

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058955.D
 Acq On : 23 May 2024 17:56
 Operator : MD/SY
 Sample : P2484-20
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHA21

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\SFAMULM052324WMA.M
 Title : VOC Analysis

Signal : TIC: VU058955.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	87	95	110	rVB	120334	138224	16.12%	2.026%
2	1.682	114	122	153	rBV	157064	217126	25.32%	3.182%
3	1.911	184	193	208	rVB	95700	128227	14.95%	1.879%
4	2.563	381	396	407	rBV	167634	278098	32.43%	4.076%
5	2.628	407	416	440	rVB	80335	165288	19.27%	2.422%
6	2.846	481	484	489	rVB3	301	216	0.03%	0.003%
7	2.914	501	505	508	rBV2	418	354	0.04%	0.005%
8	2.972	520	523	526	rVB2	371	239	0.03%	0.004%
9	2.997	526	531	534	rBV2	300	276	0.03%	0.004%
10	3.046	534	546	553	rVV6	2536	4809	0.56%	0.070%
11	3.190	575	591	619	rBV4	8710	28853	3.36%	0.423%
12	3.290	619	622	627	rBV	562	295	0.03%	0.004%
13	3.329	630	634	637	rBV2	332	294	0.03%	0.004%
14	3.441	666	669	675	rVV	242	222	0.03%	0.003%
15	3.512	688	691	699	rVB2	238	275	0.03%	0.004%
16	3.550	699	703	708	rBV2	262	254	0.03%	0.004%
17	3.586	712	714	717	rVV2	347	196	0.02%	0.003%
18	3.608	717	721	727	rVB2	224	254	0.03%	0.004%
19	3.689	742	746	750	rBV2	265	208	0.02%	0.003%
20	3.901	808	812	816	rVB	310	270	0.03%	0.004%
21	3.939	816	824	827	rBV	237	348	0.04%	0.005%
22	4.271	924	927	938	rBV2	221	246	0.03%	0.004%
23	4.457	966	985	999	rBV7	5102	17042	1.99%	0.250%
24	4.557	1014	1016	1022	rVB	837	505	0.06%	0.007%
25	4.618	1022	1035	1059	rBV	81682	221198	25.79%	3.242%
26	4.853	1105	1108	1111	rBV3	611	428	0.05%	0.006%
27	5.055	1155	1171	1197	rBV	152254	341794	39.86%	5.009%
28	5.287	1240	1243	1246	rBV2	385	303	0.04%	0.004%
29	5.357	1262	1265	1268	rVV2	265	235	0.03%	0.003%
30	5.396	1275	1277	1280	rVV2	310	195	0.02%	0.003%
31	5.721	1358	1378	1413	rBV2	315823	857545	100.00%	12.568%
32	6.132	1503	1506	1510	rVB2	387	272	0.03%	0.004%
33	6.184	1517	1522	1527	rBV2	281	241	0.03%	0.004%
34	6.245	1527	1541	1570	rBV	209962	417750	48.71%	6.122%
35	6.434	1598	1600	1604	rVB3	455	243	0.03%	0.004%
36	6.544	1621	1634	1657	rBV7	14420	46351	5.41%	0.679%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
 Title : VOC Analysis

37	6.685	1664	1678	1698	rBV	191393	385687	44.98%	5.652%
38	6.885	1735	1740	1750	rBV7	1564	2625	0.31%	0.038%
39	7.016	1778	1781	1784	rVB3	446	265	0.03%	0.004%
40	7.081	1798	1801	1806	rBV2	271	300	0.03%	0.004%
41	7.123	1806	1814	1817	rBV3	1697	2577	0.30%	0.038%
42	7.473	1916	1923	1926	rBV	207	212	0.02%	0.003%
43	7.560	1939	1950	1975	rBV	102375	187552	21.87%	2.749%
44	7.695	1988	1992	1994	rBV2	368	320	0.04%	0.005%
45	7.804	2022	2026	2030	rVB3	365	301	0.04%	0.004%
46	7.894	2041	2054	2076	rBV	362974	643191	75.00%	9.426%
47	8.177	2130	2142	2158	rBV	70983	125385	14.62%	1.838%
48	8.470	2221	2233	2242	rVB3	2709	4849	0.57%	0.071%
49	8.553	2250	2259	2264	rBV4	863	924	0.11%	0.014%
50	8.627	2271	2282	2323	rBV	219641	454286	52.98%	6.658%
51	8.788	2327	2332	2339	rVB7	3233	4709	0.55%	0.069%
52	8.907	2366	2369	2371	rBV2	369	241	0.03%	0.004%
53	9.216	2461	2465	2468	rBV	253	262	0.03%	0.004%
54	9.412	2514	2526	2549	rBV	324487	552485	64.43%	8.097%
55	9.557	2569	2571	2573	rBV3	461	278	0.03%	0.004%
56	9.656	2594	2602	2604	rBV2	737	1001	0.12%	0.015%
57	9.968	2696	2699	2705	rBV2	209	197	0.02%	0.003%
58	10.065	2726	2729	2733	rVB2	273	214	0.02%	0.003%
59	10.100	2733	2740	2743	rBV2	440	458	0.05%	0.007%
60	10.139	2744	2752	2755	rBV4	1330	1616	0.19%	0.024%
61	10.238	2774	2783	2798	rBV2	14940	27845	3.25%	0.408%
62	10.348	2814	2817	2821	rVB4	533	317	0.04%	0.005%
63	10.650	2907	2911	2915	rBV2	395	336	0.04%	0.005%
64	10.749	2928	2942	2965	rBV	271502	447371	52.17%	6.556%
65	10.884	2974	2984	2997	rBV6	4500	7221	0.84%	0.106%
66	10.958	3004	3007	3015	rVB2	253	245	0.03%	0.004%
67	11.023	3024	3027	3032	rBV2	182	208	0.02%	0.003%
68	11.068	3038	3041	3045	rBV	249	216	0.03%	0.003%
69	11.093	3046	3049	3051	rBV	374	244	0.03%	0.004%
70	11.126	3056	3059	3061	rBV	311	196	0.02%	0.003%
71	11.267	3100	3103	3110	rVB2	408	397	0.05%	0.006%
72	11.450	3156	3160	3163	rBV2	349	249	0.03%	0.004%
73	11.470	3163	3166	3170	rVV2	498	381	0.04%	0.006%
74	11.582	3196	3201	3203	rBV2	432	330	0.04%	0.005%
75	11.746	3248	3252	3257	rVV	984	881	0.10%	0.013%
76	11.807	3260	3271	3294	rBV	314335	517923	60.40%	7.590%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	11.971	3318	3322	3326	rBV3	351	449	0.05%	0.007%
78	12.077	3345	3355	3363	rBV5	3649	8080	0.94%	0.118%
79	12.187	3377	3389	3414	rBV	331785	562710	65.62%	8.247%
80	12.296	3421	3423	3426	rBV2	309	212	0.02%	0.003%
81	12.399	3451	3455	3459	rVB2	323	288	0.03%	0.004%
82	12.643	3526	3531	3533	rBV2	356	241	0.03%	0.004%
83	12.701	3546	3549	3552	rBV	387	263	0.03%	0.004%
84	12.769	3565	3570	3580	rVB3	1224	1920	0.22%	0.028%
85	12.836	3587	3591	3593	rBV	349	241	0.03%	0.004%
86	12.852	3593	3596	3600	rVV2	207	211	0.02%	0.003%
87	13.081	3664	3667	3672	rBV2	235	236	0.03%	0.003%
88	13.228	3710	3713	3720	rVB3	818	845	0.10%	0.012%
89	13.495	3792	3796	3799	rVB	407	278	0.03%	0.004%
90	13.608	3828	3831	3836	rBV	437	357	0.04%	0.005%
91	13.849	3902	3906	3910	rBV5	793	720	0.08%	0.011%
92	13.907	3921	3924	3927	rBV	343	234	0.03%	0.003%
93	14.116	3983	3989	3991	rBV2	563	528	0.06%	0.008%
94	14.466	4095	4098	4102	rBV	420	415	0.05%	0.006%
95	14.508	4108	4111	4114	rBV2	320	222	0.03%	0.003%
96	14.547	4119	4123	4125	rBV	411	308	0.04%	0.005%
97	14.569	4125	4130	4134	rBV4	510	548	0.06%	0.008%
98	14.675	4159	4163	4166	rBV2	439	398	0.05%	0.006%
99	14.958	4248	4251	4253	rBV2	596	373	0.04%	0.005%
100	16.000	4573	4575	4577	rBV2	497	318	0.04%	0.005%

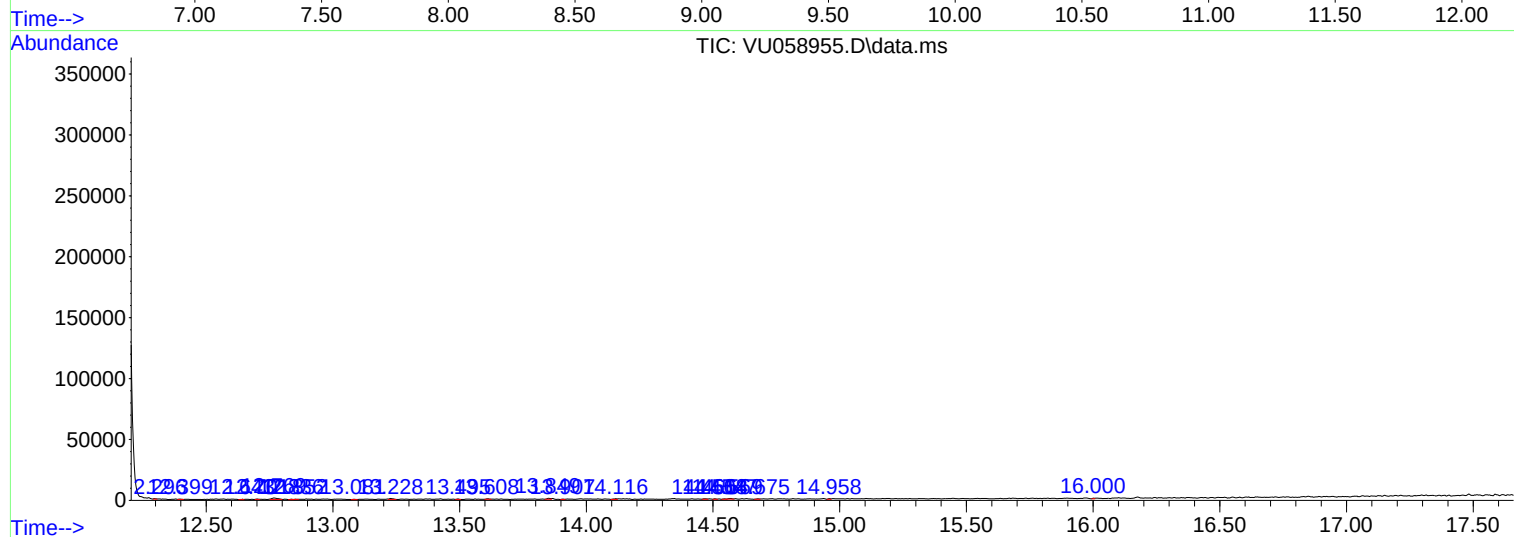
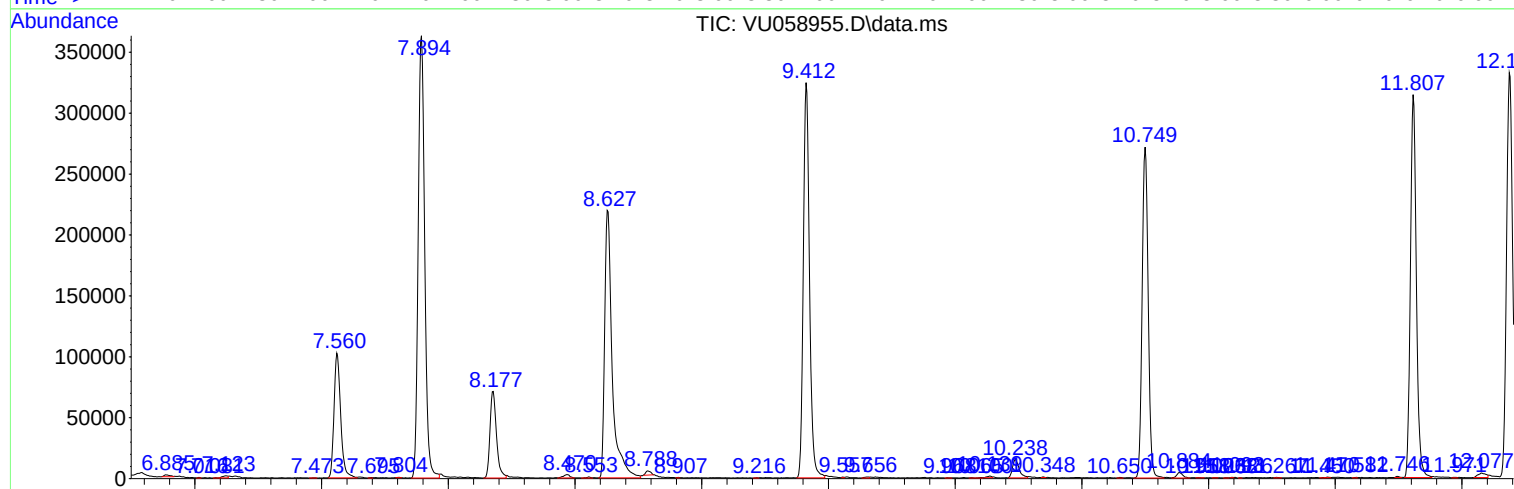
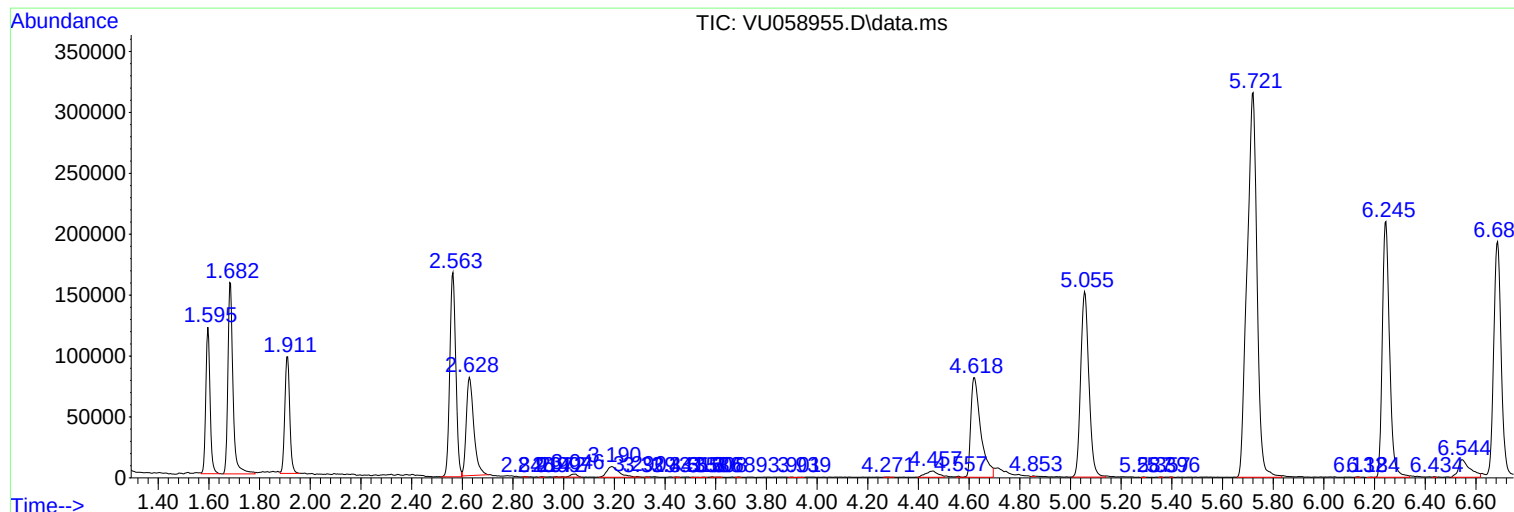
Sum of corrected areas: 6823364

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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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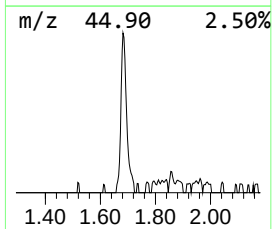
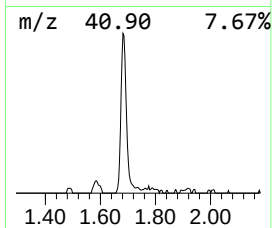
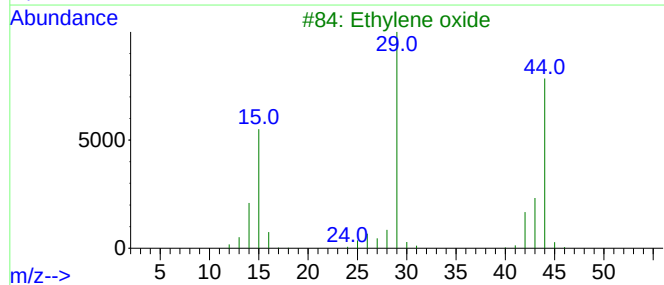
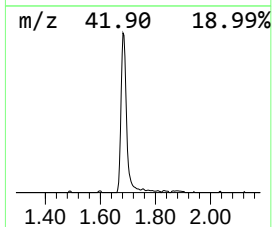
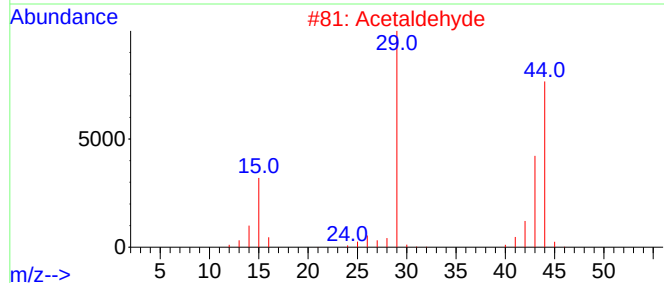
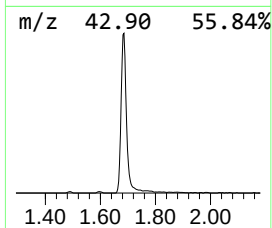
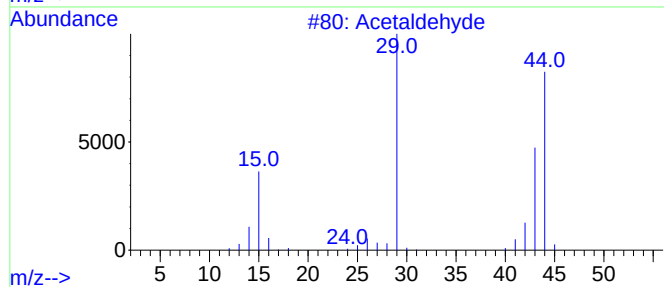
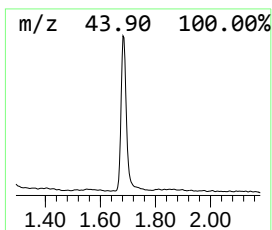
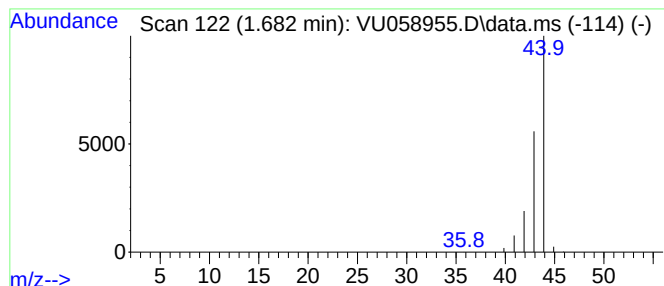
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.682	25.99 ug/L	217126	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Acetaldehyde	44	C2H4O	000075-07-0	9
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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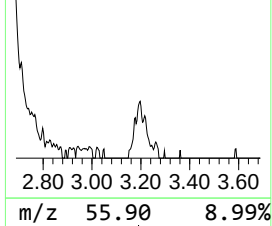
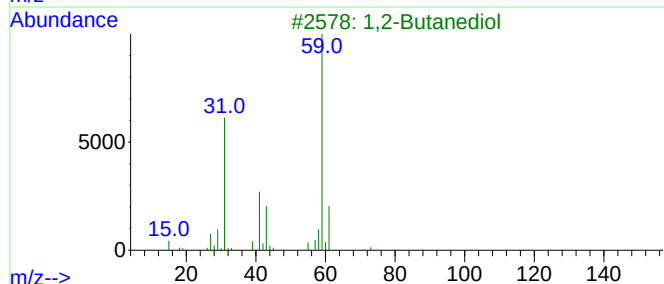
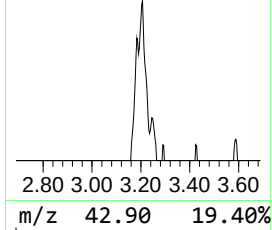
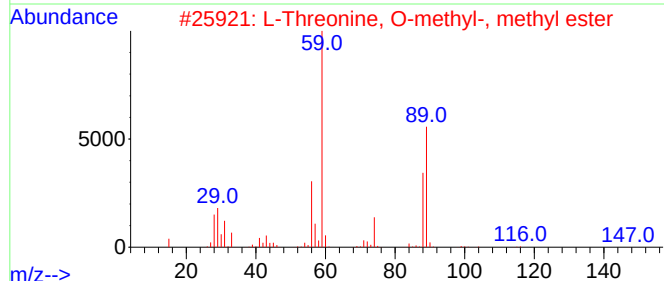
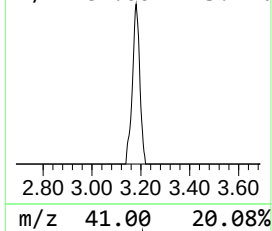
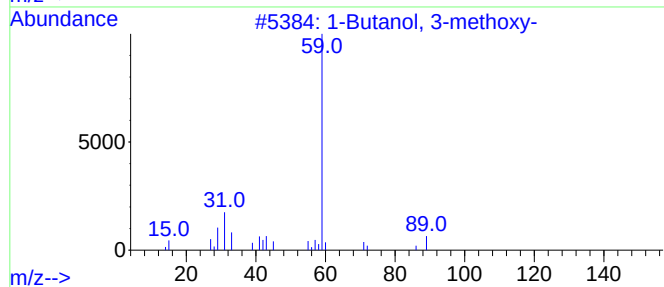
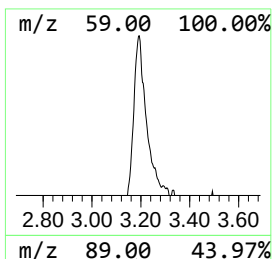
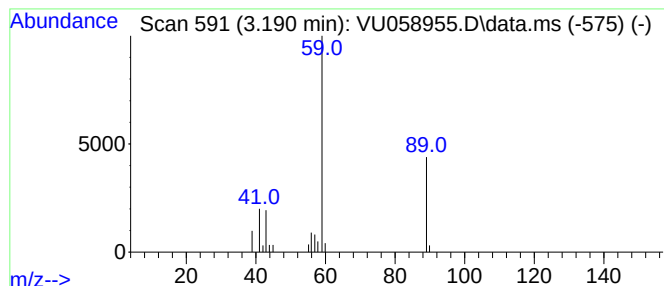
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 1-Butanol, 3-methoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.190	3.45 ug/L	28853	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 3-methoxy-			104	C5H12O2	002517-43-3	64
2	L-Threonine, O-methyl-, methyl e...			147	C6H13NO3	1000452-62-7	40
3	1,2-Butanediol			90	C4H10O2	000584-03-2	40
4	3-Pentanol			88	C5H12O	000584-02-1	33
5	1,8-Nonanediol, 8-methyl-			174	C10H22O2	054725-73-4	33



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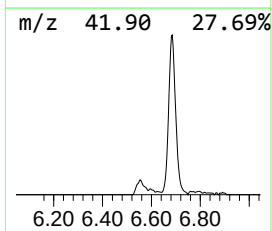
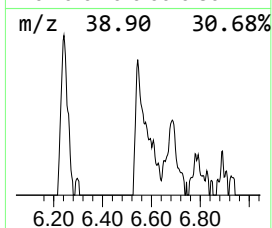
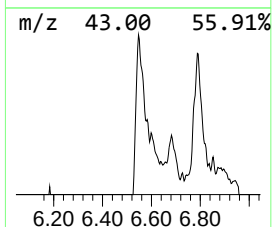
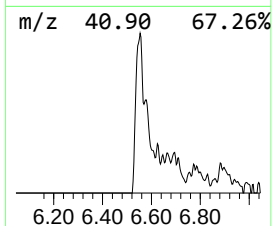
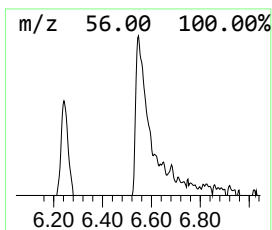
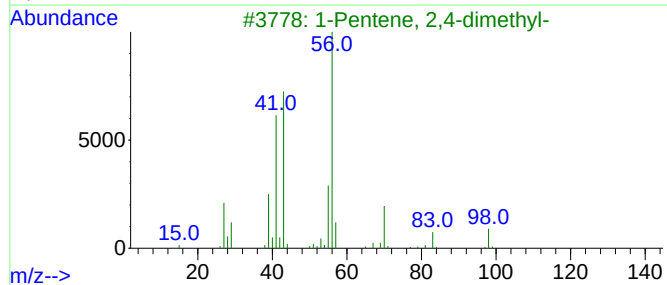
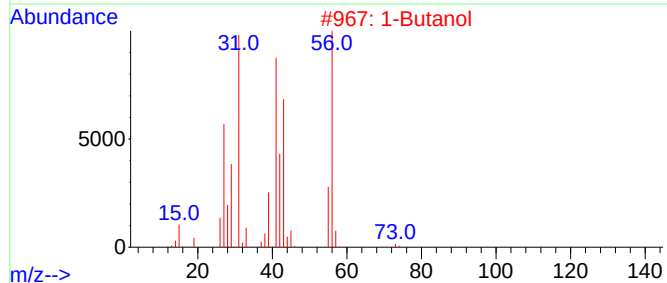
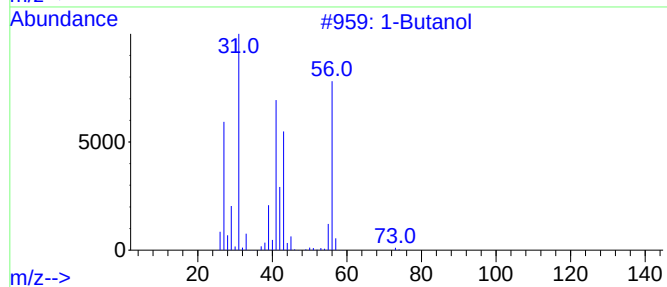
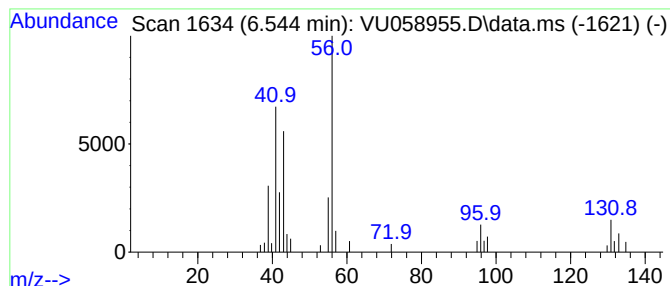
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.544	5.55 ug/L	46351	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	50
2	1-Butanol			74	C4H10O	000071-36-3	50
3	1-Pentene, 2,4-dimethyl-			98	C7H14	002213-32-3	47
4	1-Pentene, 2,4-dimethyl-			98	C7H14	002213-32-3	47
5	1-Hexene, 2-methyl-			98	C7H14	006094-02-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
Data File : VU058955.D
Acq On : 23 May 2024 17:56
Operator : MD/SY
Sample : P2484-20
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA21

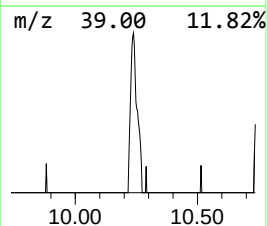
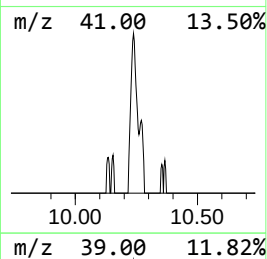
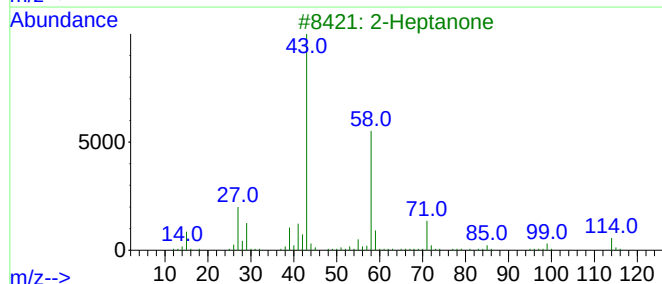
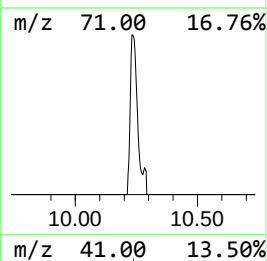
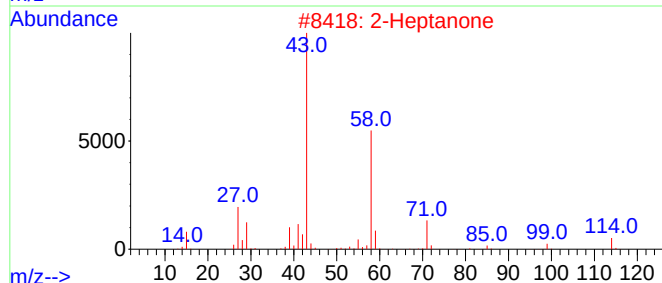
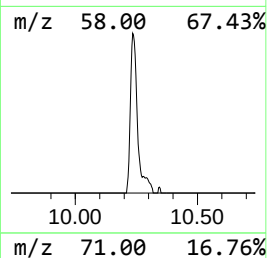
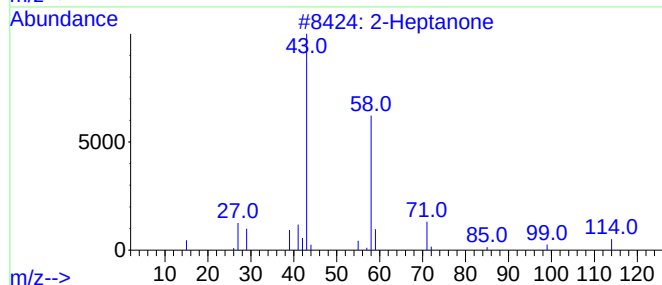
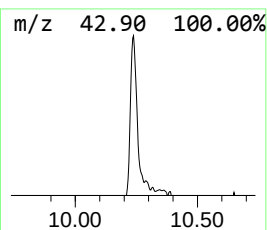
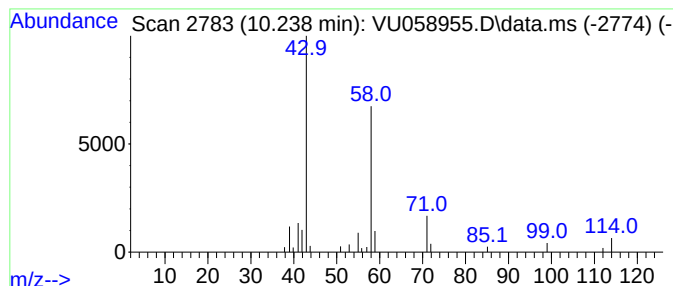
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 2-Heptanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.238	2.52 ug/L	27845	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	91
2	2-Heptanone			114	C7H14O	000110-43-0	91
3	2-Heptanone			114	C7H14O	000110-43-0	91
4	2-Heptanone			114	C7H14O	000110-43-0	90
5	2-Hexanone, 4-methyl-			114	C7H14O	000105-42-0	80



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MSVOA_U
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BHA21

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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
unknown-01	1.682	26.0	ug/L	217126	1	6.245	417750	50.0
1-Butanol, 3-me...	3.190	3.5	ug/L	28853	1	6.245	417750	50.0
1-Butanol	6.544	5.5	ug/L	46351	1	6.245	417750	50.0
2-Heptanone	10.238	2.5	ug/L	27845	2	9.412	552485	50.0