

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
 Data File : VV033327.D
 Acq On : 14 Dec 2023 12:07
 Operator : SY/MD
 Sample : PB157773TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB773

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\SFAMVLM120123WMA.M
 Title : VOC Analysis

Signal : TIC: VV033327.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	33	39	59	rBV	31942	38978	4.44%	0.518%
2	1.278	68	74	87	rBV	111766	119043	13.55%	1.583%
3	1.532	146	153	166	rVB	84334	97326	11.08%	1.294%
4	2.060	306	317	329	rBV	177275	261675	29.79%	3.479%
5	2.172	349	352	358	rBV4	356	426	0.05%	0.006%
6	2.449	429	438	452	rVB	6749	11114	1.27%	0.148%
7	2.552	465	470	472	rBV3	764	554	0.06%	0.007%
8	2.696	512	515	518	rBB	336	236	0.03%	0.003%
9	2.995	603	608	610	rBV2	242	205	0.02%	0.003%
10	3.095	634	639	640	rBV	825	649	0.07%	0.009%
11	3.372	722	725	732	rVV2	314	400	0.05%	0.005%
12	3.439	743	746	750	rBV	190	202	0.02%	0.003%
13	3.648	803	811	815	rBV3	661	870	0.10%	0.012%
14	3.780	842	852	878	rBV2	40722	107894	12.28%	1.434%
15	4.163	967	971	974	rBV3	280	229	0.03%	0.003%
16	4.246	979	997	1029	rBV	147646	378068	43.04%	5.026%
17	4.394	1041	1043	1047	rBV2	405	321	0.04%	0.004%
18	4.446	1055	1059	1062	rVB4	450	395	0.04%	0.005%
19	4.584	1099	1102	1105	rBV	437	318	0.04%	0.004%
20	4.613	1108	1111	1114	rVB4	515	309	0.04%	0.004%
21	4.674	1126	1130	1132	rBV2	251	207	0.02%	0.003%
22	4.690	1132	1135	1142	rVB2	439	475	0.05%	0.006%
23	4.725	1143	1146	1147	rBV2	478	269	0.03%	0.004%
24	4.954	1200	1217	1251	rBV2	323290	878402	100.00%	11.678%
25	5.204	1286	1295	1317	rVB4	7179	18290	2.08%	0.243%
26	5.420	1359	1362	1364	rBV	387	284	0.03%	0.004%
27	5.471	1375	1378	1384	rBV3	281	269	0.03%	0.004%
28	5.532	1384	1397	1431	rBV2	276053	579901	66.02%	7.710%
29	5.986	1522	1538	1560	rBV	176770	370890	42.22%	4.931%
30	6.179	1595	1598	1599	rBV2	624	411	0.05%	0.005%
31	6.246	1615	1619	1621	rBV2	402	289	0.03%	0.004%
32	6.391	1655	1664	1687	rBV2	78335	153709	17.50%	2.044%
33	6.828	1797	1800	1802	rBV2	325	222	0.03%	0.003%
34	6.912	1814	1826	1849	rBV	107857	203771	23.20%	2.709%
35	7.117	1881	1890	1905	rBV2	22010	38430	4.37%	0.511%
36	7.243	1917	1929	1961	rBV	421551	752187	85.63%	10.000%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
 Title : VOC Analysis

37	7.551	2014	2025	2053	rBV2	101998	188230	21.43%	2.503%
38	7.741	2080	2084	2085	rBV	331	242	0.03%	0.003%
39	7.767	2088	2092	2097	rBV3	523	454	0.05%	0.006%
40	7.809	2101	2105	2109	rBV	293	281	0.03%	0.004%
41	7.860	2109	2121	2135	rBV2	29462	52832	6.01%	0.702%
42	8.024	2163	2172	2197	rBV2	152239	282891	32.21%	3.761%
43	8.243	2233	2240	2257	rVB2	22543	40759	4.64%	0.542%
44	8.471	2306	2311	2312	rBV	441	228	0.03%	0.003%
45	8.619	2346	2357	2373	rBV	90915	151584	17.26%	2.015%
46	8.728	2387	2391	2396	rBV5	733	729	0.08%	0.010%
47	8.783	2397	2408	2438	rVV	466433	761492	86.69%	10.124%
48	8.950	2458	2460	2465	rVB4	501	320	0.04%	0.004%
49	9.008	2471	2478	2480	rBV3	539	568	0.06%	0.008%
50	9.127	2510	2515	2516	rBV3	358	284	0.03%	0.004%
51	9.175	2528	2530	2532	rBV	397	212	0.02%	0.003%
52	9.268	2557	2559	2565	rVB	316	286	0.03%	0.004%
53	9.301	2565	2569	2572	rVB2	354	278	0.03%	0.004%
54	9.342	2572	2582	2586	rBV4	1014	1518	0.17%	0.020%
55	9.449	2611	2615	2619	rBV2	267	305	0.03%	0.004%
56	9.590	2657	2659	2662	rVB2	407	251	0.03%	0.003%
57	9.629	2669	2671	2675	rVB	383	221	0.03%	0.003%
58	9.683	2682	2688	2690	rBV2	317	346	0.04%	0.005%
59	9.789	2718	2721	2724	rBV	277	217	0.02%	0.003%
60	9.831	2731	2734	2739	rBV2	270	285	0.03%	0.004%
61	9.969	2774	2777	2780	rBV2	283	198	0.02%	0.003%
62	10.085	2810	2813	2816	rVB2	365	299	0.03%	0.004%
63	10.153	2822	2834	2854	rBV	268680	422683	48.12%	5.620%
64	10.330	2879	2889	2898	rVB3	3434	5339	0.61%	0.071%
65	10.432	2916	2921	2923	rBV	381	260	0.03%	0.003%
66	10.481	2930	2936	2938	rVV2	444	352	0.04%	0.005%
67	10.555	2956	2959	2961	rBV	320	257	0.03%	0.003%
68	10.641	2983	2986	2990	rVB2	330	307	0.03%	0.004%
69	10.735	3010	3015	3019	rVB2	261	238	0.03%	0.003%
70	10.786	3027	3031	3033	rBV2	362	310	0.04%	0.004%
71	10.863	3050	3055	3060	rBV2	548	582	0.07%	0.008%
72	10.966	3082	3087	3092	rVB2	409	440	0.05%	0.006%
73	11.002	3093	3098	3102	rBB	224	232	0.03%	0.003%
74	11.037	3105	3109	3113	rBB2	380	346	0.04%	0.005%
75	11.063	3114	3117	3118	rBV2	297	207	0.02%	0.003%
76	11.120	3130	3135	3137	rBV	567	520	0.06%	0.007%

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77	11.185	3143	3155	3174	rBV	499366	776806	88.43%	10.328%
78	11.397	3219	3221	3224	rBV	572	390	0.04%	0.005%
79	11.455	3235	3239	3243	rBV2	305	221	0.03%	0.003%
80	11.561	3260	3272	3297	rBV	498573	793773	90.37%	10.553%
81	11.844	3358	3360	3364	rVB	373	272	0.03%	0.004%
82	11.966	3394	3398	3399	rBV	315	277	0.03%	0.004%
83	12.079	3431	3433	3437	rVB	412	221	0.03%	0.003%
84	12.111	3437	3443	3445	rBV2	344	403	0.05%	0.005%
85	12.194	3465	3469	3477	rVB6	1549	2037	0.23%	0.027%
86	12.500	3561	3564	3567	rBV2	375	321	0.04%	0.004%
87	12.551	3576	3580	3583	rBV2	334	219	0.02%	0.003%
88	12.590	3588	3592	3597	rBV4	884	751	0.09%	0.010%
89	12.802	3656	3658	3661	rBV2	394	224	0.03%	0.003%
90	12.821	3661	3664	3667	rVV2	332	216	0.02%	0.003%
91	12.866	3673	3678	3682	rBV2	307	331	0.04%	0.004%
92	12.956	3702	3706	3707	rBV	360	258	0.03%	0.003%
93	13.194	3778	3780	3781	rBV	762	277	0.03%	0.004%
94	13.278	3801	3806	3808	rBV2	353	296	0.03%	0.004%
95	13.333	3818	3823	3825	rBV2	433	406	0.05%	0.005%
96	13.410	3844	3847	3850	rBV2	447	272	0.03%	0.004%
97	13.455	3850	3861	3869	rBV2	4027	6429	0.73%	0.085%
98	13.545	3887	3889	3891	rBV2	420	213	0.02%	0.003%
99	13.686	3927	3933	3940	rVB4	1834	2120	0.24%	0.028%
100	13.841	3978	3981	3983	rBV	470	294	0.03%	0.004%

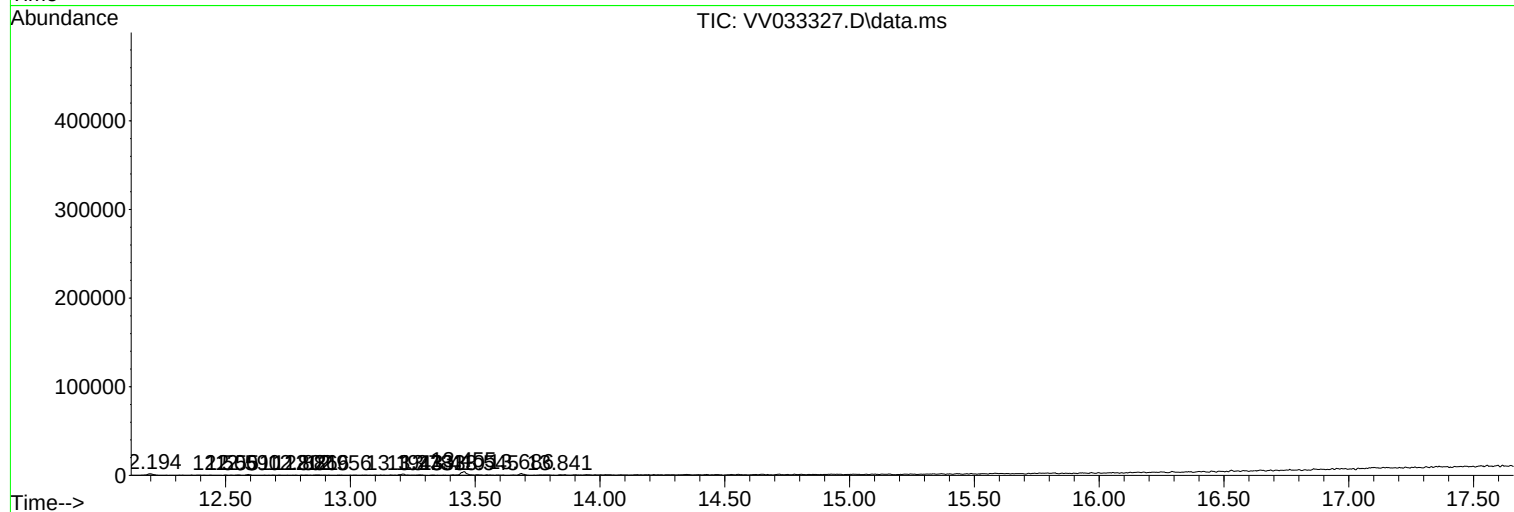
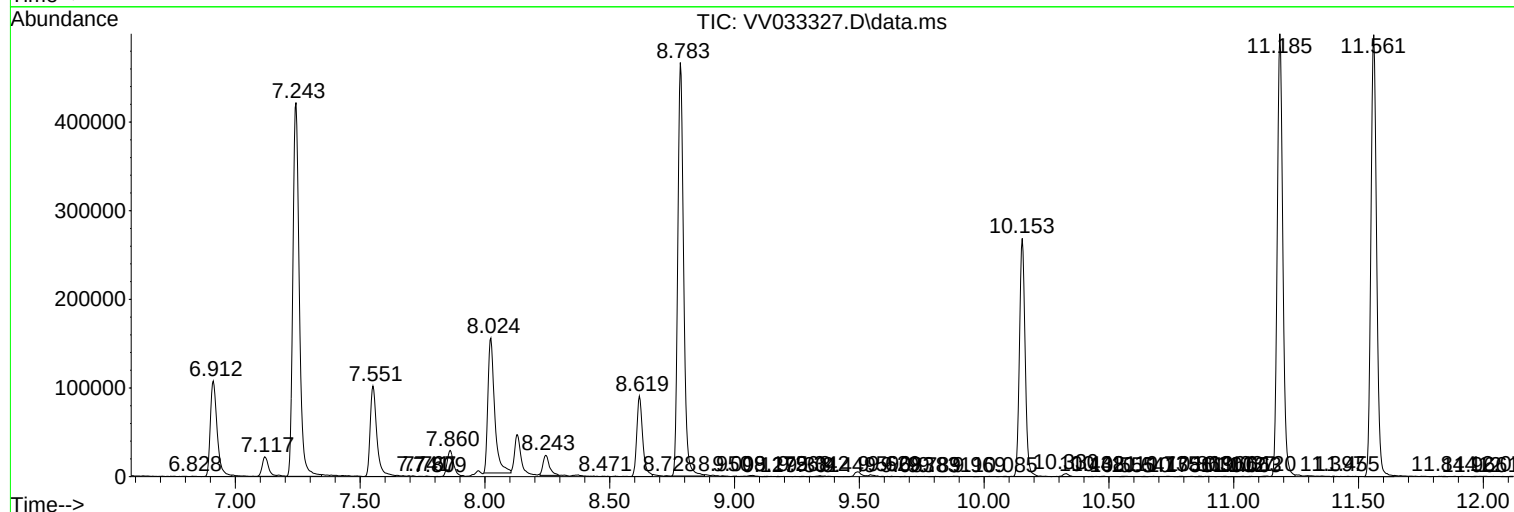
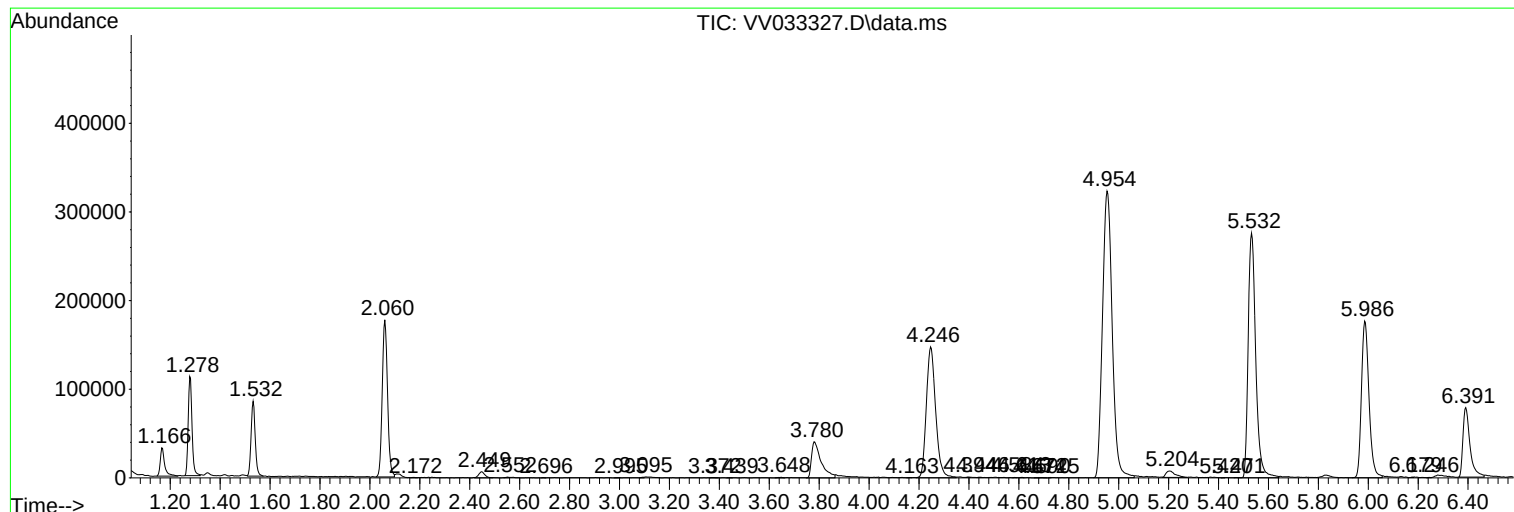
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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



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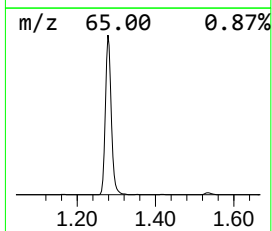
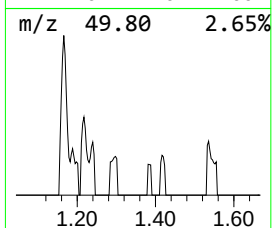
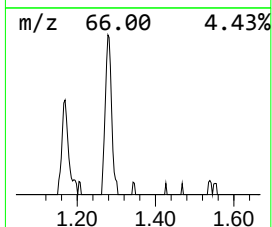
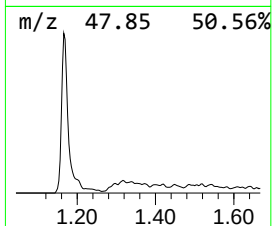
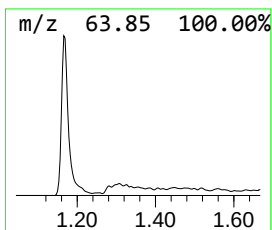
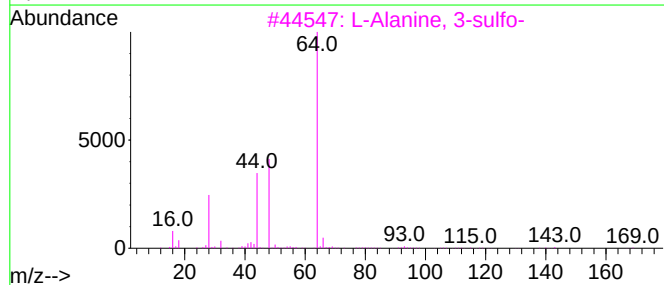
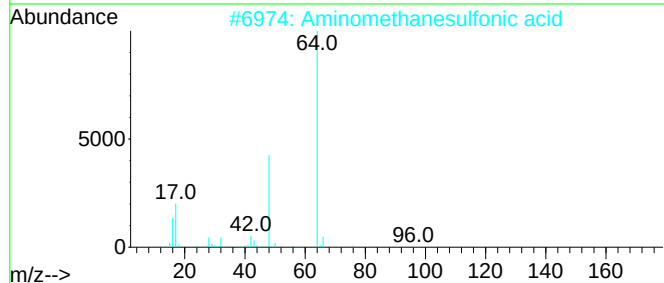
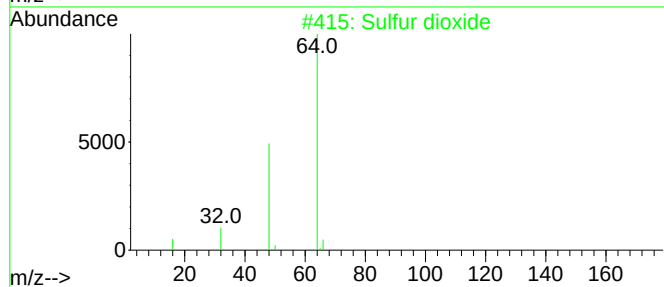
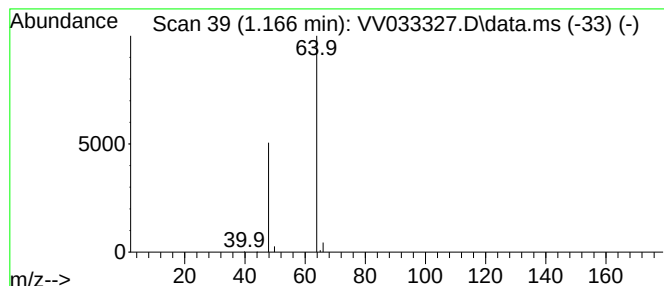
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	3.36 ug/L	38978	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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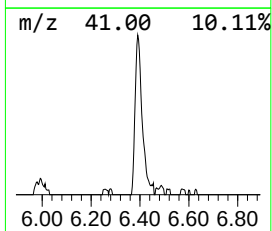
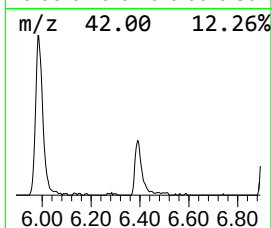
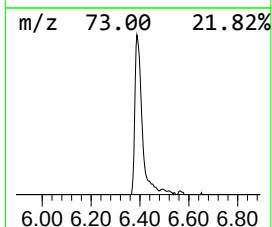
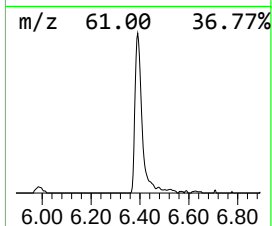
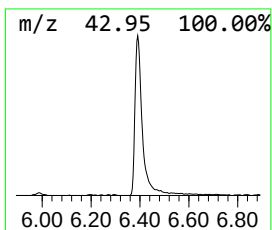
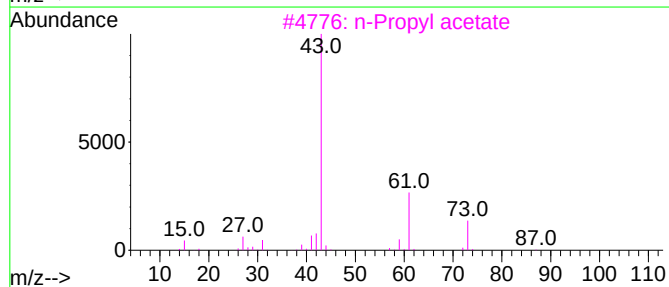
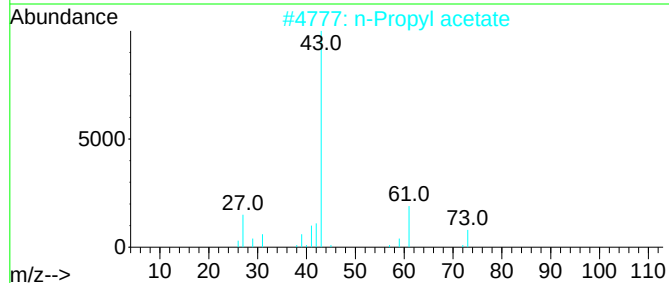
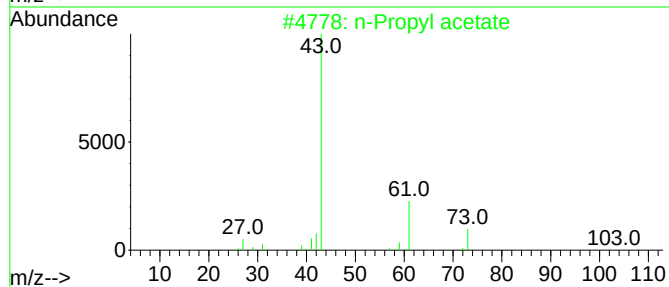
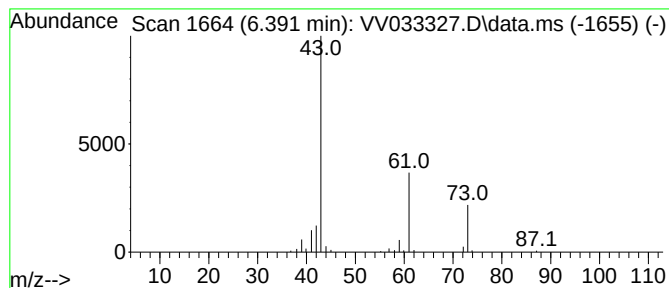
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.391	13.25 ug/L	153709	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	83
2	n-Propyl acetate			102	C5H10O2	000109-60-4	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	74
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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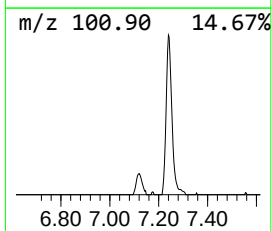
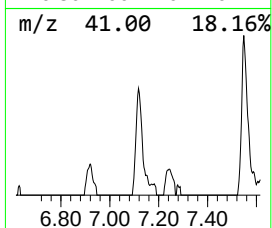
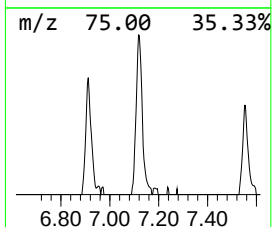
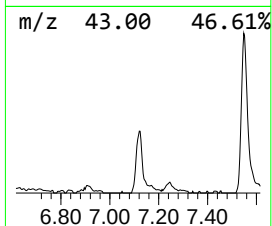
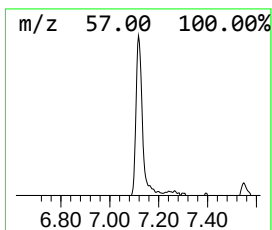
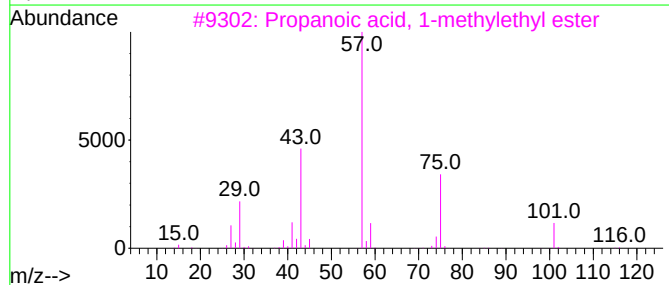
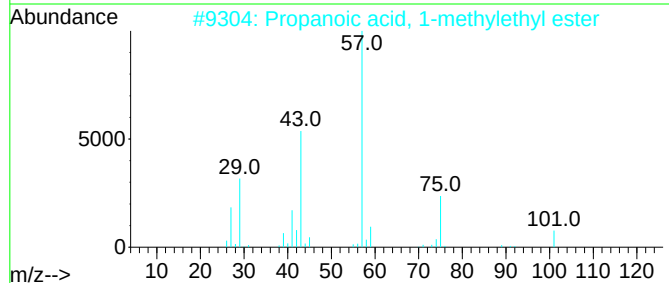
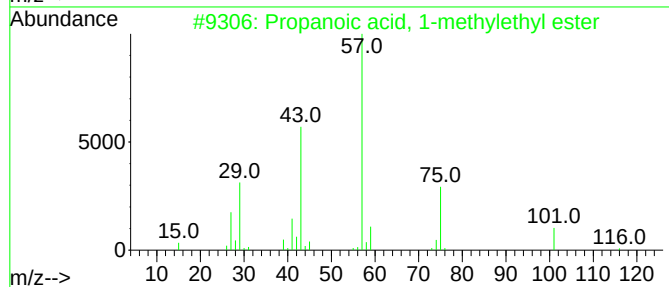
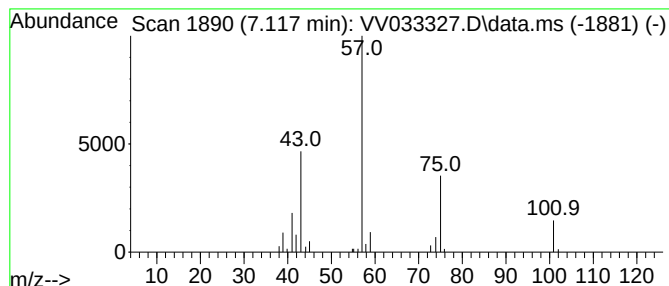
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.117	3.31 ug/L	38430	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033327.D
Acq On : 14 Dec 2023 12:07
Operator : SY/MD
Sample : PB157773TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB773

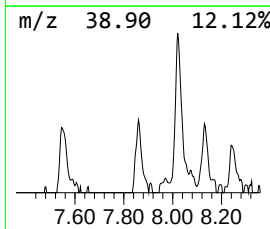
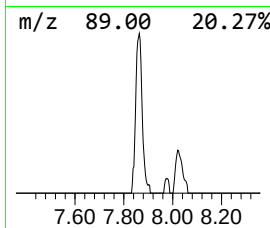
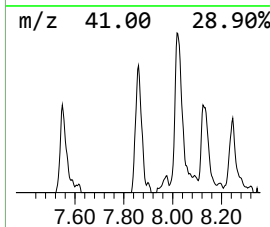
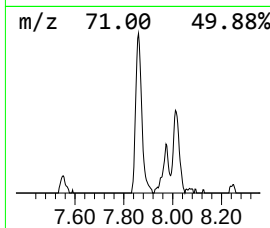
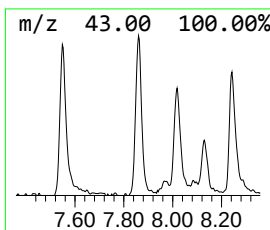
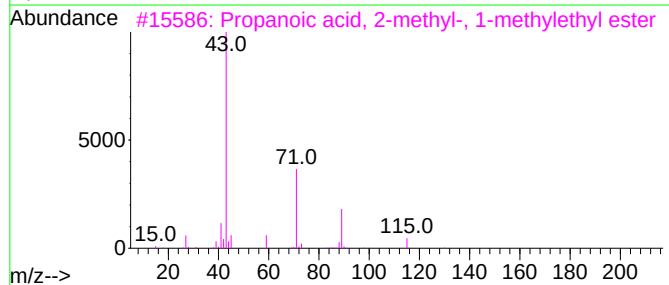
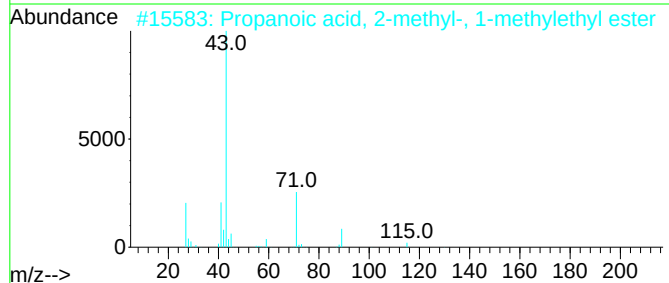
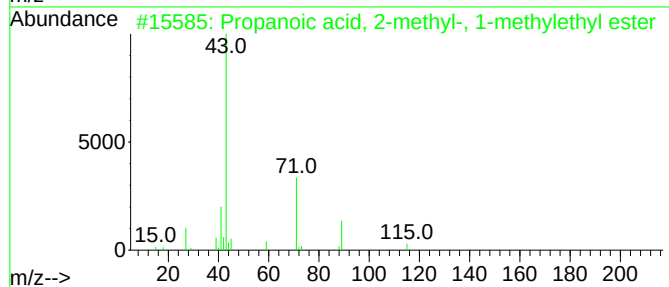
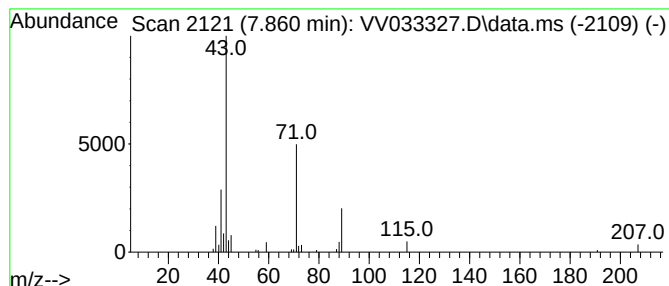
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.860	3.47 ug/L	52832	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033327.D
Acq On : 14 Dec 2023 12:07
Operator : SY/MD
Sample : PB157773TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB773

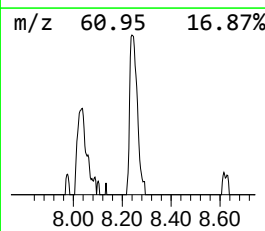
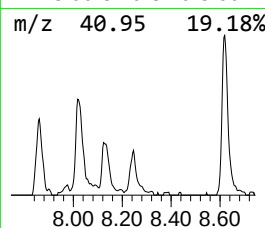
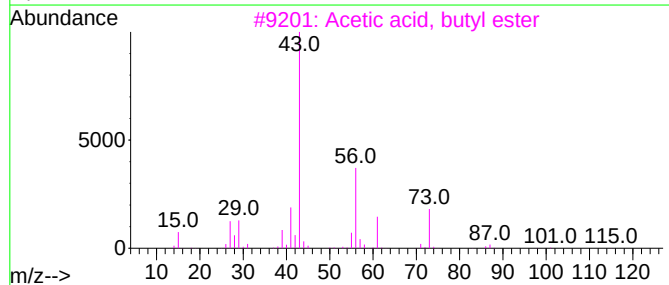
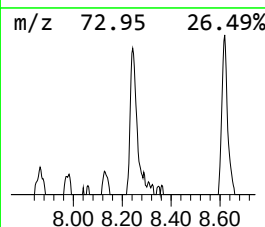
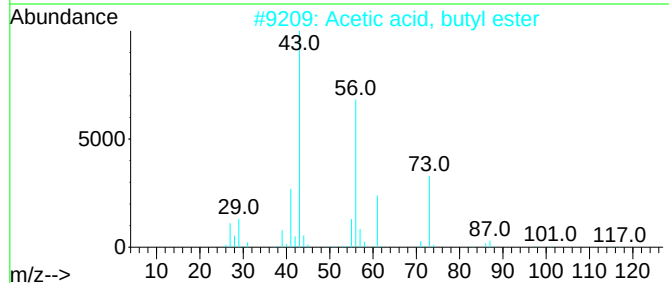
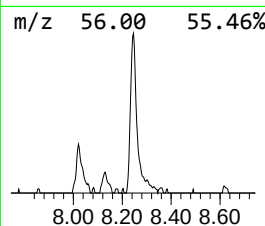
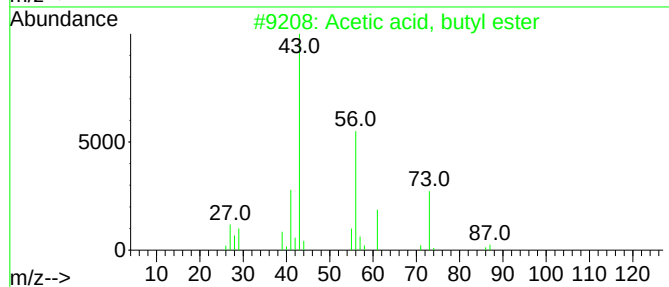
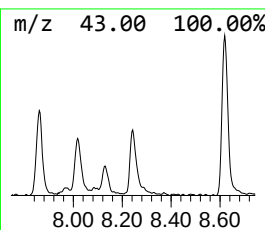
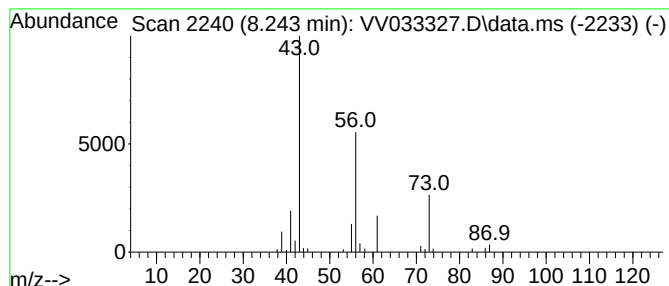
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.243	2.68 ug/L	40759	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78		
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	40		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	39		
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	10		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033327.D
Acq On : 14 Dec 2023 12:07
Operator : SY/MD
Sample : PB157773TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB773

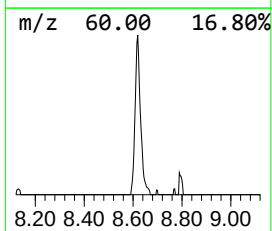
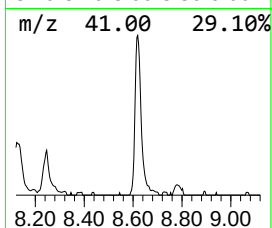
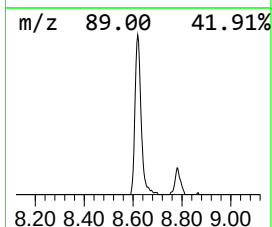
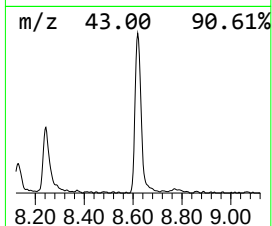
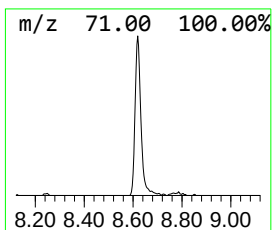
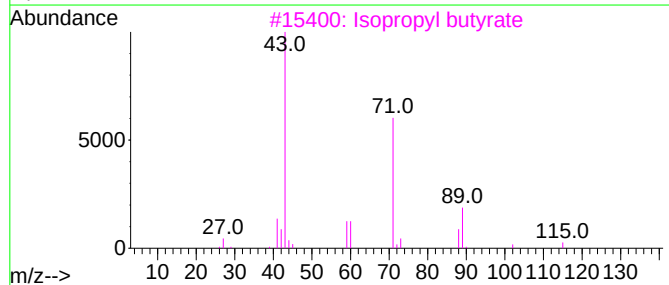
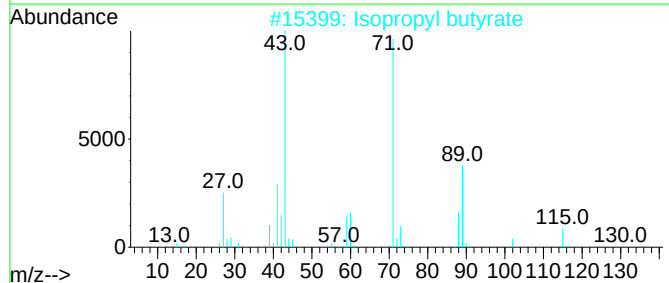
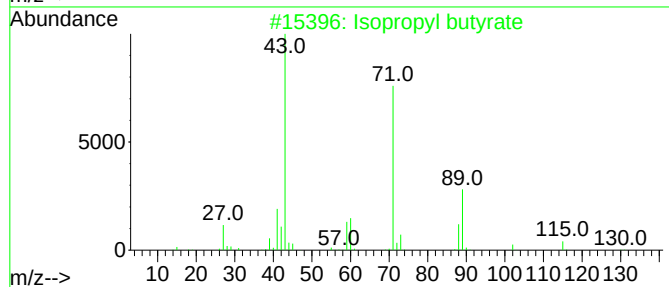
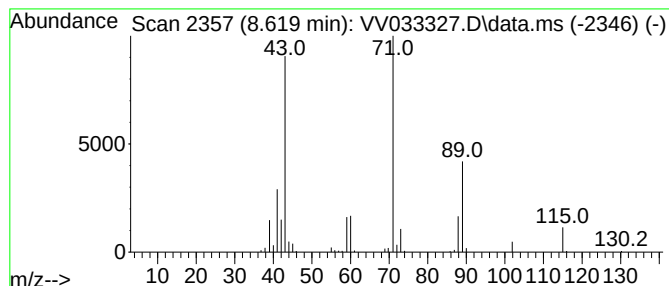
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	9.95 ug/L	151584	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW121423\
Data File : VV033327.D
Acq On : 14 Dec 2023 12:07
Operator : SY/MD
Sample : PB157773TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB773

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	3.4	ug/L	38978	1	5.532	579901	50.0
n-Propyl acetate	6.391	13.3	ug/L	153709	1	5.532	579901	50.0
Propanoic acid,...	7.117	3.3	ug/L	38430	1	5.532	579901	50.0
Propanoic acid,...	7.860	3.5	ug/L	52832	2	8.783	761492	50.0
Acetic acid, bu...	8.243	2.7	ug/L	40759	2	8.783	761492	50.0
Isopropyl butyrate	8.619	9.9	ug/L	151584	2	8.783	761492	50.0