

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
 Data File : VV028015.D
 Acq On : 21 Sep 2022 14:41
 Operator : SY/MD
 Sample : PB147776TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB776

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\SFAMVLM092022WMA.M

Title : VOC Analysis

Signal : TIC: VV028015.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	96	rVB	185474	186540	14.43%	1.694%
2	1.558	155	161	180	rVB	156816	180095	13.93%	1.635%
3	2.098	320	329	346	rBV	319780	458742	35.48%	4.166%
4	2.500	446	454	465	rVB4	7311	12695	0.98%	0.115%
5	2.597	479	484	486	rBV3	1176	1265	0.10%	0.011%
6	2.732	524	526	527	rBV	427	140	0.01%	0.001%
7	2.841	556	560	562	rBV3	592	374	0.03%	0.003%
8	2.953	592	595	596	rBV2	566	275	0.02%	0.002%
9	2.986	602	605	608	rBV3	393	255	0.02%	0.002%
10	3.053	620	626	627	rBV3	596	581	0.04%	0.005%
11	3.069	628	631	636	rVB3	1012	694	0.05%	0.006%
12	3.095	636	639	641	rBV2	784	453	0.04%	0.004%
13	3.172	661	663	665	rBV	455	180	0.01%	0.002%
14	3.233	680	682	685	rVB	779	361	0.03%	0.003%
15	3.259	688	690	693	rBV3	429	263	0.02%	0.002%
16	3.333	711	713	717	rVB3	311	138	0.01%	0.001%
17	3.355	717	720	723	rBV2	426	222	0.02%	0.002%
18	3.400	730	734	735	rBV4	530	391	0.03%	0.004%
19	3.429	741	743	746	rVB2	447	219	0.02%	0.002%
20	3.548	778	780	781	rBV2	345	193	0.01%	0.002%
21	3.593	788	794	798	rBV3	814	773	0.06%	0.007%
22	3.642	807	809	811	rBV2	304	117	0.01%	0.001%
23	3.661	813	815	818	rVB	421	250	0.02%	0.002%
24	3.690	822	824	825	rBV	219	99	0.01%	0.001%
25	3.715	831	832	835	rVB3	541	252	0.02%	0.002%
26	3.732	835	837	841	rBV2	384	209	0.02%	0.002%
27	3.764	841	847	850	rBV2	217	205	0.02%	0.002%
28	3.780	850	852	858	rVV3	450	395	0.03%	0.004%
29	3.822	863	865	867	rVB	314	117	0.01%	0.001%
30	3.873	867	881	921	rBV2	120629	391823	30.31%	3.558%
31	4.339	1012	1026	1047	rBV	224818	550648	42.59%	5.000%
32	4.664	1122	1127	1129	rBV5	1633	1061	0.08%	0.010%
33	4.709	1139	1141	1145	rBV3	725	510	0.04%	0.005%
34	4.735	1147	1149	1151	rVB3	927	415	0.03%	0.004%
35	4.773	1156	1161	1163	rBV3	463	445	0.03%	0.004%
36	4.818	1169	1175	1178	rBV3	1029	1102	0.09%	0.010%

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37	4.908	1199	1203	1205	rBV4	609	431	0.03%	0.004%
38	4.982	1224	1226	1227	rBV	303	114	0.01%	0.001%
39	5.040	1227	1244	1273	rBV2	504230	1292828	100.00%	11.740%
40	5.236	1303	1305	1308	rBV3	561	249	0.02%	0.002%
41	5.461	1372	1375	1376	rBV2	436	209	0.02%	0.002%
42	5.487	1380	1383	1384	rBV2	239	149	0.01%	0.001%
43	5.497	1384	1386	1391	rVB2	410	227	0.02%	0.002%
44	5.519	1391	1393	1396	rVB4	401	181	0.01%	0.002%
45	5.539	1396	1399	1400	rBV2	644	340	0.03%	0.003%
46	5.571	1406	1409	1410	rBV	1004	574	0.04%	0.005%
47	5.609	1410	1421	1440	rBV	401573	810673	62.71%	7.361%
48	6.063	1551	1562	1592	rVB	314095	637208	49.29%	5.786%
49	6.458	1677	1685	1712	rBV	127618	245501	18.99%	2.229%
50	6.982	1837	1848	1871	rBV	166619	309382	23.93%	2.809%
51	7.185	1904	1911	1927	rVB2	24047	40366	3.12%	0.367%
52	7.310	1939	1950	1974	rBV	588562	1041121	80.53%	9.454%
53	7.616	2035	2045	2066	rBV2	142273	248911	19.25%	2.260%
54	7.924	2130	2141	2155	rBV	35138	64024	4.95%	0.581%
55	8.085	2181	2191	2213	rBV	446755	774025	59.87%	7.029%
56	8.301	2253	2258	2271	rVB	34801	53073	4.11%	0.482%
57	8.680	2366	2376	2393	rBV2	104150	169599	13.12%	1.540%
58	8.847	2418	2428	2457	rBV	619588	1009772	78.11%	9.169%
59	9.252	2553	2554	2559	rVB2	860	511	0.04%	0.005%
60	9.275	2559	2561	2563	rBV	529	335	0.03%	0.003%
61	9.326	2572	2577	2579	rBV3	566	495	0.04%	0.004%
62	9.522	2635	2638	2639	rBV	770	437	0.03%	0.004%
63	9.548	2639	2646	2655	rVV3	7768	12737	0.99%	0.116%
64	9.709	2694	2696	2697	rBV	261	103	0.01%	0.001%
65	9.728	2700	2702	2703	rBV2	274	90	0.01%	0.001%
66	9.789	2716	2721	2723	rBV2	449	328	0.03%	0.003%
67	9.799	2723	2724	2727	rVB2	440	226	0.02%	0.002%
68	9.879	2746	2749	2752	rBV	369	286	0.02%	0.003%
69	9.924	2756	2763	2765	rBV3	1168	1012	0.08%	0.009%
70	10.014	2787	2791	2794	rVB3	723	620	0.05%	0.006%
71	10.043	2794	2800	2802	rBV4	810	722	0.06%	0.007%
72	10.059	2802	2805	2808	rBV2	616	474	0.04%	0.004%
73	10.072	2808	2809	2811	rBV2	557	262	0.02%	0.002%
74	10.114	2819	2822	2823	rBV2	1233	657	0.05%	0.006%
75	10.165	2834	2838	2839	rBV3	482	343	0.03%	0.003%
76	10.214	2841	2853	2869	rVV	458224	720710	55.75%	6.544%

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77	10.352	2895	2896	2897	rBV	550	169	0.01%	0.002%
78	10.445	2922	2925	2926	rBV3	601	368	0.03%	0.003%
79	10.526	2946	2950	2951	rBV2	696	525	0.04%	0.005%
80	10.635	2982	2984	2986	rBV2	674	406	0.03%	0.004%
81	10.828	3042	3044	3048	rVB4	502	321	0.02%	0.003%
82	10.979	3089	3091	3093	rBV	414	220	0.02%	0.002%
83	11.014	3099	3102	3104	rBV3	592	369	0.03%	0.003%
84	11.181	3152	3154	3156	rBV2	952	315	0.02%	0.003%
85	11.246	3163	3174	3193	rBV	564529	863585	66.80%	7.842%
86	11.497	3249	3252	3254	rBV	494	413	0.03%	0.004%
87	11.619	3280	3290	3311	rBV	561558	907676	70.21%	8.242%
88	11.821	3350	3353	3355	rBV2	736	416	0.03%	0.004%
89	11.857	3362	3364	3368	rBV3	777	562	0.04%	0.005%
90	12.050	3422	3424	3426	rBV2	450	179	0.01%	0.002%
91	12.062	3426	3428	3430	rBV3	560	279	0.02%	0.003%
92	12.378	3520	3526	3529	rBV4	759	888	0.07%	0.008%
93	12.458	3549	3551	3554	rBV3	670	447	0.03%	0.004%
94	13.332	3821	3823	3829	rVB3	923	758	0.06%	0.007%
95	13.384	3837	3839	3840	rBV3	614	280	0.02%	0.003%
96	13.805	3967	3970	3975	rBV5	652	740	0.06%	0.007%
97	13.908	4000	4002	4003	rBV2	751	270	0.02%	0.002%
98	14.143	4071	4075	4078	rBV3	804	832	0.06%	0.008%
99	14.159	4078	4080	4083	rVV4	786	405	0.03%	0.004%
100	14.258	4109	4111	4112	rBV	652	287	0.02%	0.003%

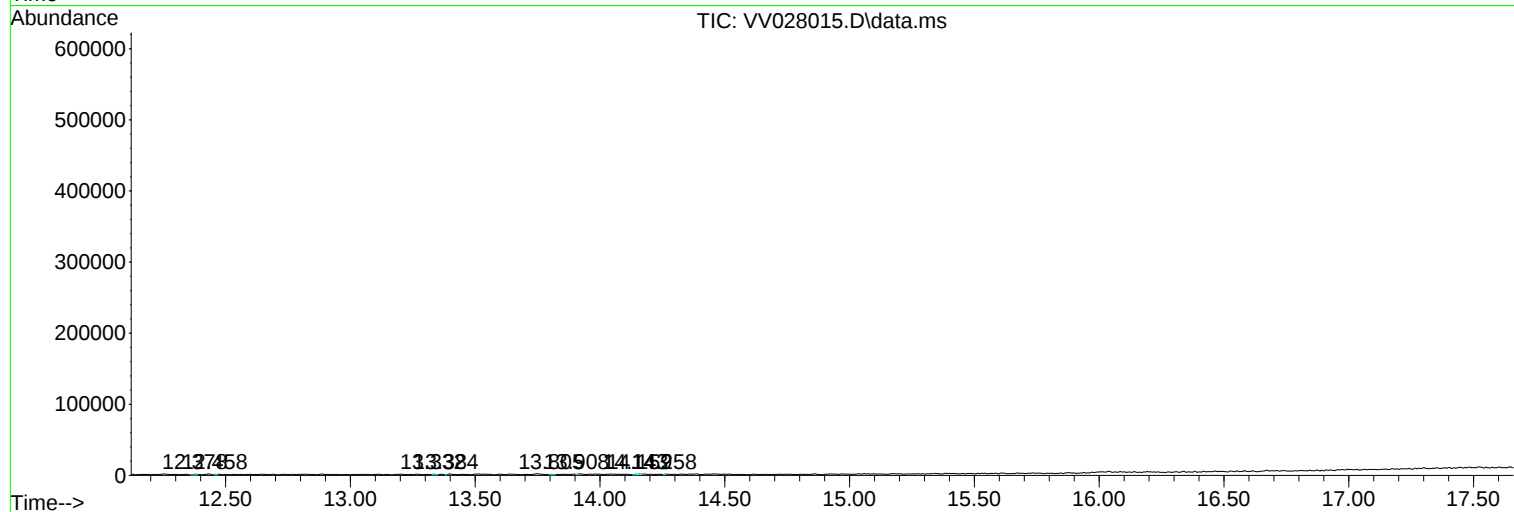
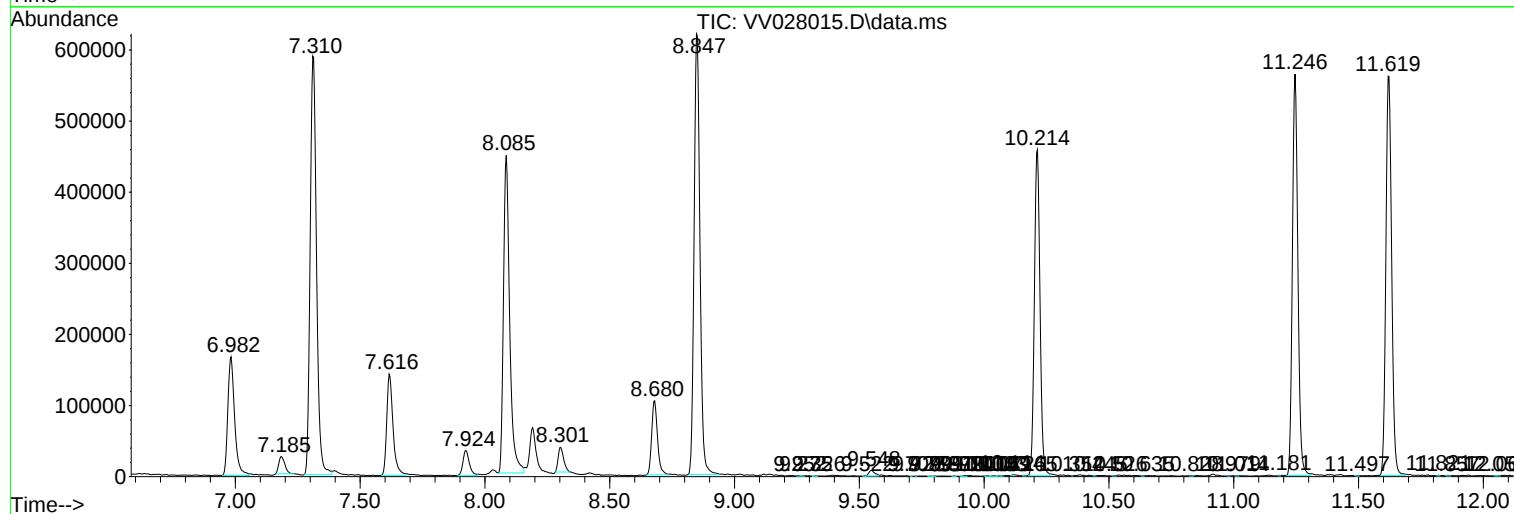
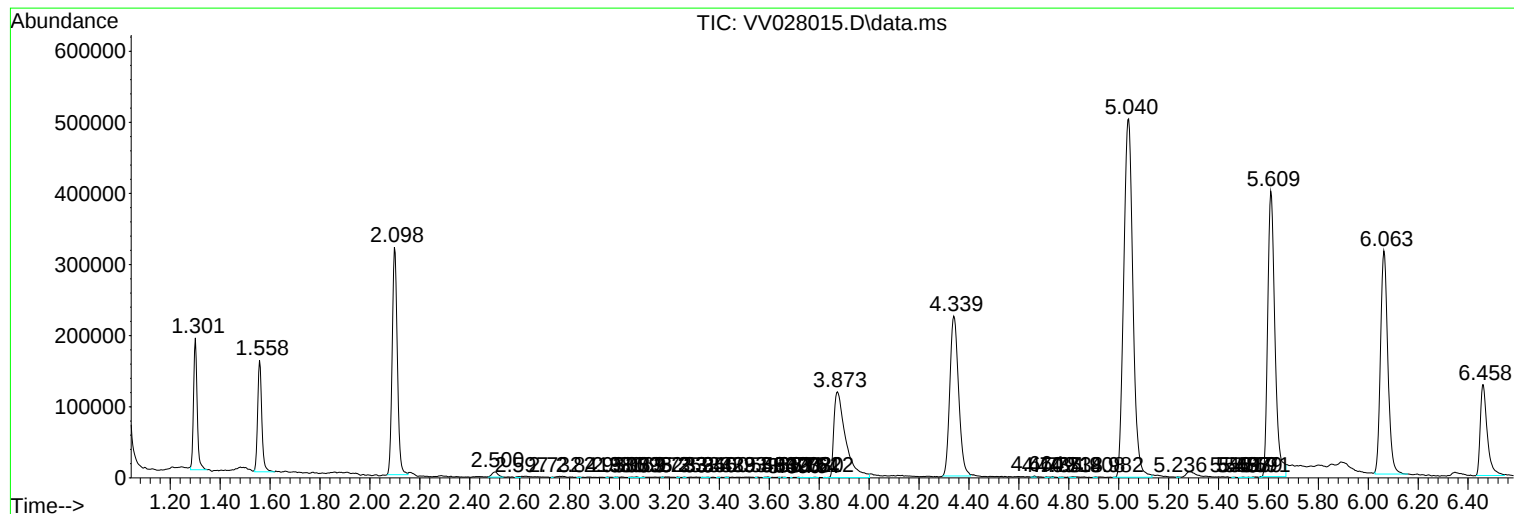
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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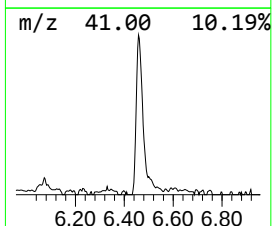
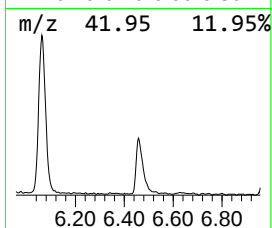
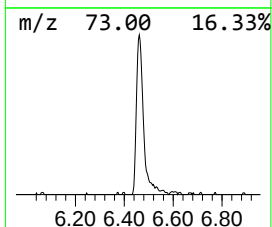
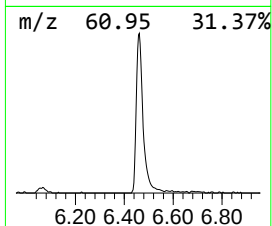
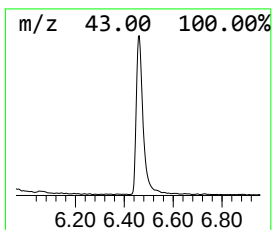
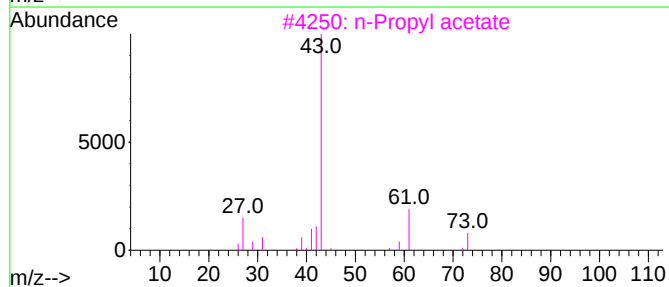
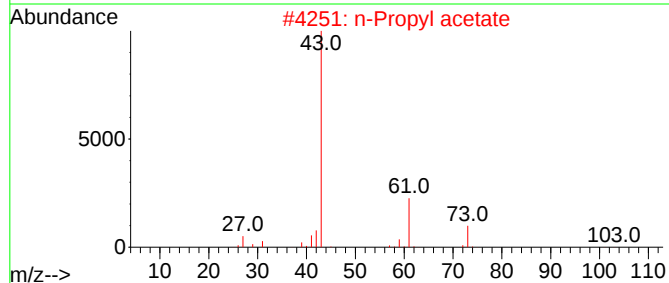
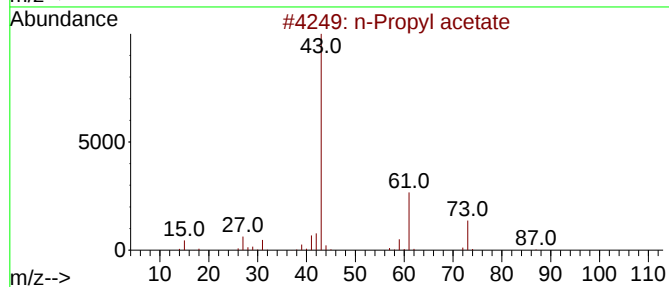
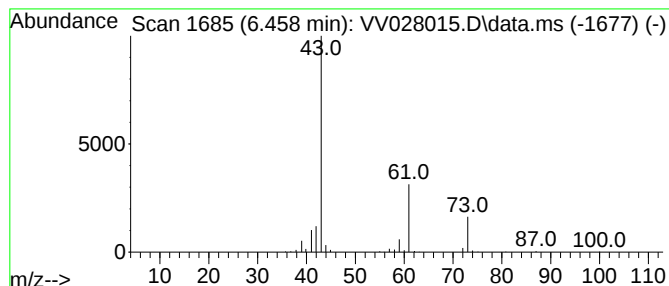
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.458	15.14 ug/L	245501	1,4-Difluorobenzene	5.609

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	72
4	Isopropyl acetate			102	C5H10O2	000108-21-4	36
5	Isopropyl acetate			102	C5H10O2	000108-21-4	33



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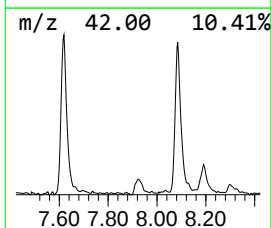
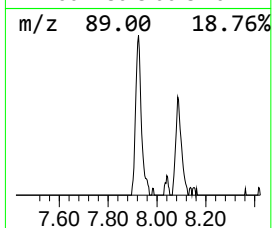
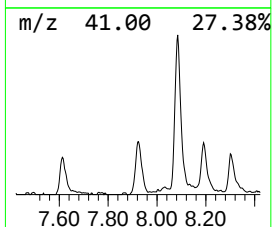
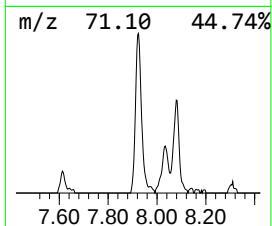
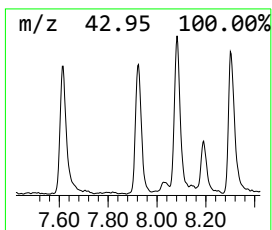
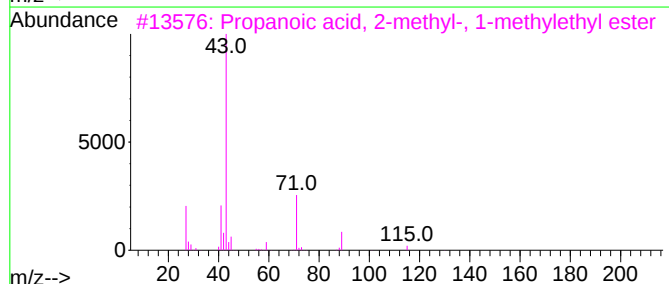
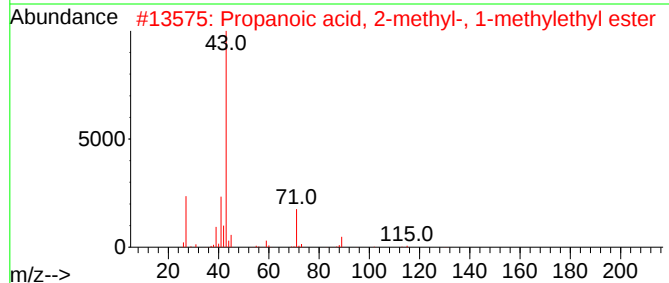
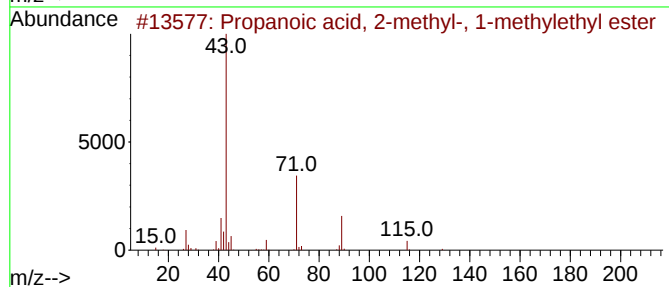
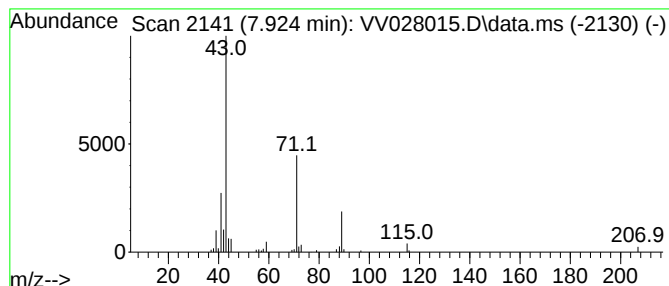
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.924	3.17 ug/L	64024	Chlorobenzene-d5	8.850

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	72
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	45



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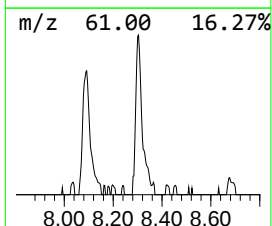
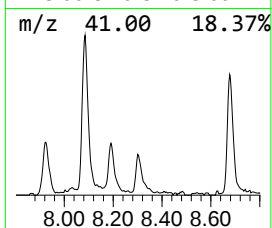
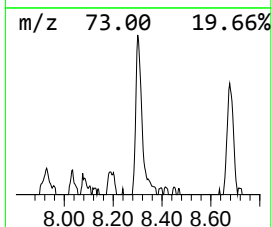
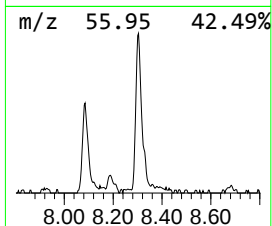
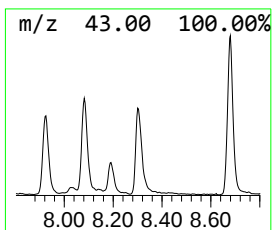
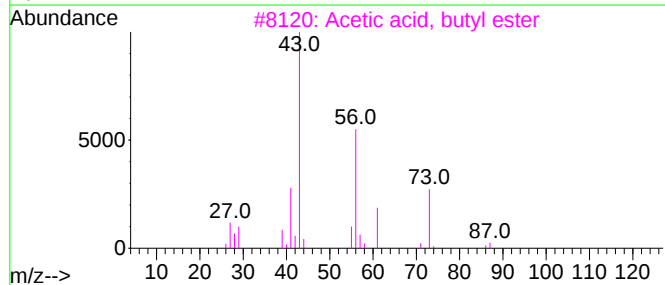
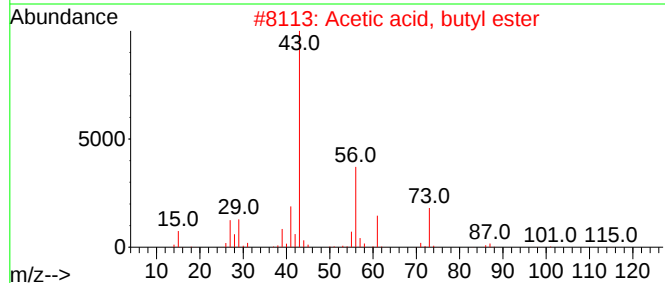
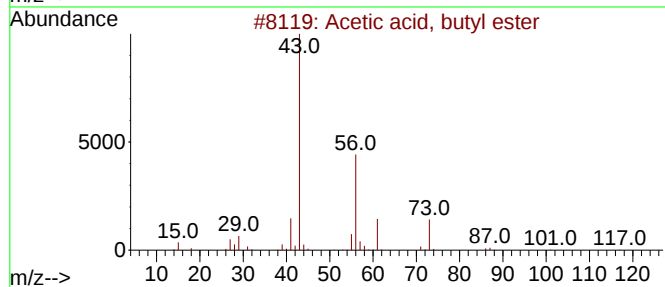
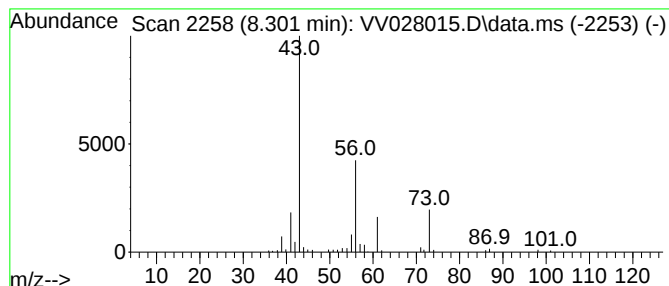
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Peak Number 4 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.301	2.63 ug/L	53073	Chlorobenzene-d5	8.850

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	72
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	59
5			Isobutyl acetate	116	C6H12O2	000110-19-0	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028015.D
Acq On : 21 Sep 2022 14:41
Operator : SY/MD
Sample : PB147776TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB776

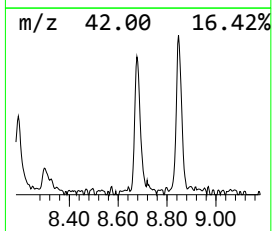
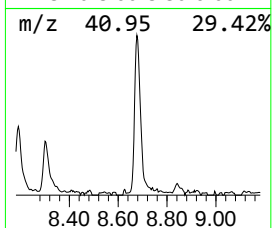
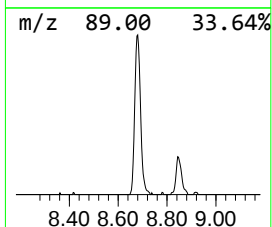
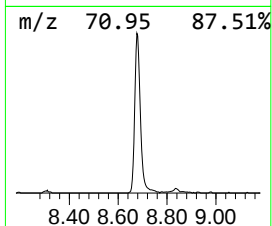
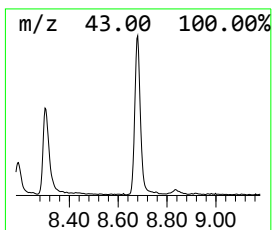
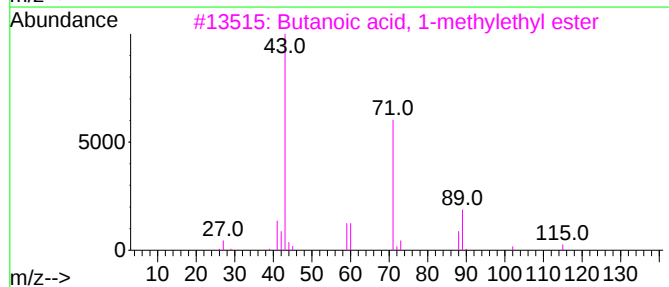
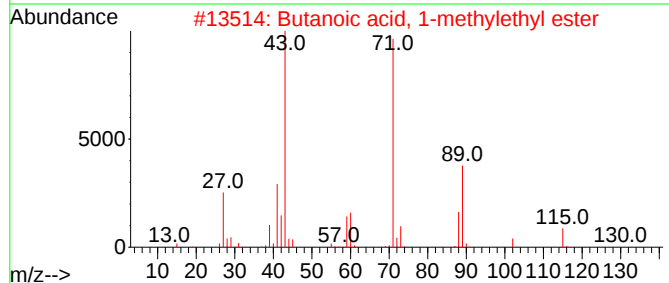
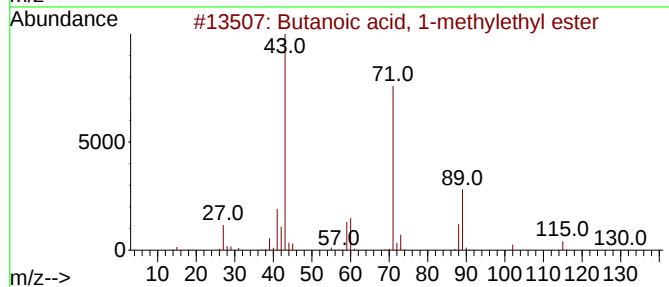
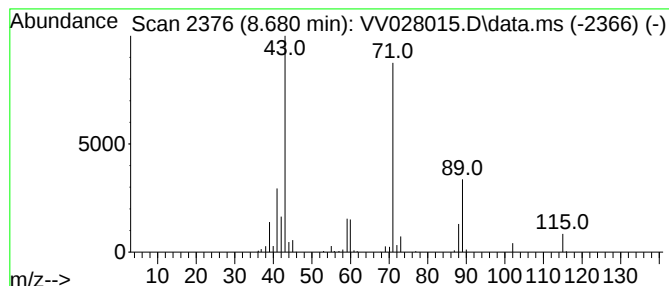
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.680	8.40 ug/L	169599	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	78
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028015.D
Acq On : 21 Sep 2022 14:41
Operator : SY/MD
Sample : PB147776TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB776

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.458	15.1	ug/L	245501	1	5.609	810673	50.0
Propanoic acid,...	7.924	3.2	ug/L	64024	2	8.850	1009770	50.0
Acetic acid, bu...	8.301	2.6	ug/L	53073	2	8.850	1009770	50.0
Butanoic acid, ...	8.680	8.4	ug/L	169599	2	8.850	1009770	50.0