338	1.01%	0.124%
40	8.030	2164	2174	2187	rBV	425303	787244	48.90%	5.997%
41	8.310	2257	2261	2265	rVB5	1707	1719	0.11%	0.013%
42	8.484	2312	2315	2317	rBV4	1752	1334	0.08%	0.010%
43	8.609	2351	2354	2358	rVB5	1355	1274	0.08%	0.010%
44	8.638	2358	2363	2366	rBV5	1845	1723	0.11%	0.013%
45	8.664	2366	2371	2375	rBV6	1811	2075	0.13%	0.016%
46	8.789	2398	2410	2438	rBV	645947	1079213	67.04%	8.221%
47	8.924	2446	2452	2453	rBV5	2963	2505	0.16%	0.019%
48	9.008	2475	2478	2482	rVB6	1657	1115	0.07%	0.008%
49	9.079	2498	2500	2504	rBV4	1434	1017	0.06%	0.008%
50	9.188	2528	2534	2540	rVB9	2620	3581	0.22%	0.027%
51	9.487	2621	2627	2628	rBV4	1298	1054	0.07%	0.008%
52	9.567	2647	2652	2655	rBV5	1285	1477	0.09%	0.011%
53	9.603	2660	2663	2667	rBV6	1171	951	0.06%	0.007%
54	9.622	2667	2669	2674	rVB5	1034	929	0.06%	0.007%
55	9.696	2689	2692	2694	rBV3	1912	1313	0.08%	0.010%
56	9.709	2694	2696	2698	rBV2	2207	1361	0.08%	0.010%
57	9.895	2743	2754	2764	rBV2	5642	10744	0.67%	0.082%
58	9.998	2782	2786	2792	rBV4	1290	1094	0.07%	0.008%
59	10.043	2796	2800	2804	rVB5	1515	1286	0.08%	0.010%
60	10.085	2808	2813	2823	rVB7	1114	1489	0.09%	0.011%
61	10.159	2823	2836	2851	rBV	515117	812217	50.46%	6.187%
62	10.329	2880	2889	2901	rVB8	6586	12644	0.79%	0.096%
63	10.461	2926	2930	2934	rBV6	1308	1162	0.07%	0.009%
64	10.571	2958	2964	2968	rBV6	4074	4677	0.29%	0.036%
65	10.712	3000	3008	3019	rBV8	5231	9047	0.56%	0.069%
66	10.773	3021	3027	3029	rBV5	2062	2149	0.13%	0.016%
67	10.837	3039	3047	3053	rBV5	2727	4317	0.27%	0.033%
68	11.001	3085	3098	3102	rBV5	5216	9838	0.61%	0.075%
69	11.091	3121	3126	3127	rBV3	1194	922	0.06%	0.007%
70	11.136	3130	3140	3146	rVV6	17967	29470	1.83%	0.225%
71	11.191	3146	3157	3178	rVV	671345	1034998	64.30%	7.885%
72	11.390	3217	3219	3224	rVB4	1394	1050	0.07%	0.008%
73	11.455	3235	3239	3240	rBV3	2037	1290	0.08%	0.010%
74	11.497	3241	3252	3262	rBV6	12512	27095	1.68%	0.206%
75	11.567	3262	3274	3291	rVB	703071	1114511	69.24%	8.490%
76	11.677	3305	3308	3312	rBV4	2981	3124	0.19%	0.024%

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

77	11.734	3323	3326	3332	rVB6	2958	2371	0.15%	0.018%
78	11.847	3356	3361	3369	rVB8	6238	8184	0.51%	0.062%
79	11.879	3369	3371	3375	rVB5	1411	878	0.05%	0.007%
80	11.943	3381	3391	3409	rBV	162954	270088	16.78%	2.058%
81	12.252	3477	3487	3500	rBV3	100477	156639	9.73%	1.193%
82	12.345	3514	3516	3520	rVB5	2824	1827	0.11%	0.014%
83	12.381	3524	3527	3530	rBV4	3247	2386	0.15%	0.018%
84	12.532	3570	3574	3578	rBV6	1985	1927	0.12%	0.015%
85	12.670	3609	3617	3618	rBV7	2670	2381	0.15%	0.018%
86	13.207	3780	3784	3785	rBV3	3166	2236	0.14%	0.017%
87	13.419	3844	3850	3860	rBV3	7545	13175	0.82%	0.100%
88	13.586	3896	3902	3908	rVB7	2164	2999	0.19%	0.023%
89	13.689	3929	3934	3939	rBV8	2645	2821	0.18%	0.021%
90	13.728	3943	3946	3950	rBV5	1201	994	0.06%	0.008%
91	13.799	3966	3968	3971	rBV2	1562	1091	0.07%	0.008%
92	13.873	3977	3991	4004	rBV	113619	190933	11.86%	1.455%
93	14.095	4056	4060	4066	rVB8	2052	2437	0.15%	0.019%
94	14.159	4077	4080	4084	rBV6	1020	963	0.06%	0.007%
95	14.181	4085	4087	4090	rVV3	1490	927	0.06%	0.007%
96	14.294	4118	4122	4128	rBV7	2925	3301	0.21%	0.025%
97	14.387	4147	4151	4153	rBV3	1590	1465	0.09%	0.011%
98	14.400	4153	4155	4159	rVB5	2332	1337	0.08%	0.010%
99	14.998	4339	4341	4344	rBV4	1614	1155	0.07%	0.009%
100	15.062	4356	4361	4365	rBV6	4968	5268	0.33%	0.040%

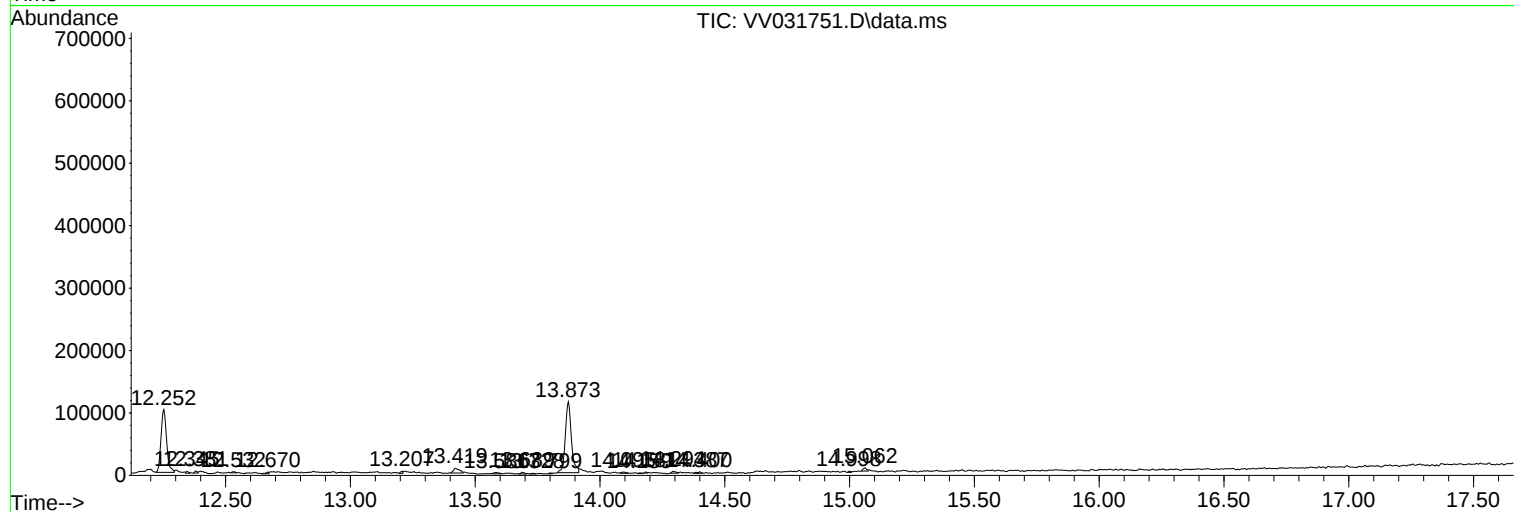
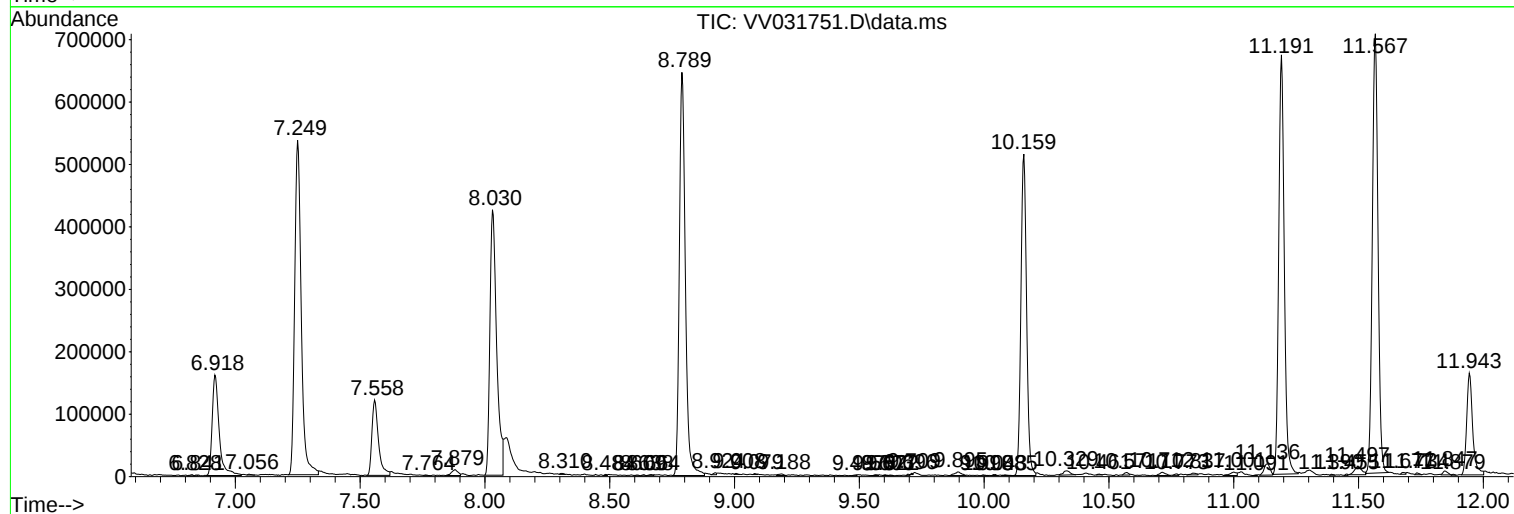
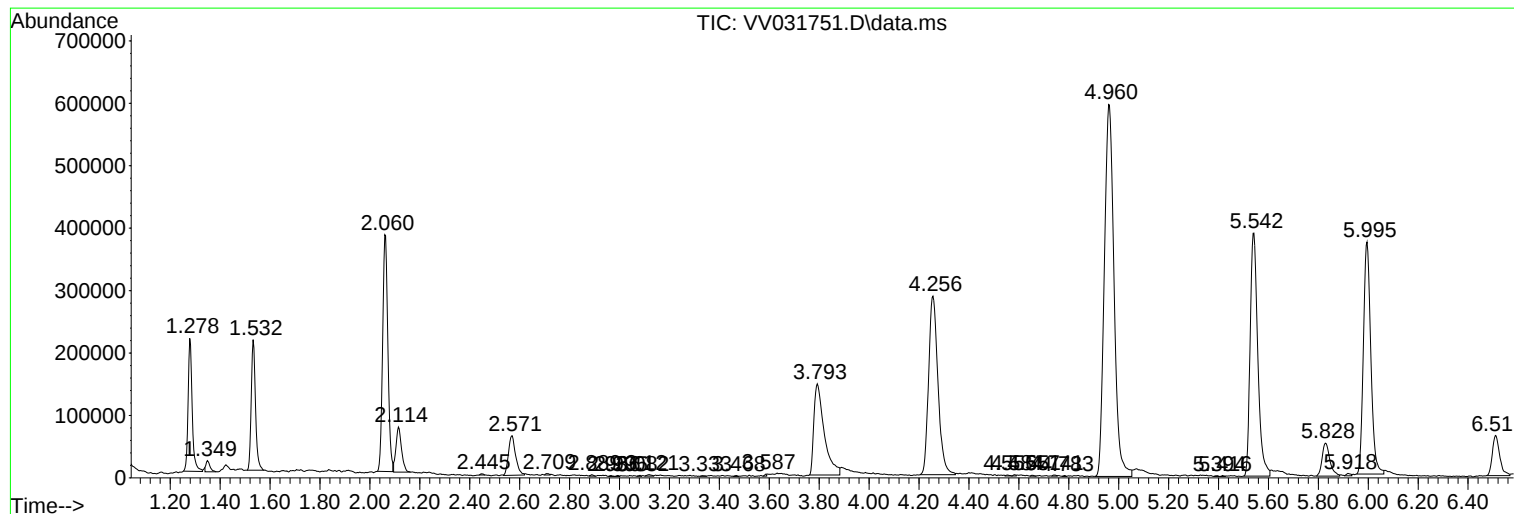
Sum of corrected areas: 13126858

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Instrument :
MSVOA_V
ClientSampleId :
BH2Y6

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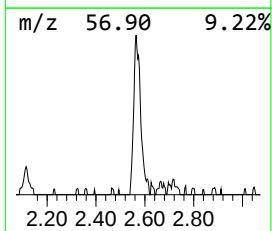
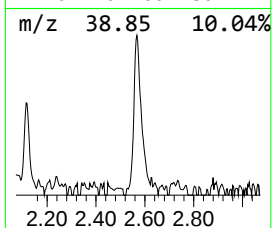
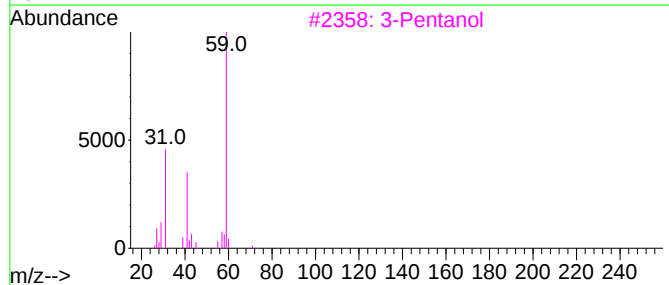
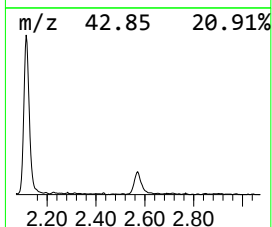
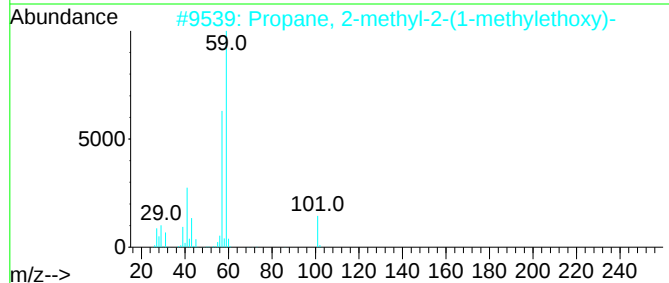
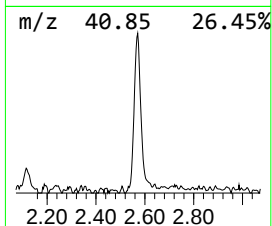
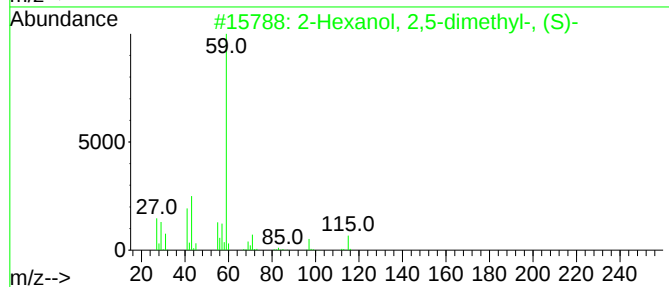
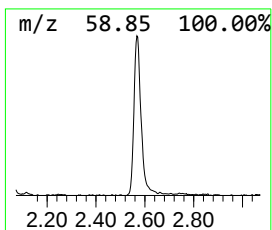
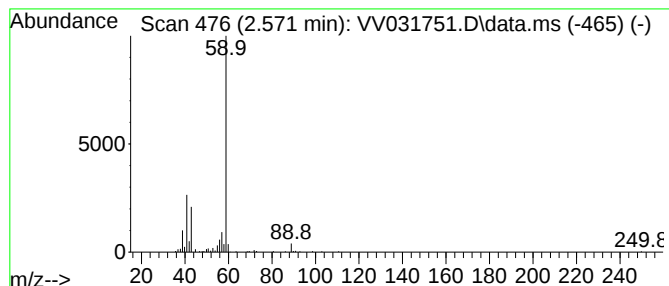
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.571	7.59 ug/L	125561	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	56		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50		
3	3-Pentanol	88	C5H12O	000584-02-1	50		
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50		
5	1,2-Butanediol	90	C4H10O2	000584-03-2	50		



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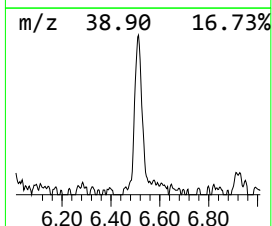
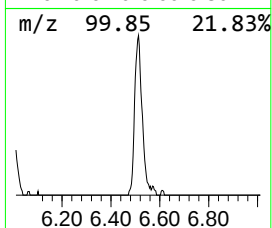
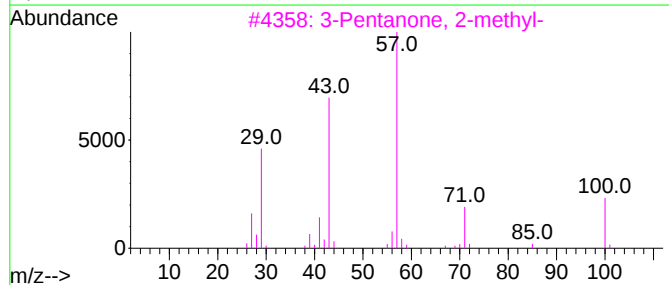
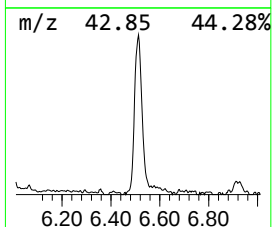
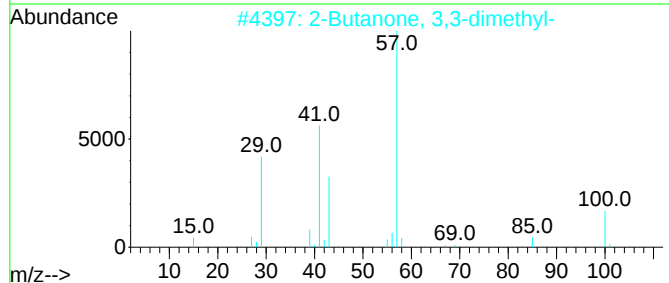
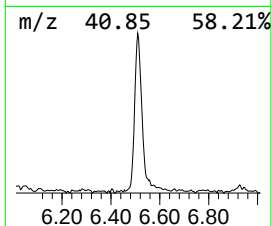
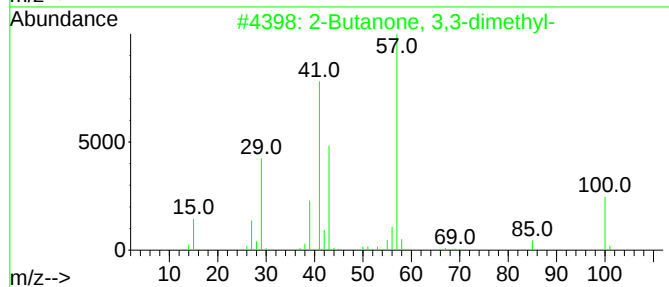
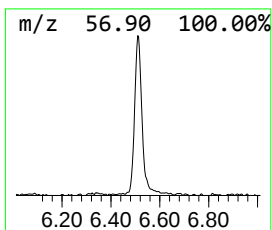
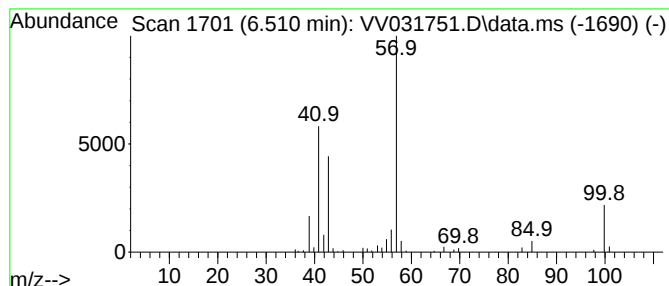
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.510	8.03 ug/L	132712	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	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	86	
3	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	80	
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72	
5	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64	



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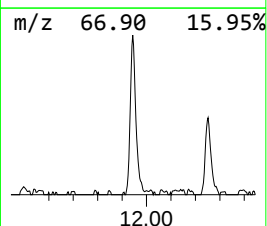
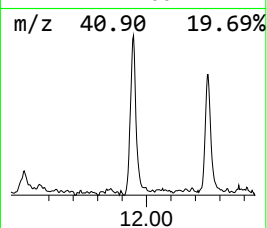
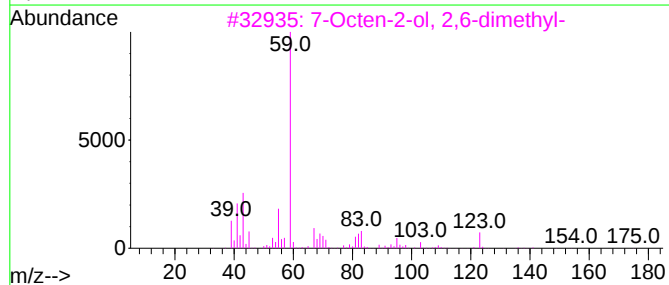
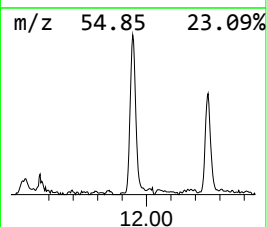
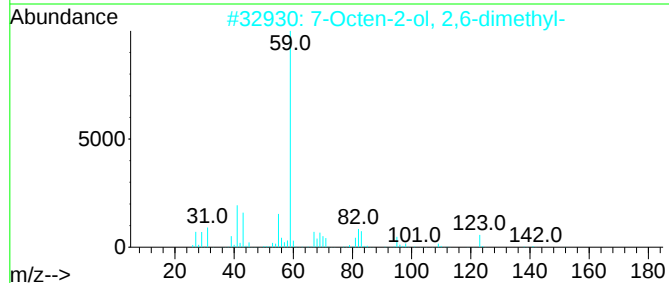
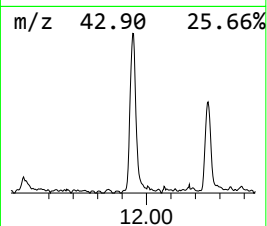
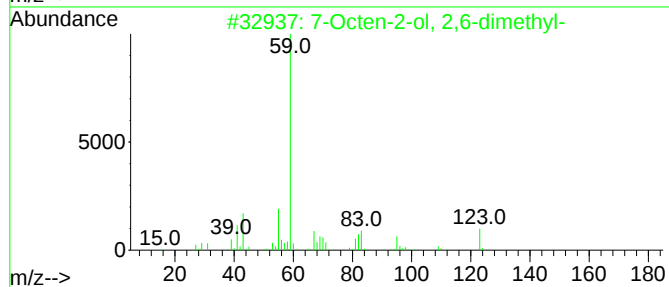
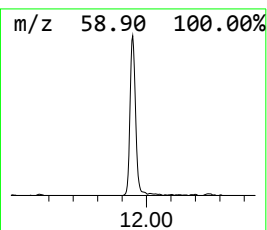
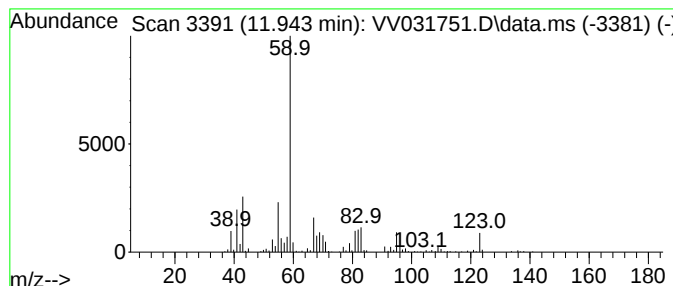
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.944	13.05 ug/L	270088	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	72
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
4			1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	72
5			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031751.D
Acq On : 25 Jul 2023 19:12
Operator : SY/MD
Sample : 03712-19
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y6

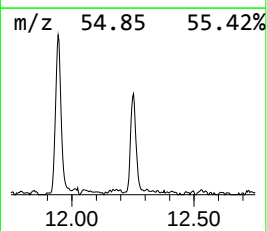
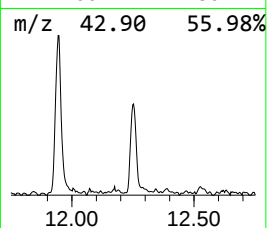
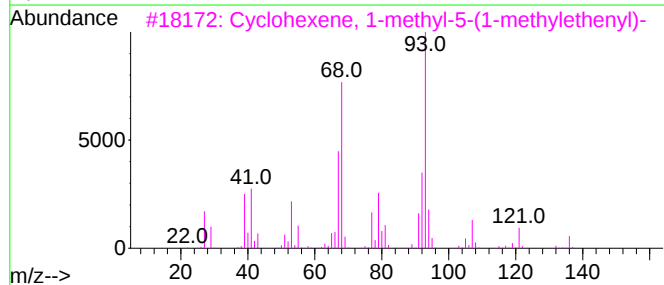
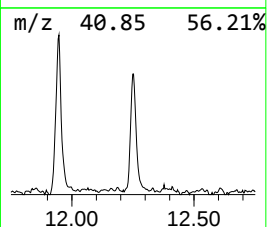
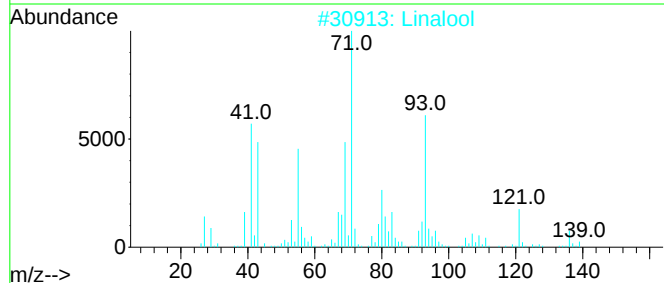
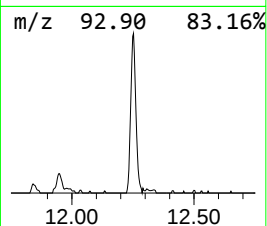
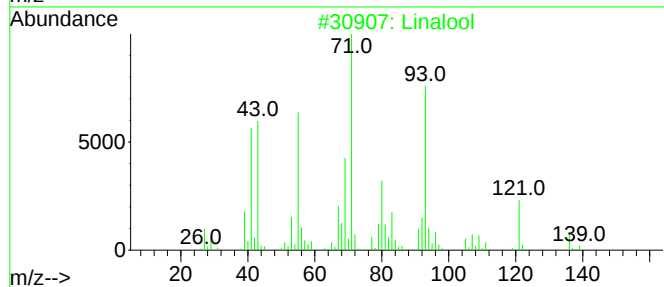
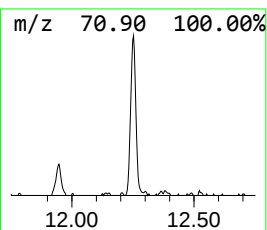
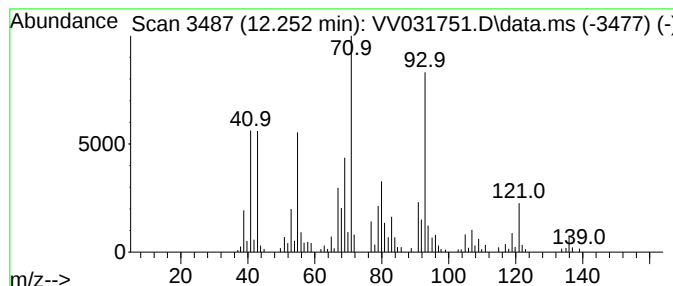
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Quant Title : VOC Analysis

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

Peak Number 6 Linalool Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.252	7.57 ug/L	156639	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	58
3			Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	55
4			1,6-Octadien-3-ol, 3,7-dimethyl-...	182	C11H18O2	000115-99-1	52
5			Linalyl acetate	196	C12H20O2	000115-95-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031751.D
Acq On : 25 Jul 2023 19:12
Operator : SY/MD
Sample : 03712-19
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y6

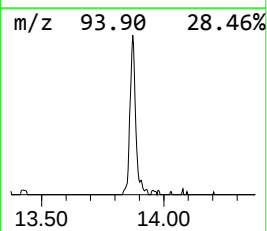
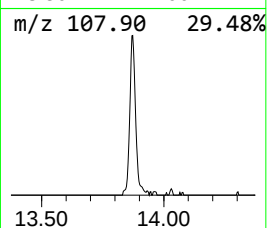
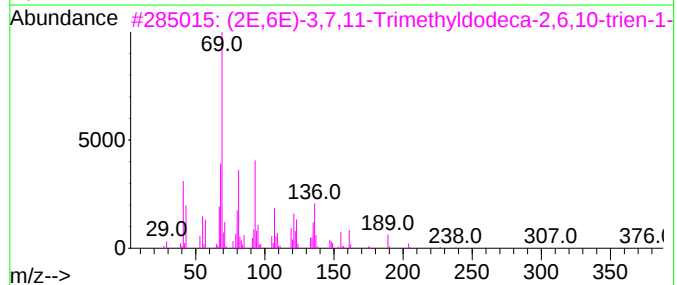
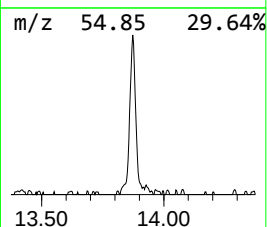
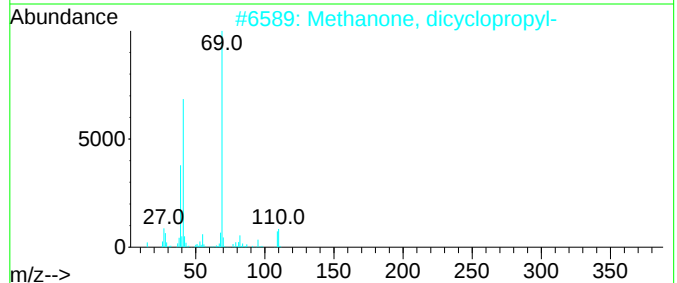
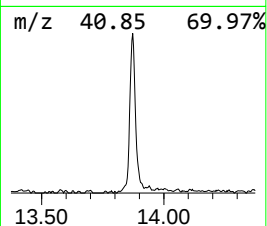
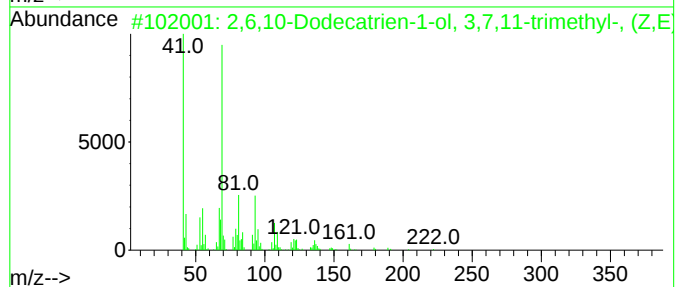
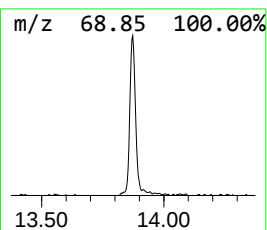
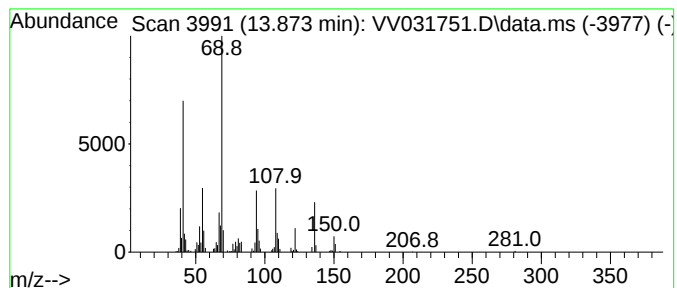
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Quant Title : VOC Analysis

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	9.22 ug/L	190933	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	43		
2	Methanone, dicyclopentyl-	110	C7H10O	001121-37-5	43		
3	(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	42		
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	40		
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	38		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031751.D
Acq On : 25 Jul 2023 19:12
Operator : SY/MD
Sample : 03712-19
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 24 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\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Hexanol, 2,5-...	2.571	7.6	ug/L	125561	1	5.539	826833	50.0
2-Butanone, 3,3...	6.510	8.0	ug/L	132712	1	5.539	826833	50.0
7-Octen-2-ol, 2...	11.944	13.1	ug/L	270088	3	11.191	1035000	50.0
Linalool	12.252	7.6	ug/L	156639	3	11.191	1035000	50.0
unknown-01	13.873	9.2	ug/L	190933	3	11.191	1035000	50.0