

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
 Data File : VV031743.D
 Acq On : 25 Jul 2023 16:04
 Operator : SY/MD
 Sample : 03712-07
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y0

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: VV031743.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	92	rVB	307287	333439	16.94%	2.149%
2	1.532	146	153	167	rVB	266344	317954	16.16%	2.050%
3	2.060	307	317	328	rBV	533540	773962	39.33%	4.989%
4	2.114	329	334	346	rVB	50059	76041	3.86%	0.490%
5	2.343	403	405	407	rBV3	1507	882	0.04%	0.006%
6	2.397	420	422	425	rBV3	1920	994	0.05%	0.006%
7	2.426	428	431	433	rBV3	1770	1212	0.06%	0.008%
8	2.571	464	476	496	rBV	62304	128585	6.53%	0.829%
9	2.838	556	559	563	rVB6	1720	1390	0.07%	0.009%
10	3.246	684	686	689	rBV4	1101	760	0.04%	0.005%
11	3.352	715	719	723	rBV6	949	939	0.05%	0.006%
12	3.503	762	766	769	rVB3	1649	1379	0.07%	0.009%
13	3.622	800	803	806	rBV5	1465	1100	0.06%	0.007%
14	3.796	847	857	894	rVV2	136918	448721	22.80%	2.893%
15	4.133	960	962	965	rVB3	1293	857	0.04%	0.006%
16	4.256	985	1000	1031	rBV	330551	861459	43.77%	5.553%
17	4.658	1122	1125	1131	rBV7	1191	1044	0.05%	0.007%
18	4.831	1177	1179	1182	rVB4	1487	795	0.04%	0.005%
19	4.963	1203	1220	1246	rBV2	740123	1967958	100.00%	12.686%
20	5.211	1295	1297	1302	rBV4	1433	1337	0.07%	0.009%
21	5.246	1306	1308	1315	rVB8	1181	1114	0.06%	0.007%
22	5.542	1387	1400	1423	rBV	430280	908931	46.19%	5.859%
23	5.828	1479	1489	1506	rVB3	57215	119844	6.09%	0.773%
24	5.995	1528	1541	1573	rBV	456860	950375	48.29%	6.126%
25	6.262	1620	1624	1626	rBV3	1699	1413	0.07%	0.009%
26	6.510	1688	1701	1716	rBV3	77863	166285	8.45%	1.072%
27	6.918	1816	1828	1855	rBV	200114	390166	19.83%	2.515%
28	7.095	1880	1883	1886	rBV4	1716	1520	0.08%	0.010%
29	7.111	1886	1888	1892	rVV5	1567	1239	0.06%	0.008%
30	7.249	1919	1931	1966	rBV	782357	1410109	71.65%	9.090%
31	7.407	1978	1980	1985	rBV6	2006	1668	0.08%	0.011%
32	7.558	2018	2027	2053	rBV	144133	261796	13.30%	1.688%
33	7.854	2115	2119	2120	rBV2	1950	1286	0.07%	0.008%
34	7.879	2122	2127	2132	rVB6	3433	4737	0.24%	0.031%
35	7.985	2153	2160	2163	rBV8	1212	1499	0.08%	0.010%
36	8.034	2163	2175	2217	rBV3	438693	988059	50.21%	6.369%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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Stop Thrs : 0

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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

37	8.622	2354	2358	2364	rVB9	1317	1599	0.08%	0.010%
38	8.715	2383	2387	2393	rBV8	1548	1688	0.09%	0.011%
39	8.789	2398	2410	2444	rBV	713041	1203516	61.16%	7.758%
40	8.989	2469	2472	2476	rVB4	1454	1277	0.06%	0.008%
41	9.046	2486	2490	2495	rBV6	1630	1533	0.08%	0.010%
42	9.069	2495	2497	2500	rBV4	1577	1186	0.06%	0.008%
43	9.349	2578	2584	2587	rBV5	1302	1105	0.06%	0.007%
44	9.397	2596	2599	2604	rVB4	1631	1295	0.07%	0.008%
45	9.426	2604	2608	2609	rBV2	1504	983	0.05%	0.006%
46	9.493	2624	2629	2630	rBV5	1262	1008	0.05%	0.006%
47	9.683	2682	2688	2691	rBV5	1279	1390	0.07%	0.009%
48	9.725	2695	2701	2711	rVB10	3046	4322	0.22%	0.028%
49	9.899	2741	2755	2759	rBV10	4715	8402	0.43%	0.054%
50	9.972	2775	2778	2782	rVB3	1056	794	0.04%	0.005%
51	10.059	2800	2805	2809	rBV6	1340	992	0.05%	0.006%
52	10.159	2823	2836	2860	rBV	532784	862103	43.81%	5.557%
53	10.329	2881	2889	2895	rBV9	3870	4219	0.21%	0.027%
54	10.365	2896	2900	2904	rVV4	1839	1347	0.07%	0.009%
55	10.413	2911	2915	2923	rVB7	2284	2786	0.14%	0.018%
56	10.474	2930	2934	2936	rBV3	994	861	0.04%	0.006%
57	10.570	2952	2964	2974	rVV3	4373	7594	0.39%	0.049%
58	10.661	2988	2992	2993	rBV3	1281	812	0.04%	0.005%
59	10.718	2999	3010	3019	rVB3	3633	6950	0.35%	0.045%
60	10.805	3029	3037	3040	rBV8	1695	2149	0.11%	0.014%
61	11.001	3092	3098	3101	rVV6	3099	3646	0.19%	0.024%
62	11.030	3103	3107	3114	rVB6	4577	6196	0.31%	0.040%
63	11.133	3129	3139	3147	rBV5	24695	40065	2.04%	0.258%
64	11.191	3147	3157	3177	rVB	693456	1084457	55.11%	6.991%
65	11.300	3186	3191	3198	rVB7	6508	8824	0.45%	0.057%
66	11.423	3224	3229	3233	rVB3	1204	969	0.05%	0.006%
67	11.458	3236	3240	3241	rBV3	1321	780	0.04%	0.005%
68	11.497	3243	3252	3260	rBV5	11287	22426	1.14%	0.145%
69	11.567	3262	3274	3293	rVB	828886	1297632	65.94%	8.365%
70	11.689	3310	3312	3319	rVB6	1225	873	0.04%	0.006%
71	11.828	3350	3355	3356	rBV4	1695	1272	0.06%	0.008%
72	11.844	3356	3360	3369	rVB7	4764	6537	0.33%	0.042%
73	11.943	3378	3391	3408	rBV	169514	271683	13.81%	1.751%
74	12.191	3465	3468	3477	rVB9	3855	4792	0.24%	0.031%
75	12.252	3477	3487	3499	rBV2	117901	182648	9.28%	1.177%
76	12.837	3666	3669	3673	rVV5	1050	839	0.04%	0.005%

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

77	12.886	3681	3684	3688	rBV5	1402	1046	0.05%	0.007%
78	13.001	3716	3720	3721	rBV3	1518	1237	0.06%	0.008%
79	13.040	3728	3732	3733	rBV3	2939	1481	0.08%	0.010%
80	13.223	3778	3789	3795	rBV3	4613	9325	0.47%	0.060%
81	13.387	3836	3840	3841	rBV4	3942	2754	0.14%	0.018%
82	13.422	3848	3851	3853	rBV4	5270	3713	0.19%	0.024%
83	13.583	3897	3901	3903	rBV4	2210	1690	0.09%	0.011%
84	13.648	3917	3921	3924	rBV5	1202	801	0.04%	0.005%
85	13.689	3924	3934	3947	rBV5	16078	26424	1.34%	0.170%
86	13.873	3976	3991	4012	rBV2	139890	236646	12.02%	1.525%
87	14.101	4059	4062	4067	rVV6	2590	2166	0.11%	0.014%
88	14.197	4090	4092	4095	rVB4	2325	1150	0.06%	0.007%
89	14.220	4095	4099	4102	rBV5	1385	1180	0.06%	0.008%
90	14.265	4109	4113	4115	rBV2	1194	901	0.05%	0.006%
91	14.352	4138	4140	4143	rBV4	1711	1037	0.05%	0.007%
92	14.390	4146	4152	4159	rBV9	3150	4758	0.24%	0.031%
93	14.567	4205	4207	4212	rVB6	1472	1061	0.05%	0.007%
94	14.593	4212	4215	4218	rBV3	1477	1387	0.07%	0.009%
95	15.059	4352	4360	4369	rBV9	14684	23338	1.19%	0.150%
96	15.229	4411	4413	4416	rBV4	1422	912	0.05%	0.006%
97	15.496	4493	4496	4498	rBV3	1360	962	0.05%	0.006%
98	15.535	4505	4508	4510	rBV3	1814	1016	0.05%	0.007%
99	15.644	4539	4542	4545	rBV5	2672	2206	0.11%	0.014%
100	15.680	4549	4553	4557	rVB6	1603	1549	0.08%	0.010%

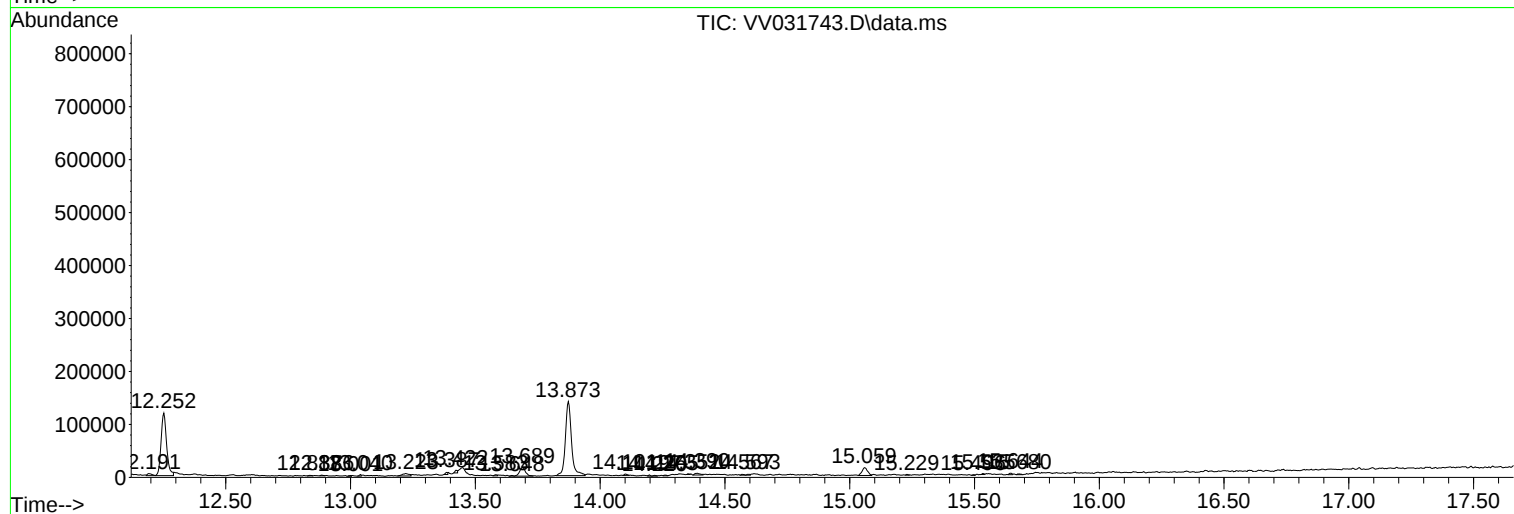
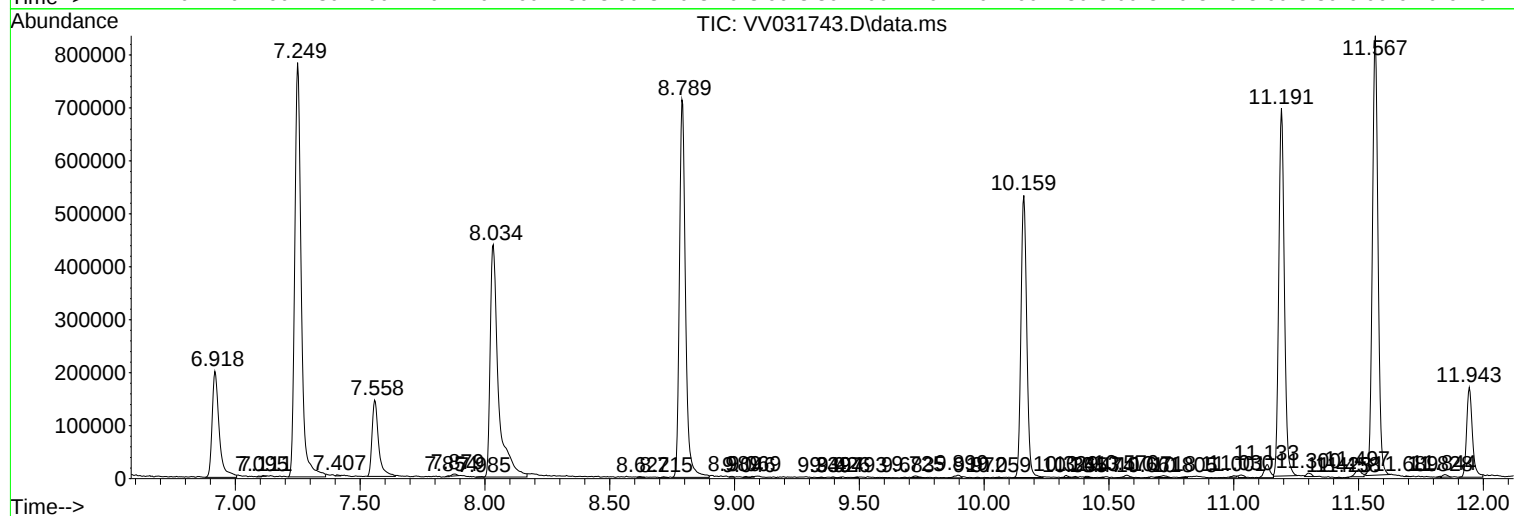
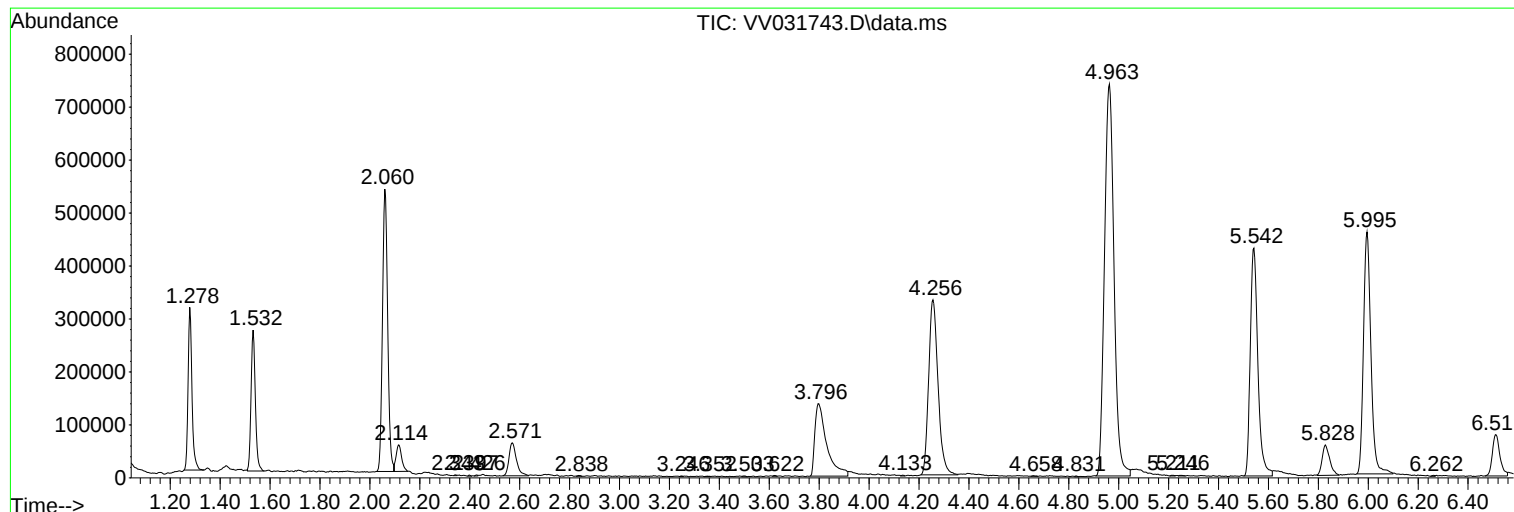
Sum of corrected areas: 15513139

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
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Instrument :
MSVOA_V
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BH2Y0

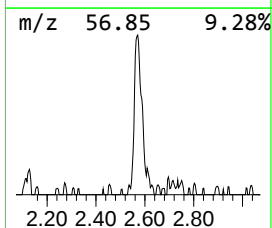
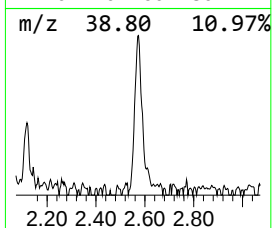
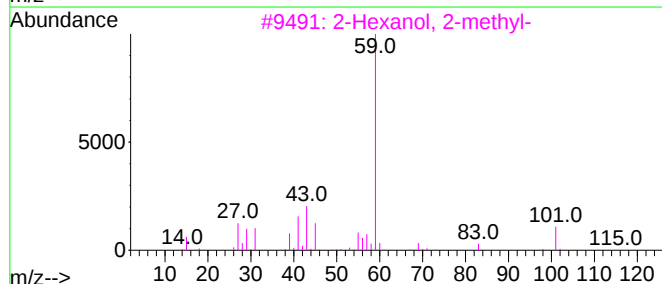
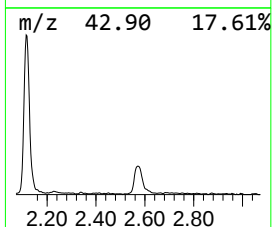
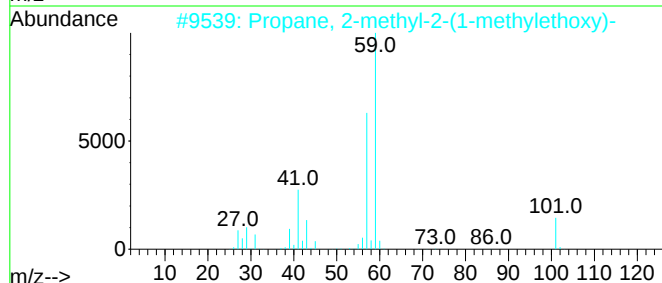
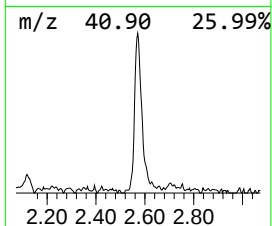
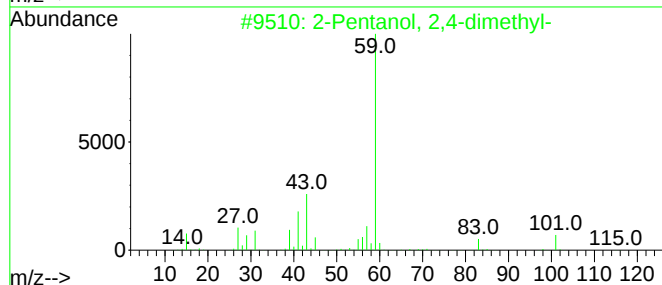
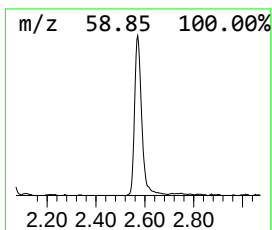
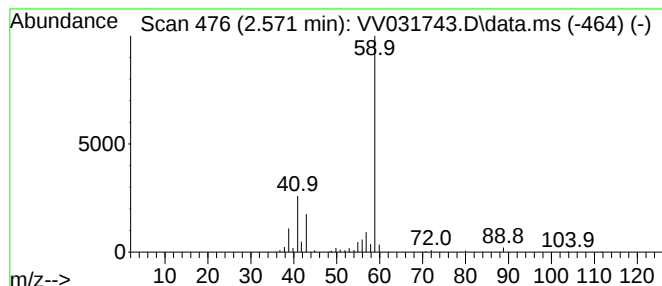
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Pentanol, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.571	7.07 ug/L	128585	1,4-Difluorobenzene	5.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2,4-dimethyl-			116	C7H16O	000625-06-9	64
2	Propane, 2-methyl-2-(1-methyleth...			116	C7H16O	017348-59-3	56
3	2-Hexanol, 2-methyl-			116	C7H16O	000625-23-0	56
4	1-Butanol, 3-methoxy-			104	C5H12O2	002517-43-3	43
5	2-Butanol, 3-methoxy-			104	C5H12O2	053778-72-6	43



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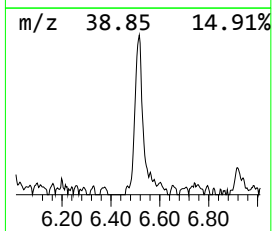
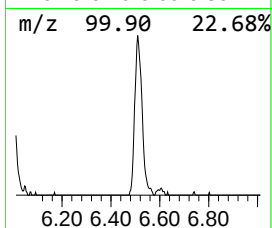
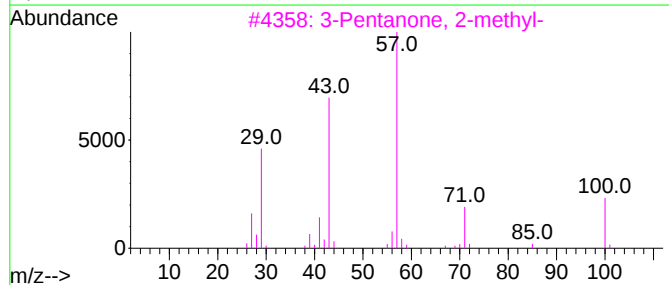
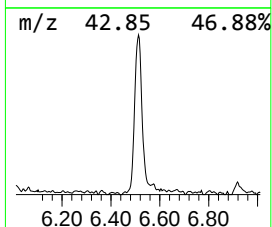
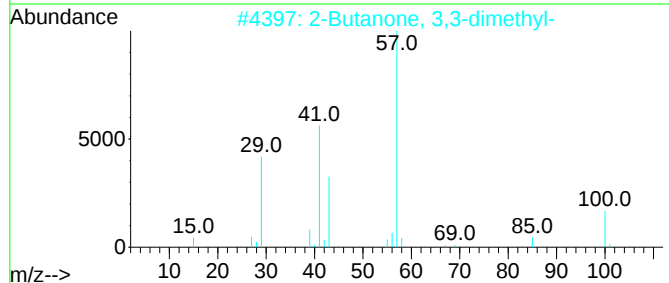
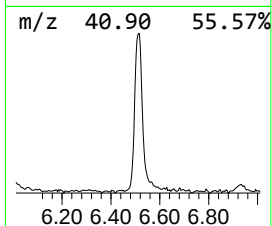
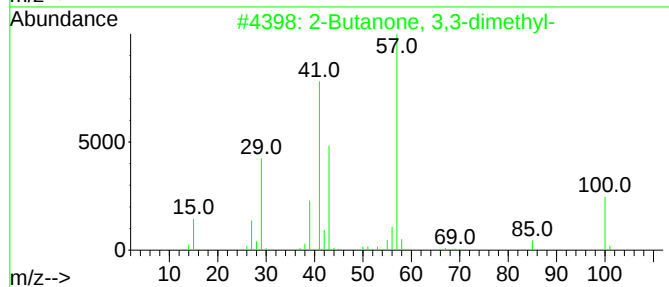
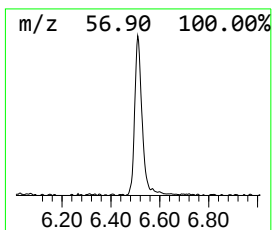
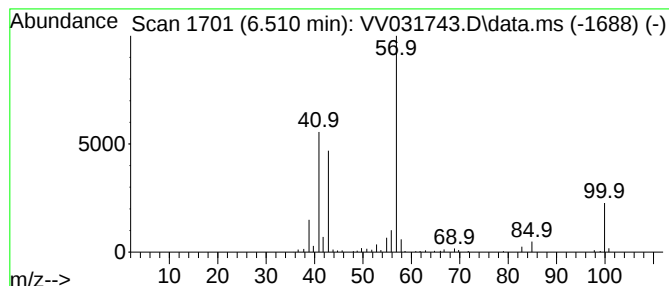
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.510	9.15 ug/L	166285	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	90	
2	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	83	
3	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	64	
4	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	64	
5	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	59	



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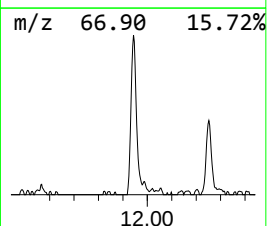
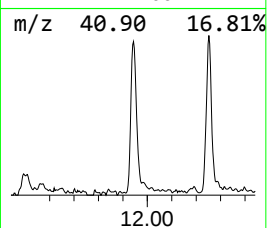
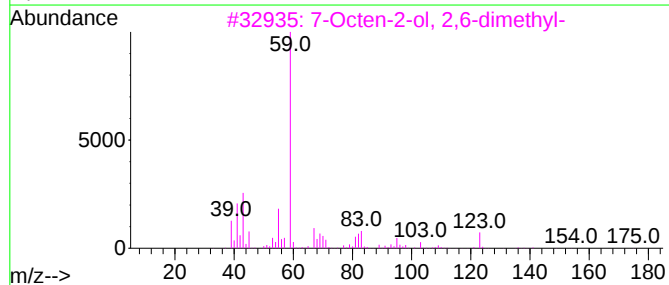
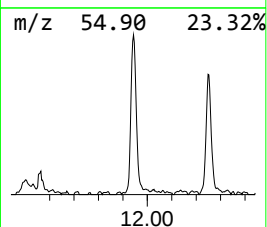
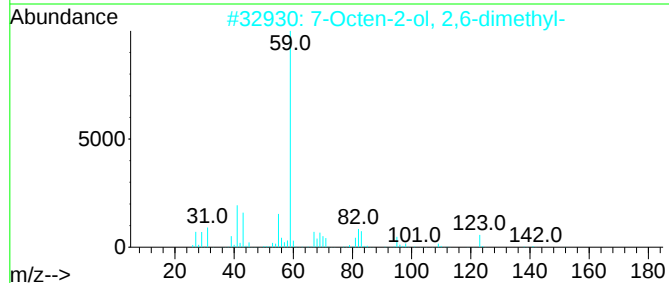
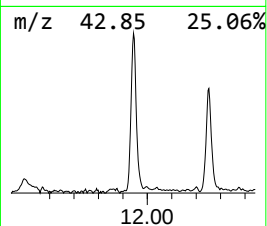
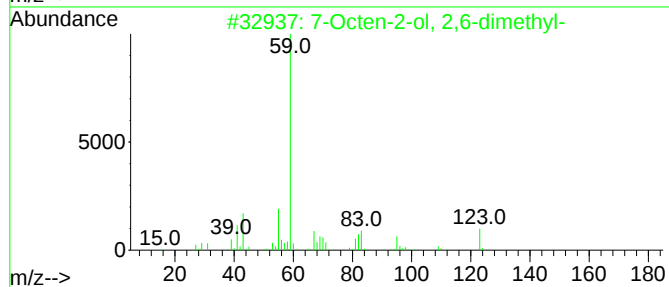
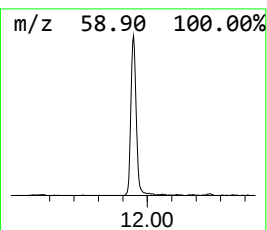
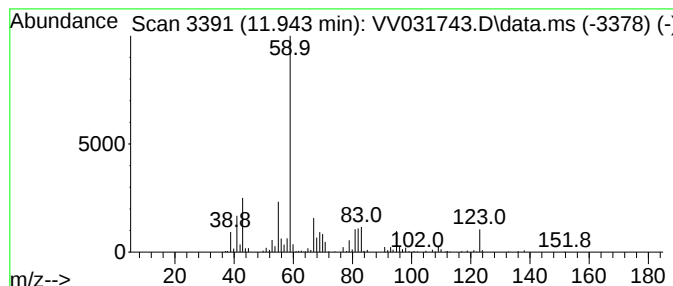
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Quant Title : VOC Analysis

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.
11.943	12.53 ug/L	271683	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	86
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			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	56
5			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031743.D
Acq On : 25 Jul 2023 16:04
Operator : SY/MD
Sample : 03712-07
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y0

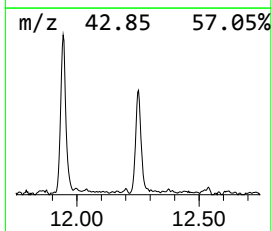
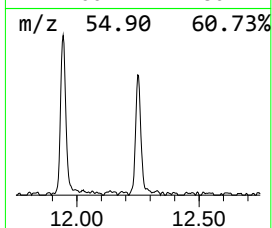
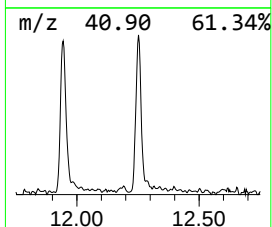
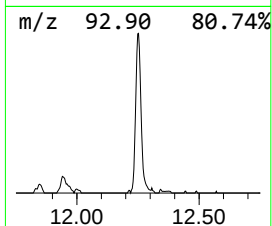
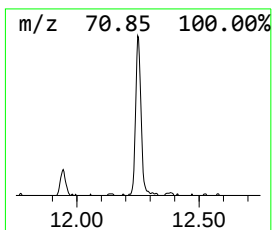
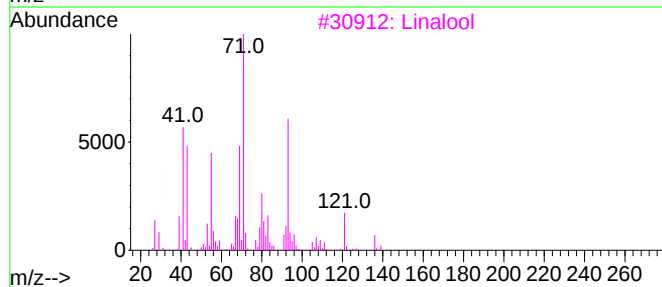
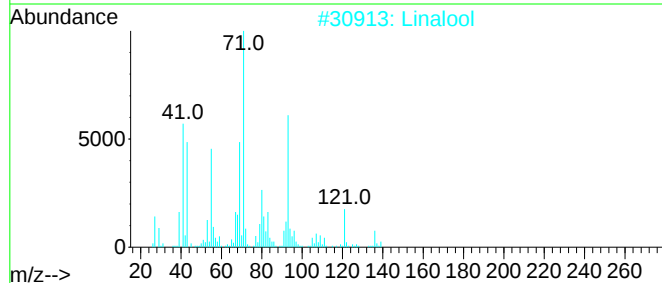
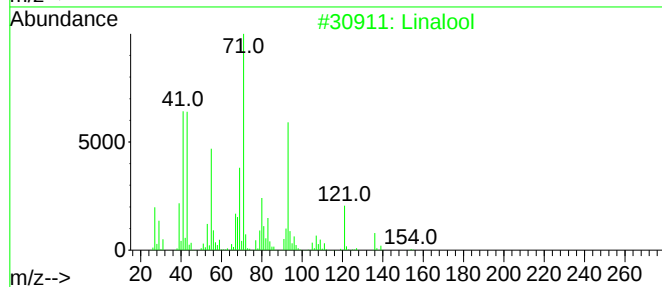
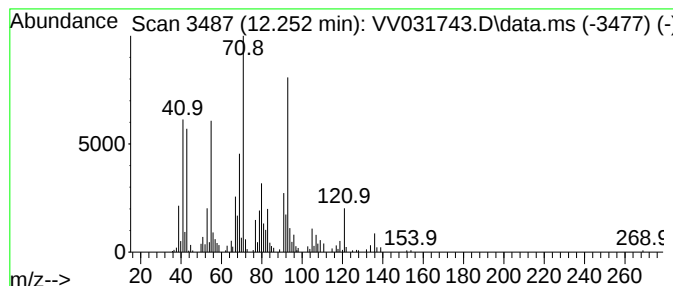
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Quant Title : VOC Analysis

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	8.42 ug/L	182648	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linalool	154	C10H18O	000078-70-6	94
2			Linalool	154	C10H18O	000078-70-6	68
3			Linalool	154	C10H18O	000078-70-6	68
4			Linalool	154	C10H18O	000078-70-6	64
5			3-Carene	136	C10H16	013466-78-9	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031743.D
Acq On : 25 Jul 2023 16:04
Operator : SY/MD
Sample : 03712-07
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y0

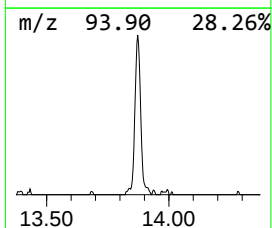
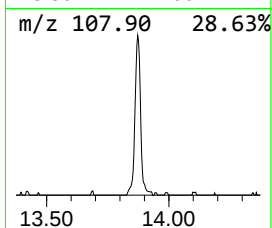
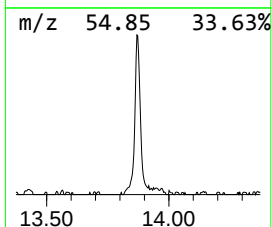
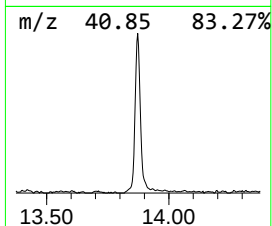
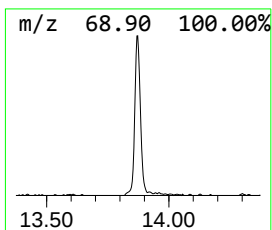
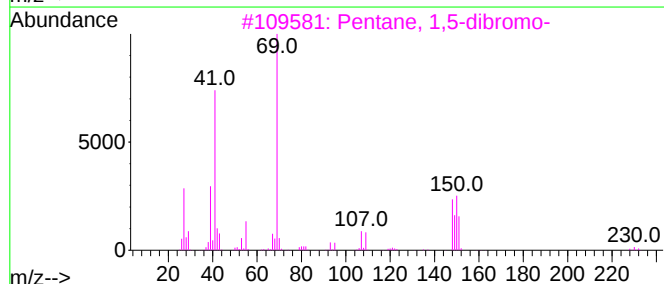
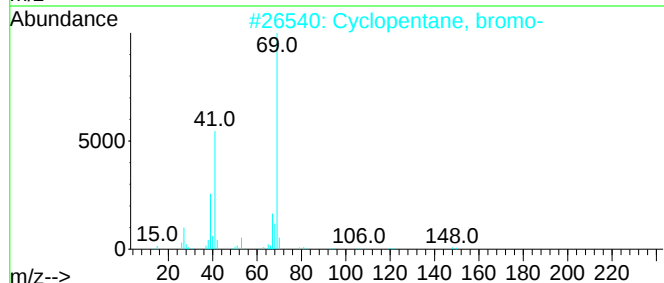
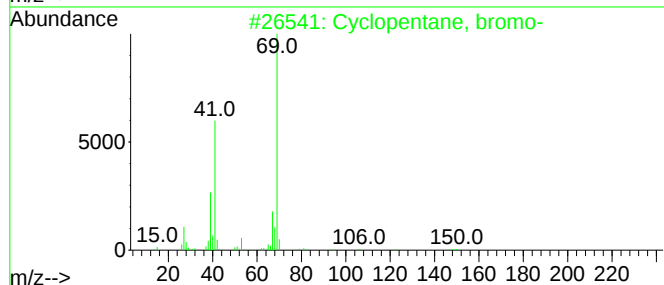
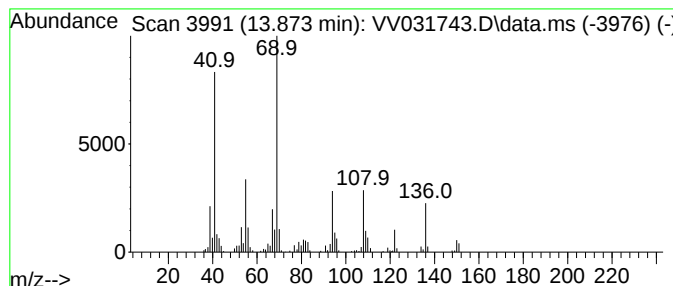
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	10.91 ug/L	236646	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	45
2			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	43
3			Pentane, 1,5-dibromo-	228	C5H10Br2	000111-24-0	38
4			Cyclopropanecarboxaldehyde, 2-me...	166	C11H18O	097231-35-1	38
5			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072523\
Data File : VV031743.D
Acq On : 25 Jul 2023 16:04
Operator : SY/MD
Sample : 03712-07
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y0

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-Pentanol, 2,4...	2.571	7.1	ug/L	128585	1	5.542	908931	50.0
2-Butanone, 3,3...	6.510	9.2	ug/L	166285	1	5.542	908931	50.0
7-Octen-2-ol, 2...	11.943	12.5	ug/L	271683	3	11.191	1084460	50.0
Linalool	12.252	8.4	ug/L	182648	3	11.191	1084460	50.0
unknown-01	13.873	10.9	ug/L	236646	3	11.191	1084460	50.0