

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
 Data File : VV033564.D
 Acq On : 10 Jan 2024 16:42
 Operator : SY/MD
 Sample : P1016-06 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMH6

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\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033564.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.220	51	56	59	rBV5	2787	3225	0.24%	0.030%
2	1.281	67	75	90	rBV	191108	203836	15.47%	1.899%
3	1.532	146	153	170	rVB	146150	178678	13.56%	1.664%
4	2.059	308	317	330	rBV	289589	421034	31.96%	3.922%
5	2.452	429	439	450	rVB	6930	11725	0.89%	0.109%
6	2.757	531	534	539	rVV4	413	334	0.03%	0.003%
7	2.783	539	542	545	rBV4	547	487	0.04%	0.005%
8	3.104	632	642	661	rBV3	6193	16595	1.26%	0.155%
9	3.240	681	684	686	rBV3	498	318	0.02%	0.003%
10	3.404	733	735	738	rBV	557	364	0.03%	0.003%
11	3.641	805	809	813	rVV6	540	551	0.04%	0.005%
12	3.722	830	834	836	rBV2	555	378	0.03%	0.004%
13	3.783	845	853	893	rBV	90069	248764	18.88%	2.317%
14	4.249	982	998	1030	rBV	194444	501473	38.07%	4.671%
15	4.577	1096	1100	1101	rBV2	536	412	0.03%	0.004%
16	4.593	1101	1105	1108	rVB5	523	454	0.03%	0.004%
17	4.670	1126	1129	1132	rVB4	523	307	0.02%	0.003%
18	4.693	1132	1136	1139	rBV4	506	483	0.04%	0.004%
19	4.760	1154	1157	1160	rVB2	563	387	0.03%	0.004%
20	4.957	1199	1218	1250	rBV2	496051	1317389	100.00%	12.272%
21	5.217	1291	1299	1314	rBV3	5665	12496	0.95%	0.116%
22	5.535	1386	1398	1425	rBV	403354	825571	62.67%	7.691%
23	5.831	1480	1490	1508	rVB4	7051	15789	1.20%	0.147%
24	5.921	1515	1518	1521	rBV6	648	499	0.04%	0.005%
25	5.989	1525	1539	1573	rBV	285782	604735	45.90%	5.633%
26	6.397	1657	1666	1704	rBV	92051	189496	14.38%	1.765%
27	6.770	1779	1782	1785	rBV3	468	363	0.03%	0.003%
28	6.915	1813	1827	1852	rBV	171480	324418	24.63%	3.022%
29	7.124	1883	1892	1906	rBV	21855	40024	3.04%	0.373%
30	7.243	1918	1929	1959	rBV	591589	1049926	79.70%	9.780%
31	7.554	2015	2026	2049	rBV2	139972	261999	19.89%	2.441%
32	7.863	2108	2122	2140	rBV2	31329	55025	4.18%	0.513%
33	7.976	2149	2157	2162	rBV3	5209	8113	0.62%	0.076%
34	8.024	2163	2172	2198	rVV	331060	621604	47.18%	5.790%
35	8.133	2200	2206	2227	rVB2	40734	76317	5.79%	0.711%
36	8.249	2235	2242	2259	rVB2	21145	37829	2.87%	0.352%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

37	8.493	2316	2318	2323	rBV5	352	314	0.02%	0.003%
38	8.525	2326	2328	2331	rVB2	714	375	0.03%	0.003%
39	8.548	2331	2335	2338	rBV4	750	522	0.04%	0.005%
40	8.619	2346	2357	2378	rBV	86648	142766	10.84%	1.330%
41	8.783	2397	2408	2446	rBV	606249	1010677	76.72%	9.415%
42	8.956	2458	2462	2468	rBV7	938	854	0.06%	0.008%
43	9.053	2488	2492	2493	rBV4	439	370	0.03%	0.003%
44	9.066	2494	2496	2499	rVV4	589	388	0.03%	0.004%
45	9.162	2521	2526	2529	rBV6	753	942	0.07%	0.009%
46	9.294	2562	2567	2570	rBV3	458	370	0.03%	0.003%
47	9.313	2571	2573	2578	rVB4	478	465	0.04%	0.004%
48	9.339	2578	2581	2582	rBV	654	320	0.02%	0.003%
49	9.419	2604	2606	2612	rBV3	372	428	0.03%	0.004%
50	9.500	2621	2631	2639	rBV8	4068	8364	0.63%	0.078%
51	9.763	2709	2713	2718	rBV5	276	298	0.02%	0.003%
52	9.863	2740	2744	2747	rBV4	676	586	0.04%	0.005%
53	9.908	2756	2758	2765	rBV3	401	415	0.03%	0.004%
54	10.098	2813	2817	2819	rBV3	602	584	0.04%	0.005%
55	10.152	2820	2834	2862	rVV	352099	563678	42.79%	5.251%
56	10.336	2887	2891	2896	rVB5	643	588	0.04%	0.005%
57	10.410	2912	2914	2918	rVB2	639	474	0.04%	0.004%
58	10.487	2931	2938	2940	rBV4	896	1004	0.08%	0.009%
59	10.529	2949	2951	2960	rVV6	881	1098	0.08%	0.010%
60	10.770	3021	3026	3028	rBV4	600	517	0.04%	0.005%
61	10.866	3052	3056	3058	rBV4	522	499	0.04%	0.005%
62	10.905	3065	3068	3072	rVB5	580	438	0.03%	0.004%
63	10.924	3072	3074	3077	rBV2	693	470	0.04%	0.004%
64	11.130	3133	3138	3139	rBV4	834	681	0.05%	0.006%
65	11.185	3145	3155	3181	rBV	626169	978947	74.31%	9.119%
66	11.403	3219	3223	3225	rBV4	564	365	0.03%	0.003%
67	11.477	3241	3246	3249	rBV4	578	575	0.04%	0.005%
68	11.561	3260	3272	3301	rVV	579109	926424	70.32%	8.630%
69	11.876	3367	3370	3375	rBV5	549	449	0.03%	0.004%
70	11.918	3381	3383	3388	rVB5	805	617	0.05%	0.006%
71	12.059	3425	3427	3433	rVB3	357	319	0.02%	0.003%
72	12.230	3473	3480	3484	rBV5	288	471	0.04%	0.004%
73	12.300	3499	3502	3505	rVB4	501	311	0.02%	0.003%
74	12.336	3510	3513	3516	rVB4	568	334	0.03%	0.003%
75	12.371	3522	3524	3528	rBV3	378	320	0.02%	0.003%
76	12.484	3553	3559	3562	rBV4	618	512	0.04%	0.005%

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 Title : VOC Analysis

77	12.763	3642	3646	3648	rBV3	344	293	0.02%	0.003%
78	12.892	3684	3686	3691	rVB2	441	318	0.02%	0.003%
79	12.918	3691	3694	3698	rBV3	582	511	0.04%	0.005%
80	12.940	3699	3701	3705	rVB3	538	297	0.02%	0.003%
81	12.966	3705	3709	3714	rVB6	685	561	0.04%	0.005%
82	13.078	3740	3744	3746	rBV3	635	521	0.04%	0.005%
83	13.162	3768	3770	3774	rBV5	630	470	0.04%	0.004%
84	13.207	3776	3784	3791	rBV3	4707	7401	0.56%	0.069%
85	13.307	3810	3815	3816	rBV3	481	347	0.03%	0.003%
86	13.361	3830	3832	3835	rBV	443	391	0.03%	0.004%
87	13.448	3849	3859	3874	rBV2	19199	33642	2.55%	0.313%
88	13.596	3902	3905	3912	rBV3	647	527	0.04%	0.005%
89	13.631	3914	3916	3920	rBV5	463	352	0.03%	0.003%
90	13.686	3925	3933	3944	rVB9	2528	4340	0.33%	0.040%
91	13.811	3969	3972	3974	rVB	500	302	0.02%	0.003%
92	13.860	3984	3987	3989	rBV3	497	334	0.03%	0.003%
93	13.963	4015	4019	4021	rBV3	643	592	0.04%	0.006%
94	14.107	4061	4064	4068	rVB4	715	478	0.04%	0.004%
95	14.130	4068	4071	4073	rBV3	615	467	0.04%	0.004%
96	14.172	4081	4084	4087	rBV4	503	436	0.03%	0.004%
97	14.419	4157	4161	4166	rBV6	666	690	0.05%	0.006%
98	14.615	4218	4222	4226	rBV5	494	595	0.05%	0.006%
99	14.827	4284	4288	4292	rBV4	877	830	0.06%	0.008%
100	14.856	4292	4297	4298	rBV4	809	710	0.05%	0.007%

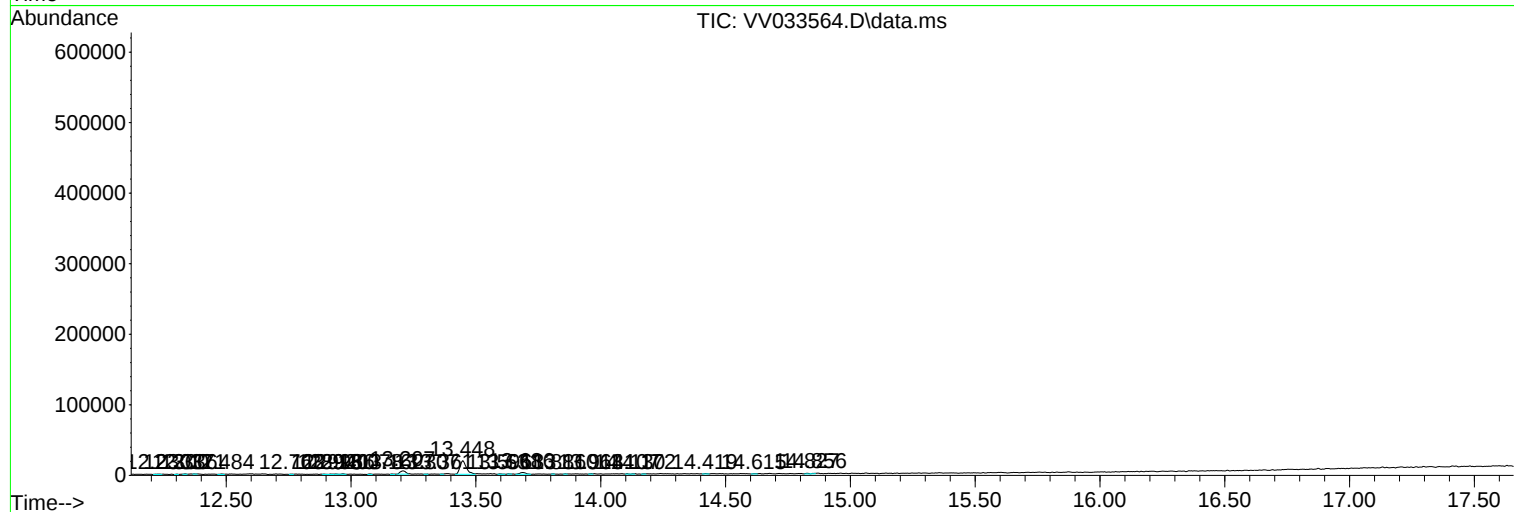
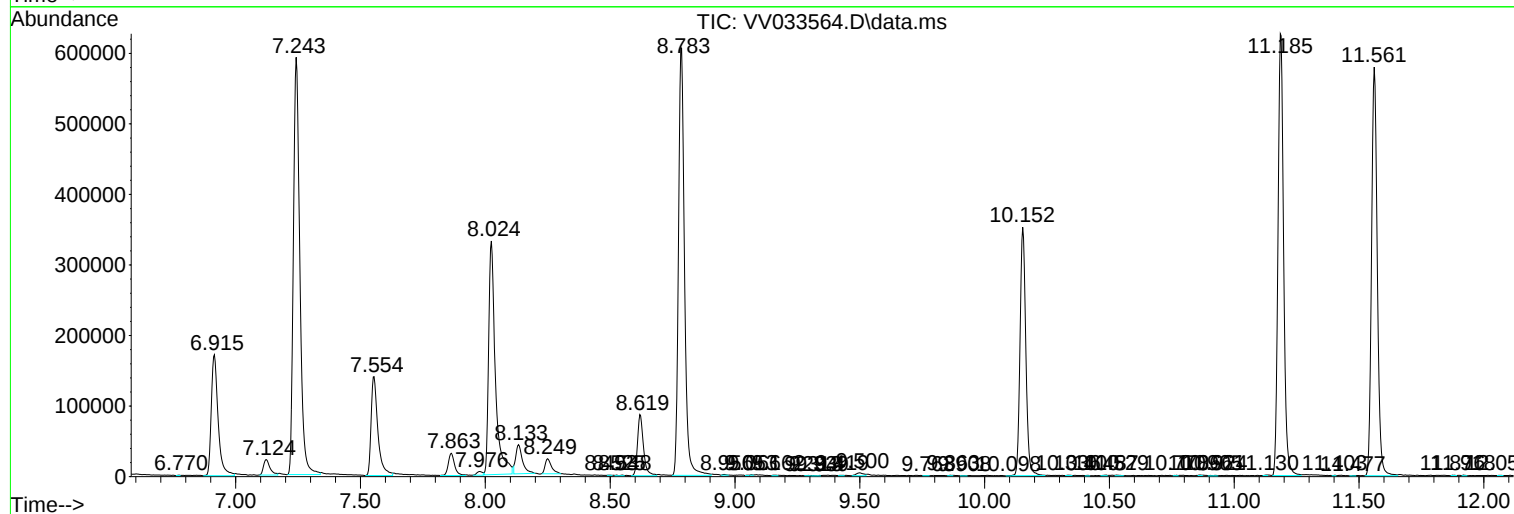
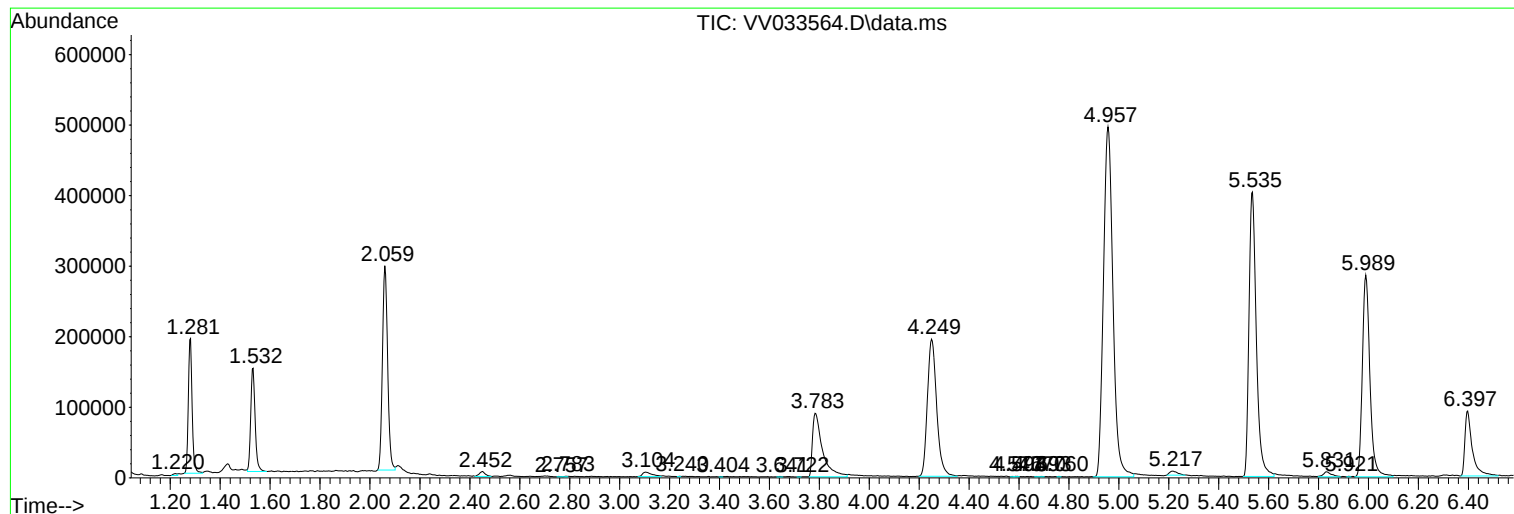
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MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



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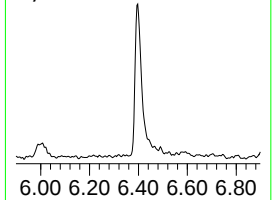
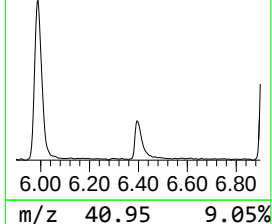
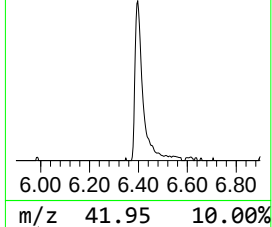
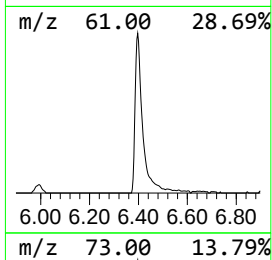
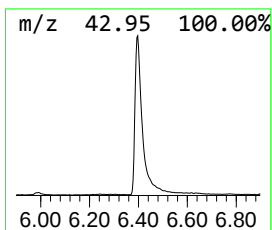
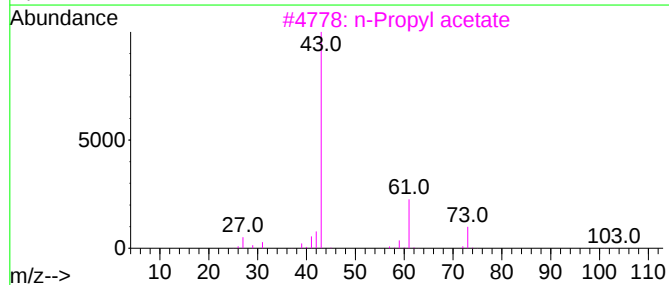
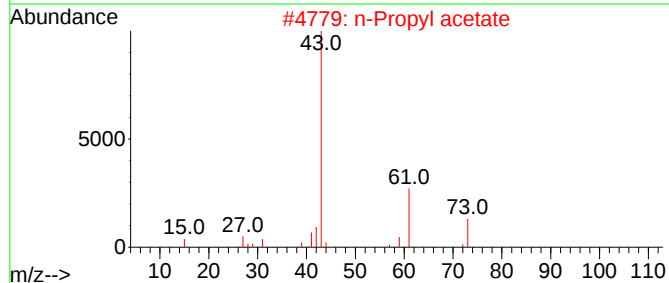
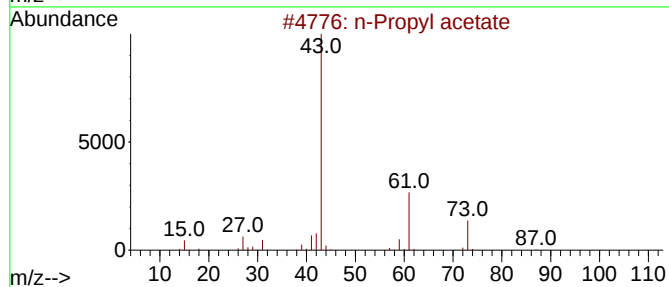
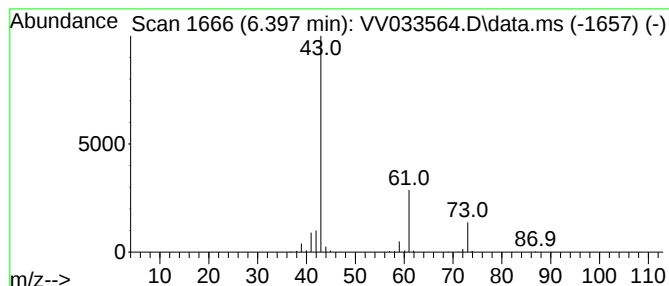
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.397	11.48 ug/L	189496	1,4-Difluorobenzene	5.535

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	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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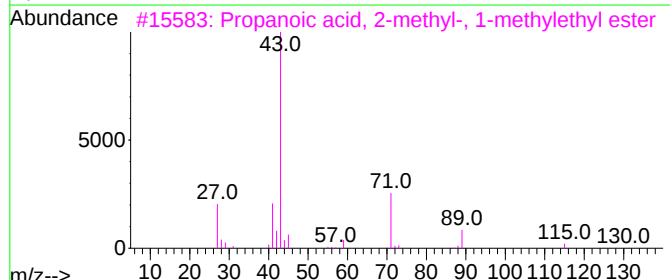
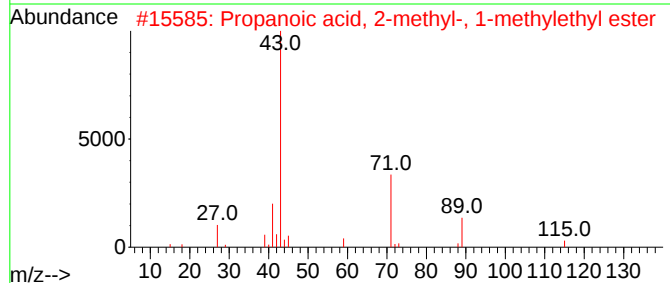
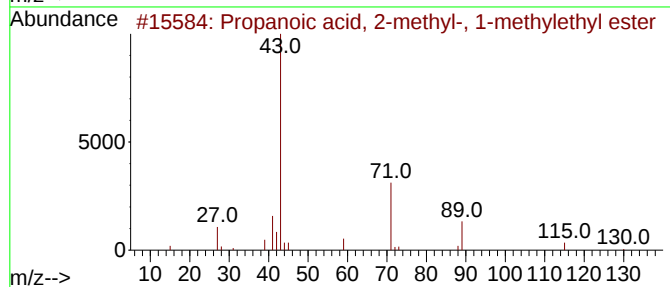
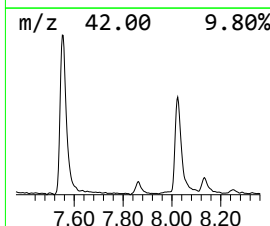
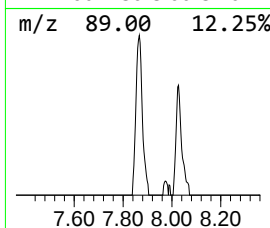
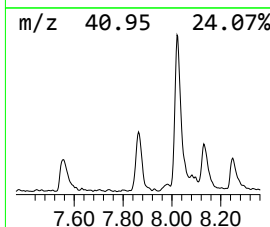
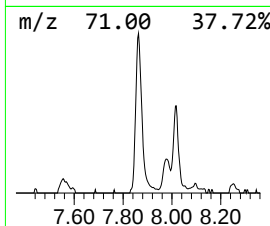
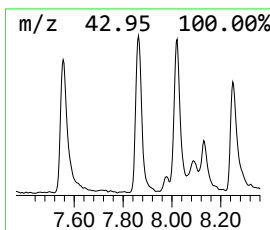
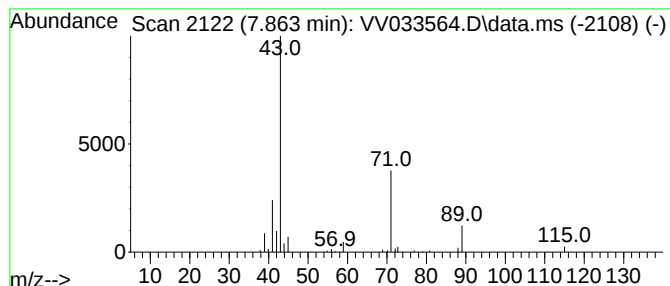
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	2.72 ug/L	55025	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



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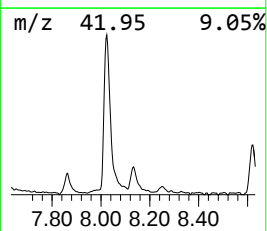
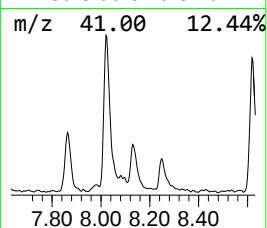
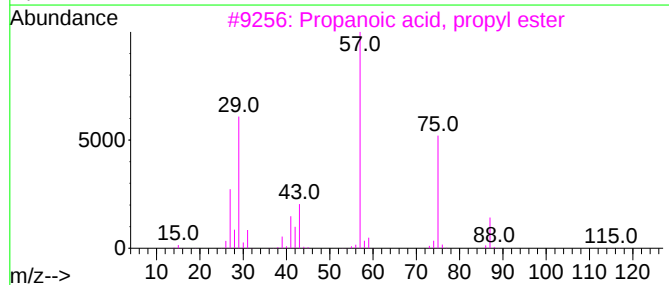
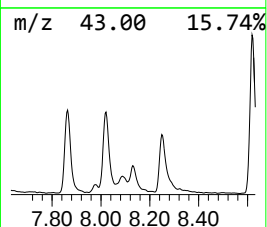
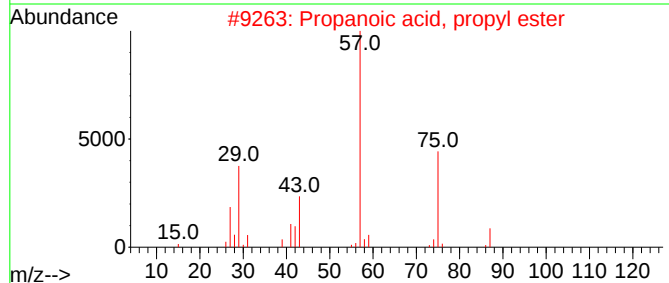
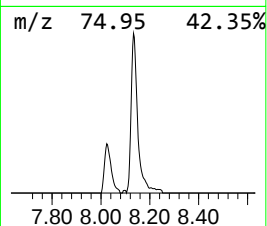
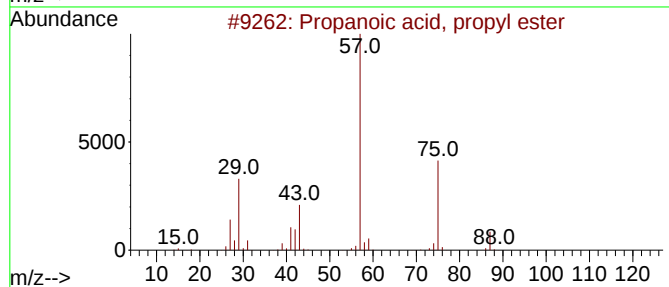
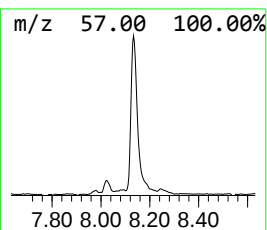
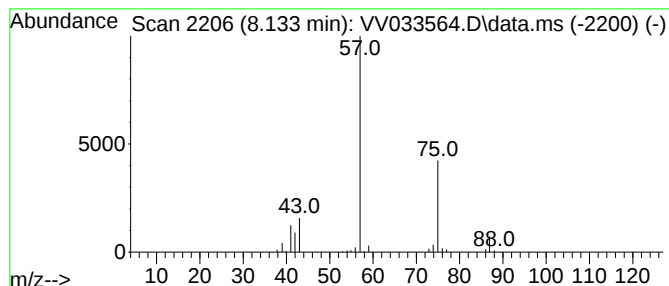
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.133	3.78 ug/L	76317	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	43
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033564.D
Acq On : 10 Jan 2024 16:42
Operator : SY/MD
Sample : P1016-06 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMH6

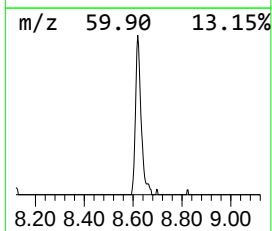
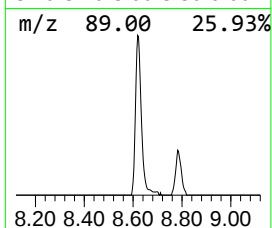
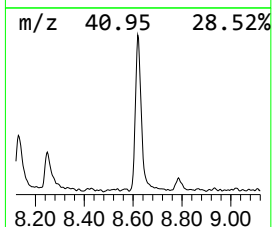
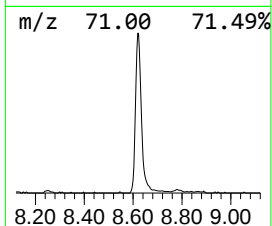
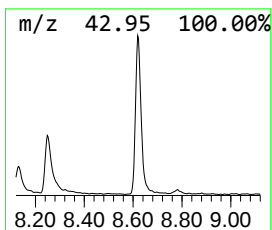
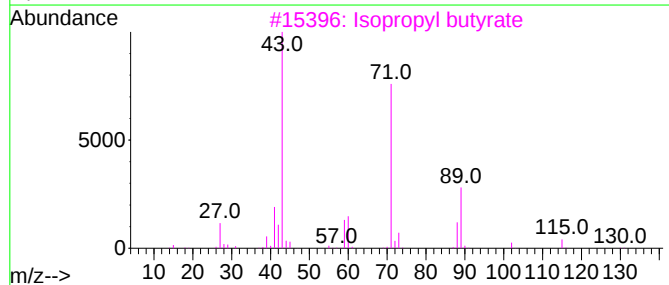
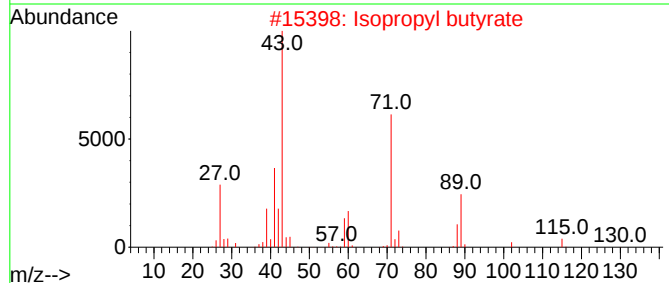
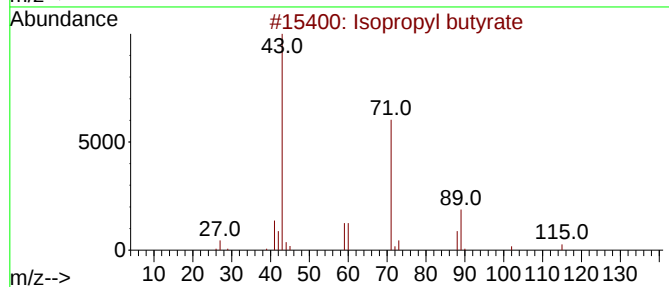
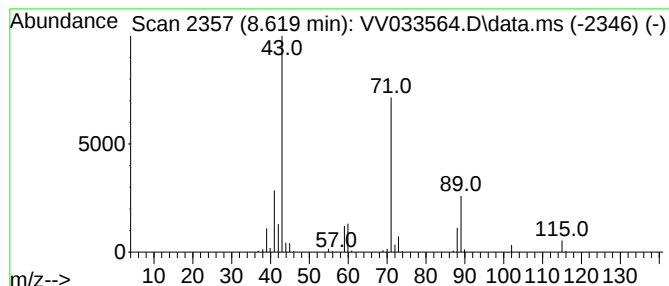
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Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	7.06 ug/L	142766	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	86
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033564.D
Acq On : 10 Jan 2024 16:42
Operator : SY/MD
Sample : P1016-06 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMH6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.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
n-Propyl acetate	6.397	11.5	ug/L	189496	1	5.535	825571	50.0
Propanoic acid,...	7.863	2.7	ug/L	55025	2	8.786	1010680	50.0
Propanoic acid,...	8.133	3.8	ug/L	76317	2	8.786	1010680	50.0
Isopropyl butyrate	8.619	7.1	ug/L	142766	2	8.786	1010680	50.0