

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
 Data File : VU048501.D
 Acq On : 10 May 2022 19:08
 Operator : SY/MD
 Sample : N2736-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEX4

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_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048501.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	96	rVB	113396	127584	12.55%	1.359%
2	1.912	171	178	193	rVB	86276	114472	11.26%	1.220%
3	2.568	369	382	394	rBV	213612	350986	34.53%	3.739%
4	2.890	480	482	485	rVB	316	157	0.02%	0.002%
5	2.954	500	502	505	rBV2	260	147	0.01%	0.002%
6	3.070	536	538	544	rBB	169	98	0.01%	0.001%
7	3.099	544	547	551	rBV2	242	170	0.02%	0.002%
8	3.253	593	595	600	rBV	268	175	0.02%	0.002%
9	3.272	600	601	604	rVB	284	120	0.01%	0.001%
10	3.391	635	638	641	rBV	162	135	0.01%	0.001%
11	3.436	648	652	654	rBV	280	223	0.02%	0.002%
12	3.498	668	671	675	rBV	213	238	0.02%	0.003%
13	3.539	681	684	688	rVB	368	279	0.03%	0.003%
14	3.575	688	695	700	rBV4	974	1420	0.14%	0.015%
15	3.620	707	709	713	rVB	199	96	0.01%	0.001%
16	3.768	754	755	760	rVB	270	126	0.01%	0.001%
17	3.797	761	764	768	rBV	193	207	0.02%	0.002%
18	3.819	768	771	773	rBV	172	109	0.01%	0.001%
19	3.867	784	786	789	rVB2	301	169	0.02%	0.002%
20	3.893	789	794	797	rBV2	335	350	0.03%	0.004%
21	3.938	804	808	809	rBV	181	121	0.01%	0.001%
22	3.977	818	820	823	rBV	199	167	0.02%	0.002%
23	3.996	824	826	829	rVV2	208	136	0.01%	0.001%
24	4.102	855	859	860	rBV	257	182	0.02%	0.002%
25	4.144	869	872	877	rVB	258	169	0.02%	0.002%
26	4.215	887	894	898	rBB	352	401	0.04%	0.004%
27	4.244	898	903	904	rBV	184	176	0.02%	0.002%
28	4.260	906	908	912	rVV	430	310	0.03%	0.003%
29	4.282	912	915	919	rVV	247	151	0.01%	0.002%
30	4.301	919	921	925	rVV2	168	113	0.01%	0.001%
31	4.324	925	928	934	rBV2	296	271	0.03%	0.003%
32	4.449	960	967	968	rBV3	578	652	0.06%	0.007%
33	4.475	973	975	979	rVB	172	103	0.01%	0.001%
34	4.543	994	996	997	rBV	269	132	0.01%	0.001%
35	4.620	1007	1020	1047	rBV	115779	281176	27.67%	2.996%
36	4.961	1123	1126	1128	rBV2	399	295	0.03%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

37	5.063	1143	1158	1180	rBV	192491	419586	41.28%	4.470%
38	5.192	1195	1198	1200	rBV2	460	284	0.03%	0.003%
39	5.227	1207	1209	1212	rVB	309	156	0.02%	0.002%
40	5.253	1213	1217	1220	rBV2	158	149	0.01%	0.002%
41	5.295	1226	1230	1231	rBV2	217	146	0.01%	0.002%
42	5.314	1235	1236	1240	rVB2	372	179	0.02%	0.002%
43	5.388	1254	1259	1261	rBV3	276	269	0.03%	0.003%
44	5.436	1272	1274	1278	rBV	137	136	0.01%	0.001%
45	5.459	1278	1281	1286	rVB2	293	294	0.03%	0.003%
46	5.488	1286	1290	1294	rBV	470	487	0.05%	0.005%
47	5.546	1304	1308	1313	rVB2	458	509	0.05%	0.005%
48	5.575	1314	1317	1318	rBV	239	156	0.02%	0.002%
49	5.616	1328	1330	1332	rBV	261	133	0.01%	0.001%
50	5.649	1337	1340	1343	rBV	200	178	0.02%	0.002%
51	5.726	1343	1364	1388	rBV2	368371	1016324	100.00%	10.828%
52	6.108	1480	1483	1487	rVV3	435	382	0.04%	0.004%
53	6.157	1487	1498	1508	rVV4	5070	10908	1.07%	0.116%
54	6.250	1513	1527	1550	rBV	337227	635879	62.57%	6.775%
55	6.372	1563	1565	1567	rBV	415	209	0.02%	0.002%
56	6.452	1587	1590	1593	rBV2	196	150	0.01%	0.002%
57	6.494	1599	1603	1604	rBV	651	392	0.04%	0.004%
58	6.610	1637	1639	1641	rBV	274	172	0.02%	0.002%
59	6.690	1647	1664	1682	rBV2	230703	449986	44.28%	4.794%
60	6.816	1701	1703	1706	rVB3	875	487	0.05%	0.005%
61	6.928	1734	1738	1741	rBV2	390	383	0.04%	0.004%
62	6.980	1752	1754	1756	rBV	317	172	0.02%	0.002%
63	7.005	1756	1762	1763	rBV3	1340	1151	0.11%	0.012%
64	7.047	1772	1775	1776	rBV3	198	109	0.01%	0.001%
65	7.163	1799	1811	1830	rVB	26697	53274	5.24%	0.568%
66	7.253	1837	1839	1845	rBV	265	315	0.03%	0.003%
67	7.311	1852	1857	1859	rBV2	388	406	0.04%	0.004%
68	7.343	1865	1867	1869	rBV	236	130	0.01%	0.001%
69	7.391	1879	1882	1886	rVV	385	274	0.03%	0.003%
70	7.449	1889	1900	1910	rBV7	4433	8101	0.80%	0.086%
71	7.565	1924	1936	1967	rBV	94472	199162	19.60%	2.122%
72	7.745	1990	1992	1996	rVB	573	311	0.03%	0.003%
73	7.767	1996	1999	2002	rBV2	301	222	0.02%	0.002%
74	7.899	2020	2040	2057	rBV	467839	819488	80.63%	8.731%
75	8.112	2104	2106	2108	rBV	190	97	0.01%	0.001%
76	8.179	2114	2127	2144	rBV2	68917	117015	11.51%	1.247%

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77	8.488	2210	2223	2239	rBV	121078	211762	20.84%	2.256%
78	8.632	2256	2268	2284	rBV	372029	667831	65.71%	7.115%
79	8.893	2343	2349	2357	rVB8	1612	2341	0.23%	0.025%
80	8.951	2364	2367	2375	rVB7	2166	2630	0.26%	0.028%
81	9.105	2404	2415	2425	rBV3	9878	17133	1.69%	0.183%
82	9.269	2454	2466	2478	rBV	196193	330412	32.51%	3.520%
83	9.417	2499	2512	2532	rBV	485201	834905	82.15%	8.895%
84	9.758	2609	2618	2632	rBV4	6299	13117	1.29%	0.140%
85	9.857	2646	2649	2651	rBV	453	321	0.03%	0.003%
86	9.970	2673	2684	2706	rVB5	42697	97943	9.64%	1.044%
87	10.076	2714	2717	2718	rBV2	902	477	0.05%	0.005%
88	10.201	2750	2756	2760	rBV3	1282	1570	0.15%	0.017%
89	10.362	2794	2806	2824	rBV2	172991	309708	30.47%	3.300%
90	10.755	2919	2928	2941	rVB	346079	548403	53.96%	5.843%
91	11.520	3163	3166	3167	rBV	754	465	0.05%	0.005%
92	11.812	3244	3257	3278	rBV	525697	853217	83.95%	9.090%
93	12.063	3325	3335	3354	rBV2	34423	67153	6.61%	0.715%
94	12.192	3364	3375	3393	rVB	491669	798444	78.56%	8.507%
95	12.494	3466	3469	3471	rBV3	438	245	0.02%	0.003%
96	12.832	3570	3574	3582	rVB4	763	1073	0.11%	0.011%
97	12.867	3582	3585	3586	rBV	638	334	0.03%	0.004%
98	13.452	3765	3767	3769	rBV2	533	243	0.02%	0.003%
99	13.742	3848	3857	3863	rBV7	3585	5329	0.52%	0.057%
100	13.848	3885	3890	3895	rBV4	884	924	0.09%	0.010%

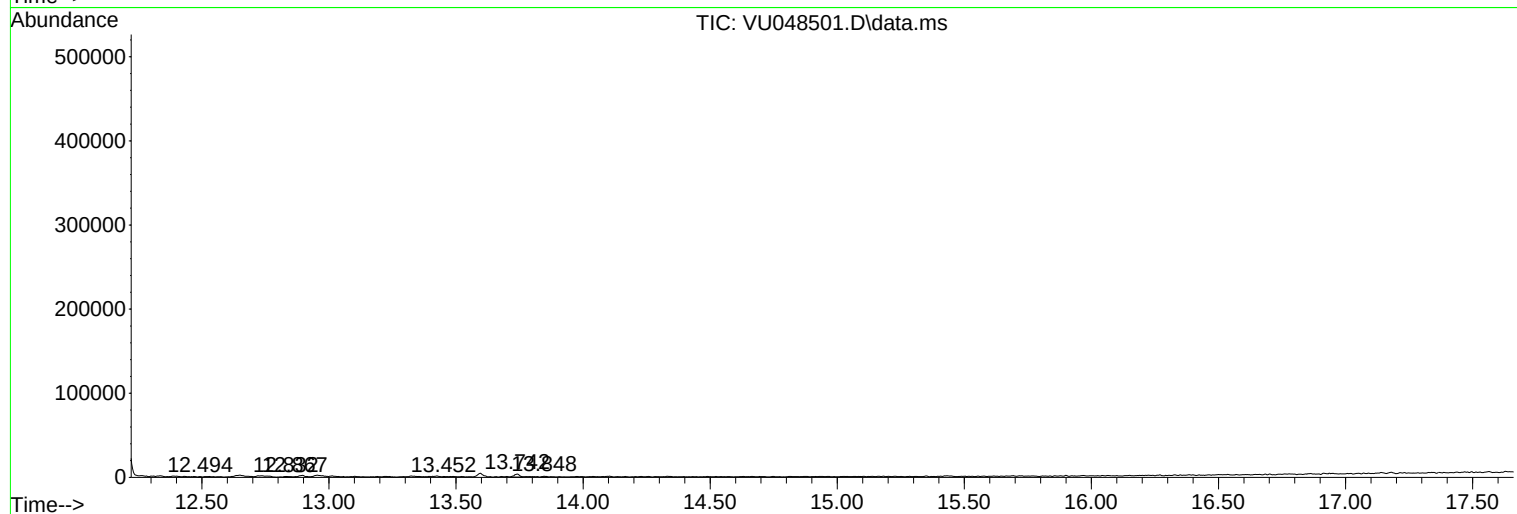
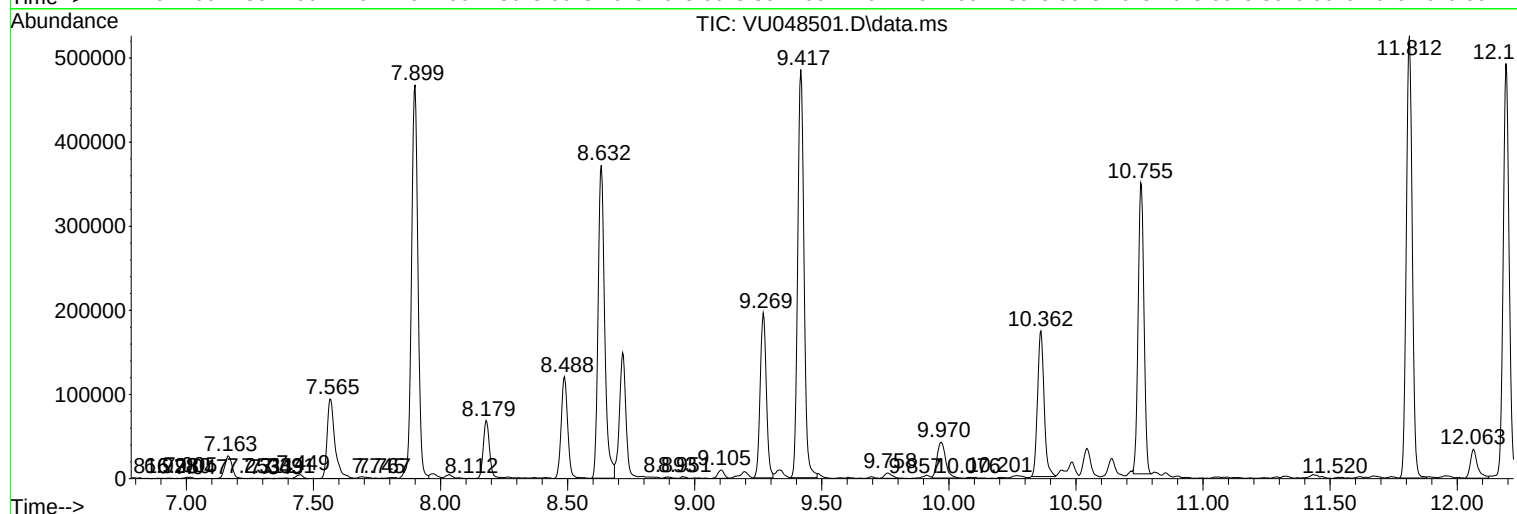
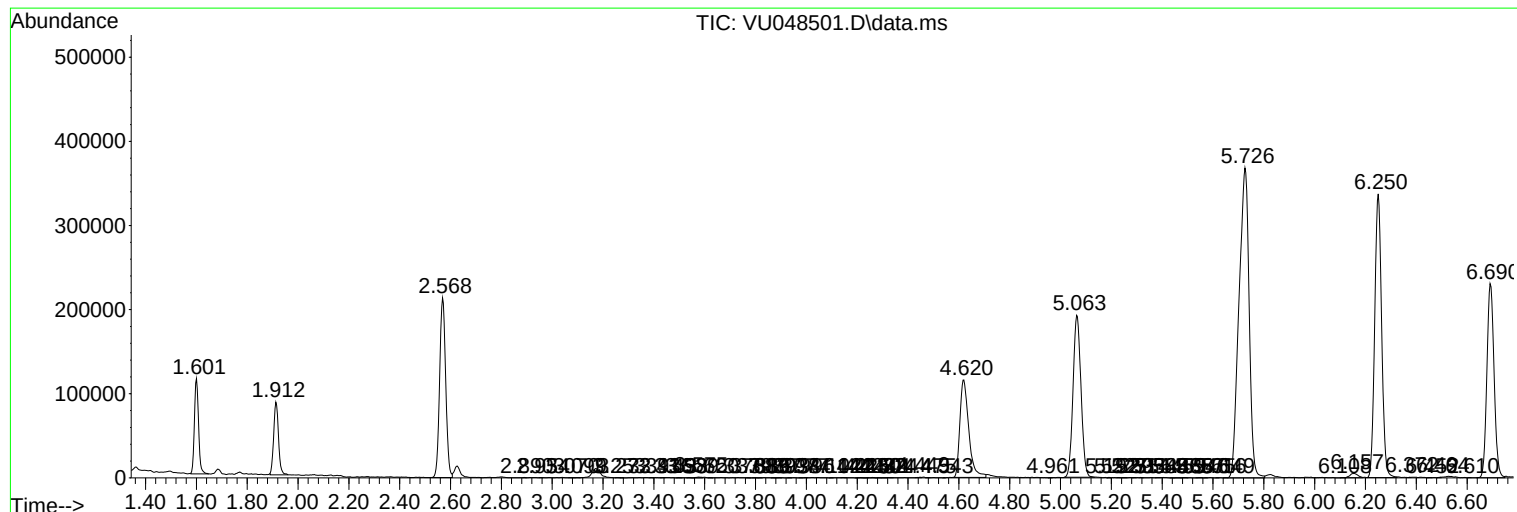
Sum of corrected areas: 9385957

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Instrument :
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ClientSampleId :
EXEX4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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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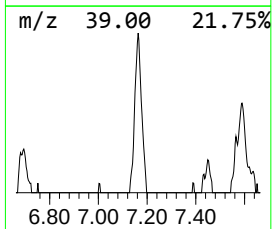
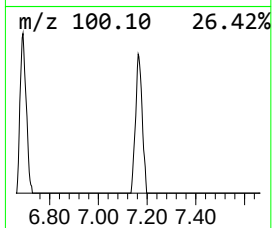
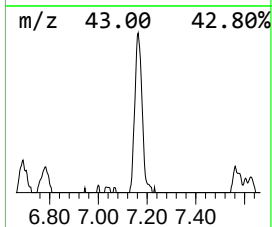
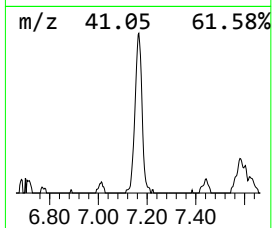
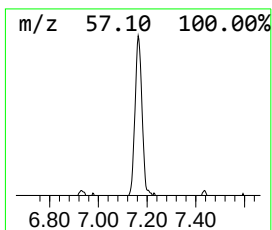
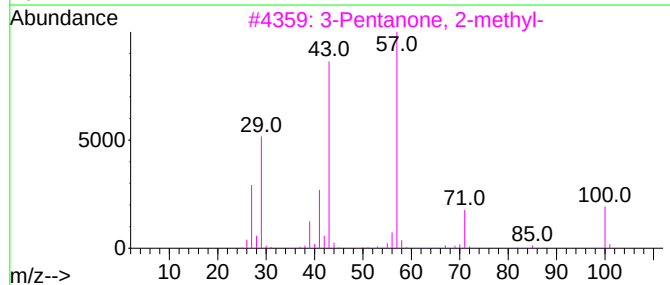
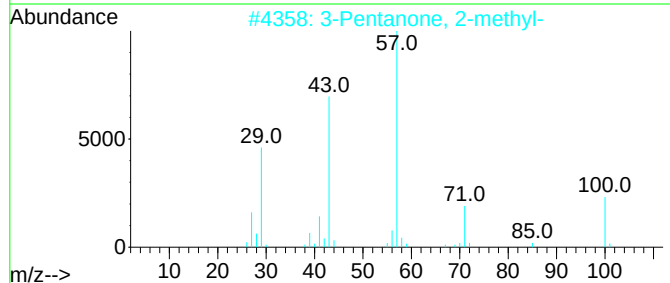
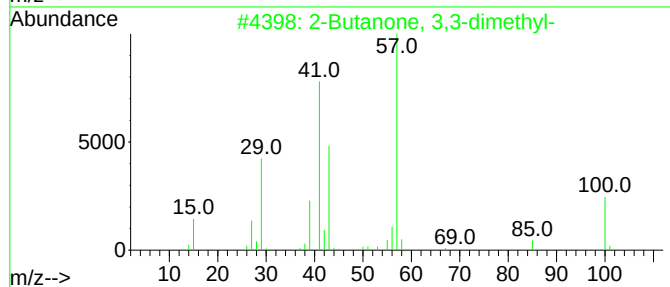
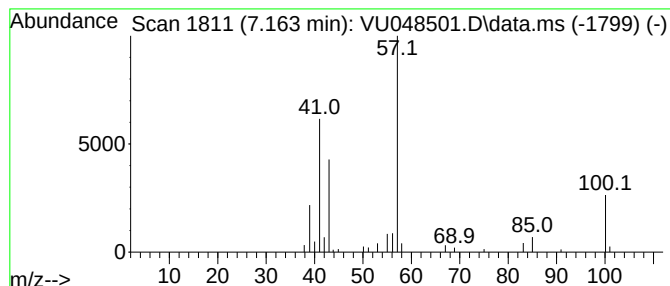
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.163	4.19 ug/L	53274	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	87	
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64	
3	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59	
4	trans-1-Ethoxy-1-butene	100	C6H12O	1000139-43-9	58	
5	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	43	



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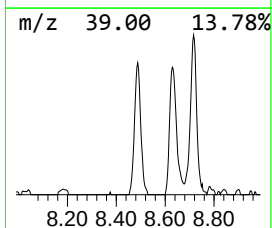
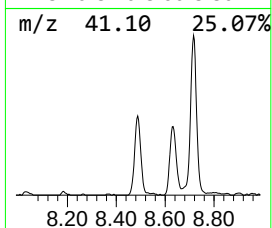
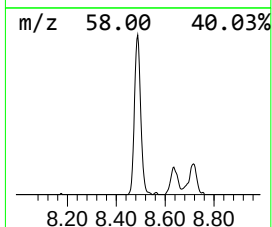
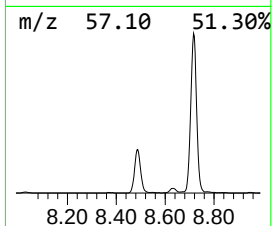
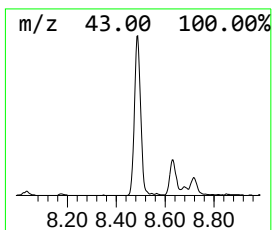
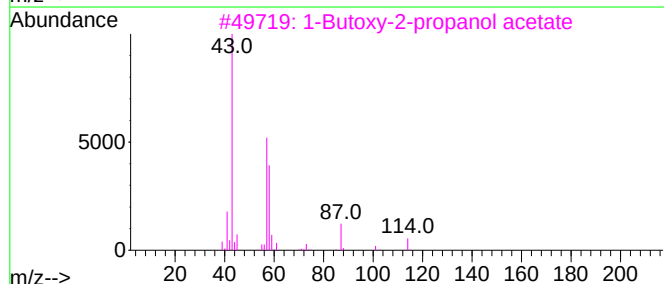
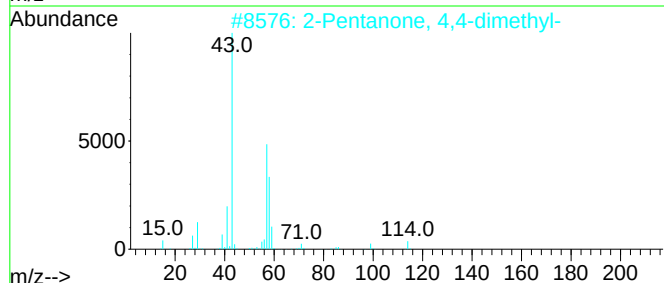
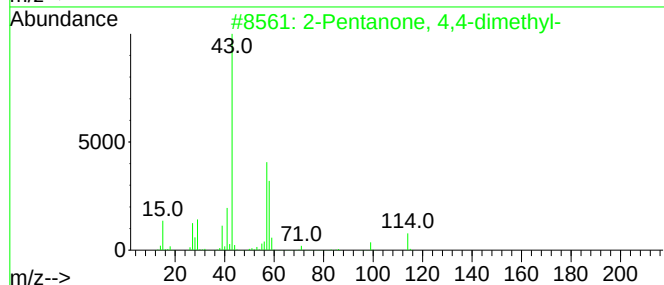
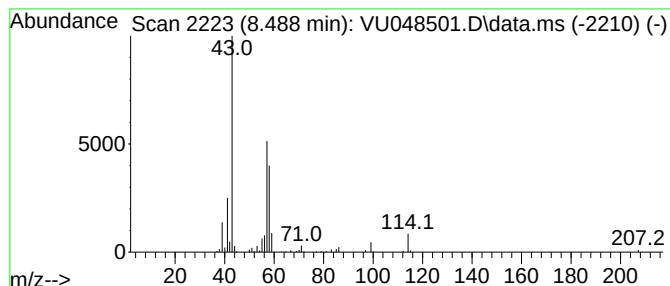
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.488	12.68 ug/L	211762	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	91		
2	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	78		
3	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	72		
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64		
5	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	59		



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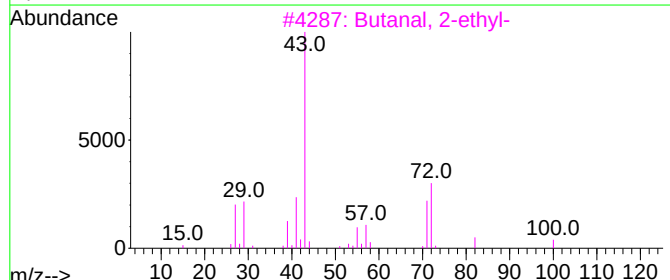
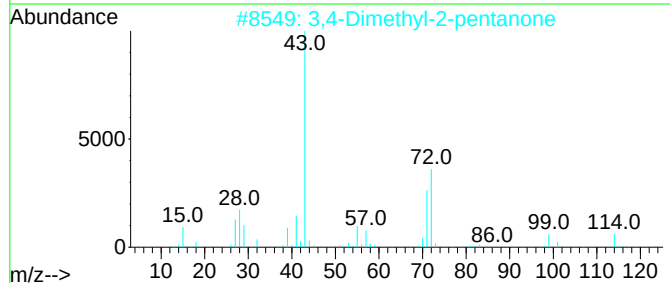
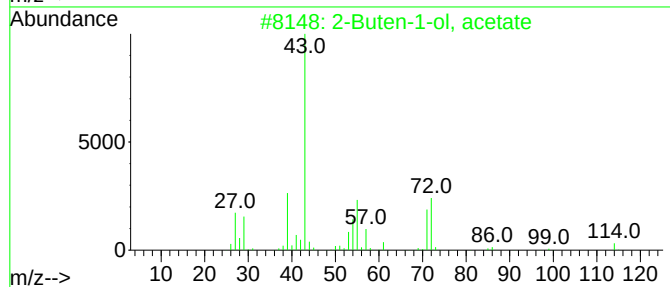
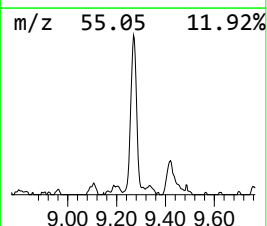
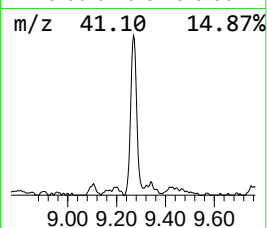
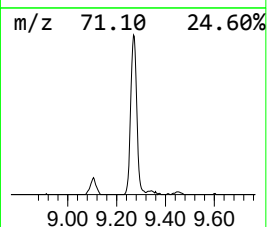
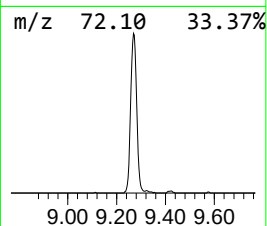
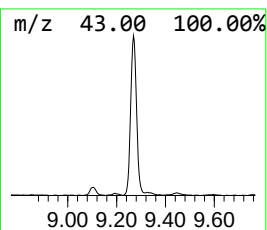
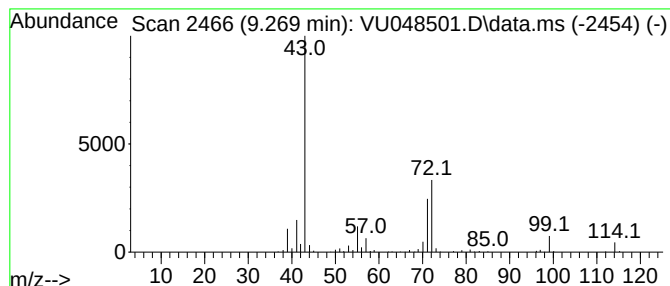
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 2-Buten-1-ol, acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.269	19.79 ug/L	330412	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	59
2			3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	59
3			Butanal, 2-ethyl-	100	C6H12O	000097-96-1	59
4			2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	53
5			2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048501.D
Acq On : 10 May 2022 19:08
Operator : SY/MD
Sample : N2736-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEX4

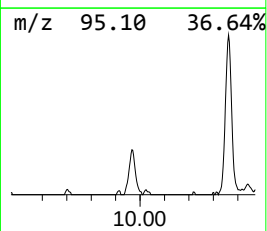
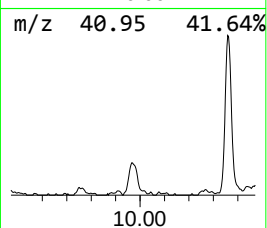
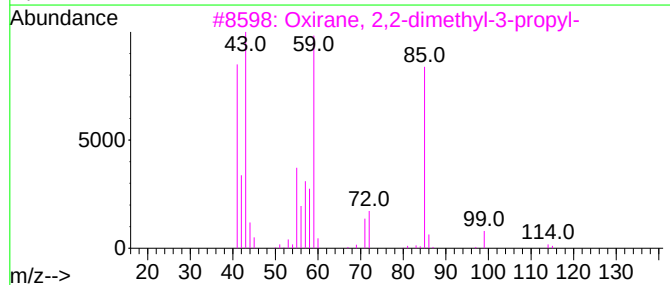
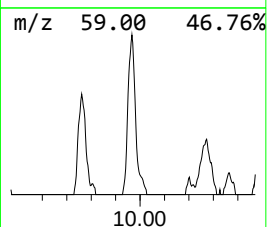
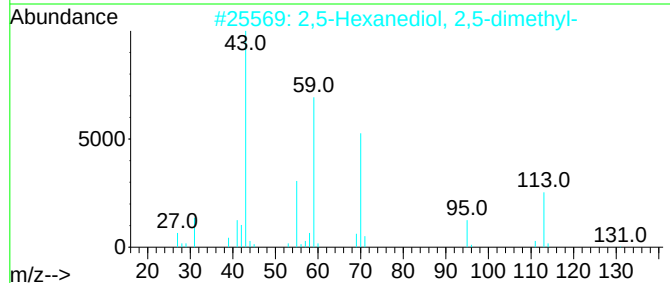
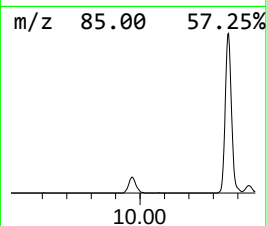
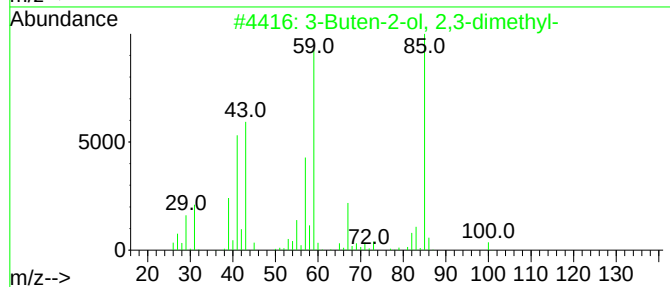
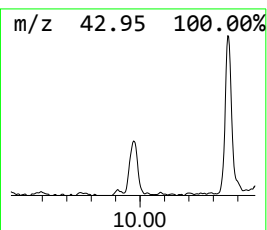
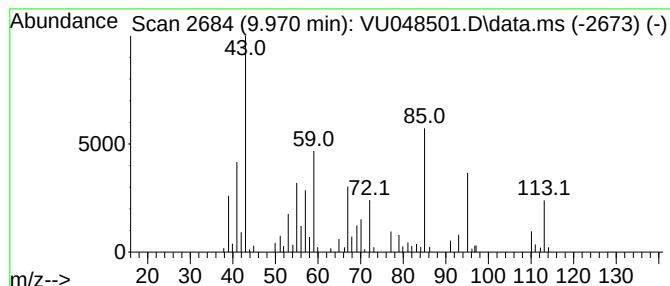
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.970	5.87 ug/L	97943	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	32
2			2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	27
3			Oxirane, 2,2-dimethyl-3-propyl-	114	C7H14O	017612-35-0	25
4			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	22
5			2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048501.D
Acq On : 10 May 2022 19:08
Operator : SY/MD
Sample : N2736-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEX4

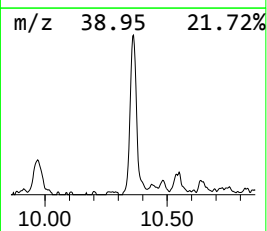
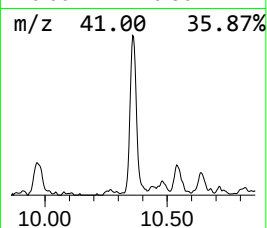
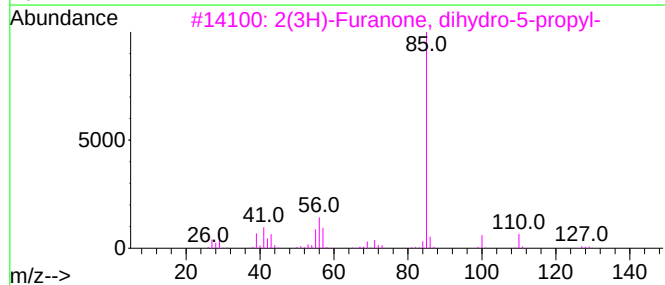
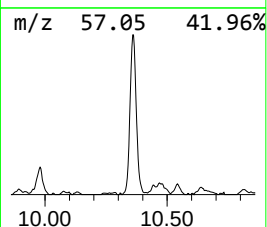
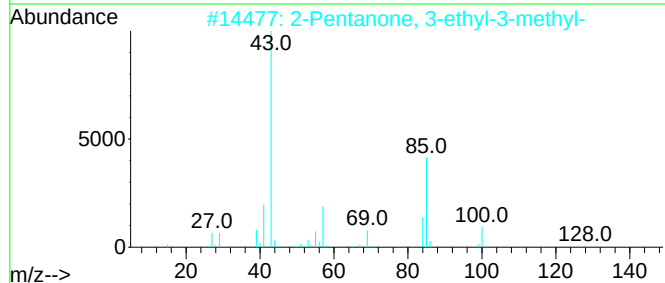
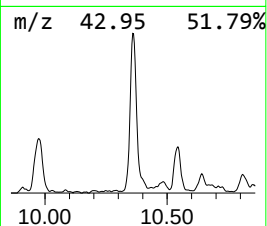
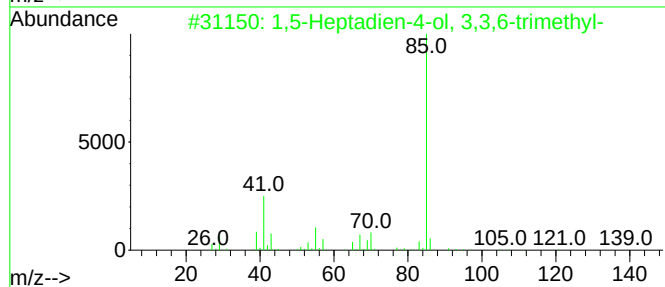
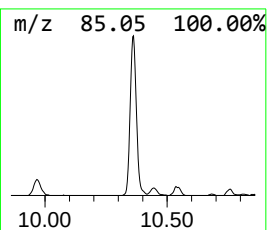
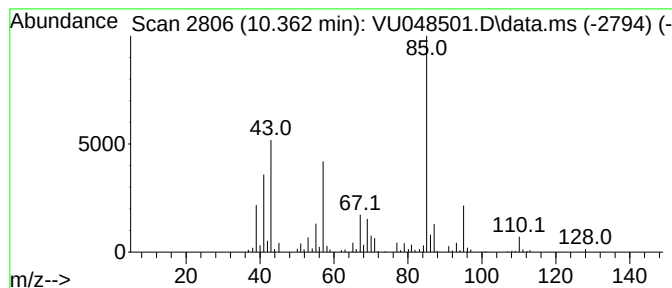
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 1,5-Heptadien-4-ol, 3,3,6-t... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.362	18.55 ug/L	309708	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Heptadien-4-ol, 3,3,6-trimet...	154	C10H18O	027644-04-8	59
2			2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	58
3			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	52
4			2-Methylbutanoic anhydride	186	C10H18O3	001468-39-9	50
5			Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048501.D
Acq On : 10 May 2022 19:08
Operator : SY/MD
Sample : N2736-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEX4

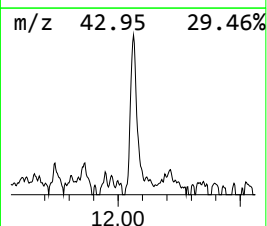
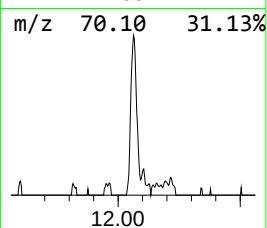
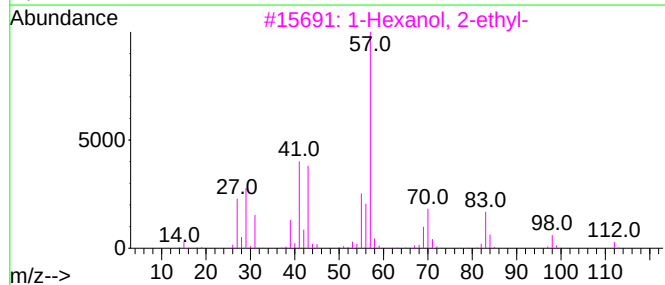
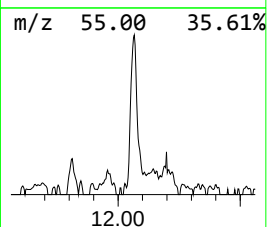
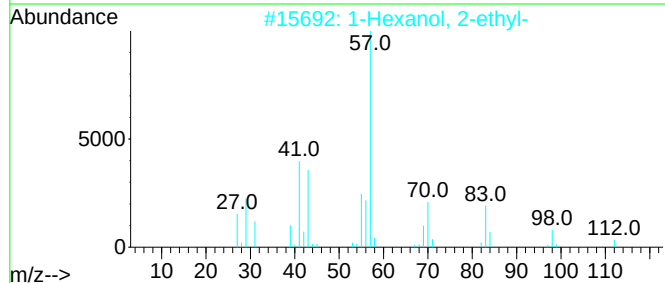
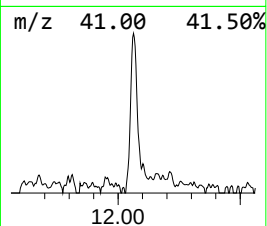
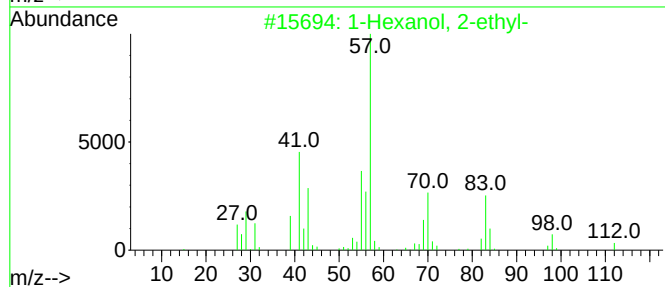
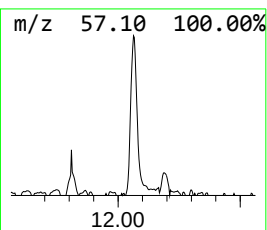
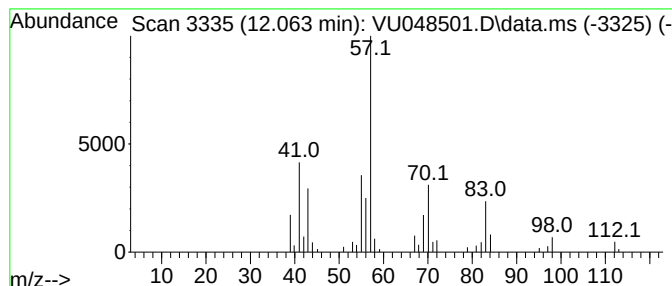
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	3.94 ug/L	67153	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048501.D
Acq On : 10 May 2022 19:08
Operator : SY/MD
Sample : N2736-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEX4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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-Butanone, 3,3...	7.163	4.2	ug/L	53274	1	6.250	635879	50.0
2-Pentanone, 4,...	8.488	12.7	ug/L	211762	2	9.417	834905	50.0
2-Buten-1-ol, a...	9.269	19.8	ug/L	330412	2	9.417	834905	50.0
unknown-01	9.970	5.9	ug/L	97943	2	9.417	834905	50.0
1,5-Heptadien-4...	10.362	18.6	ug/L	309708	2	9.417	834905	50.0
1-Hexanol, 2-et...	12.063	3.9	ug/L	67153	3	11.812	853217	50.0