

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
 Data File : VX026082.D
 Acq On : 27 Dec 2021 23:50
 Operator : JC/MD
 Sample : PB141699TB 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VLEB699

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_X\Method\SFAMXLM122321WMA.M

Title : VOC Analysis

Signal : TIC: VX026082.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	53	rBV	96889	100837	3.44%	0.690%
2	1.672	92	96	104	rVB	92495	106528	3.64%	0.729%
3	2.313	195	201	209	rBV	172654	276425	9.44%	1.891%
4	2.392	210	214	222	rVB	14598	26176	0.89%	0.179%
5	2.660	256	258	259	rBV	786	514	0.02%	0.004%
6	2.794	274	280	288	rVB	48788	90808	3.10%	0.621%
7	3.032	316	319	321	rBV2	502	562	0.02%	0.004%
8	3.215	346	349	352	rVB2	844	1124	0.04%	0.008%
9	3.245	352	354	356	rBV2	556	620	0.02%	0.004%
10	3.325	365	367	368	rBV	810	599	0.02%	0.004%
11	3.501	394	396	397	rVB	1306	696	0.02%	0.005%
12	3.520	397	399	401	rBV2	723	992	0.03%	0.007%
13	3.684	424	426	428	rVB	813	586	0.02%	0.004%
14	4.044	484	485	488	rBV2	498	608	0.02%	0.004%
15	4.129	497	499	501	rVV2	584	521	0.02%	0.004%
16	4.263	518	521	522	rBV	787	578	0.02%	0.004%
17	4.294	522	526	528	rVB2	479	600	0.02%	0.004%
18	4.324	528	531	532	rBV	607	578	0.02%	0.004%
19	4.458	544	553	568	rBV	72671	215762	7.37%	1.476%
20	4.745	597	600	601	rBV	697	744	0.03%	0.005%
21	4.952	632	634	636	rBV2	774	485	0.02%	0.003%
22	5.068	640	653	665	rBV	124301	364915	12.46%	2.496%
23	5.318	690	694	696	rBV2	855	1092	0.04%	0.007%
24	5.471	717	719	721	rBV2	713	834	0.03%	0.006%
25	5.708	756	758	759	rVB	862	486	0.02%	0.003%
26	5.727	759	761	764	rBV	463	548	0.02%	0.004%
27	5.977	788	802	816	rBV2	290035	876261	29.91%	5.993%
28	6.342	855	862	872	rVV	13363	34536	1.18%	0.236%
29	6.434	875	877	880	rBV2	517	577	0.02%	0.004%
30	6.665	913	915	918	rVB2	1222	1070	0.04%	0.007%
31	6.763	922	931	944	rBV	180153	456755	15.59%	3.124%
32	7.312	1013	1021	1038	rVB	190870	415312	14.18%	2.841%
33	7.464	1040	1046	1052	rBV3	7859	18286	0.62%	0.125%
34	7.604	1064	1069	1071	rBV3	3509	5717	0.20%	0.039%
35	7.647	1071	1076	1080	rVV	9114	16008	0.55%	0.109%
36	7.799	1094	1101	1115	rBV	1194551	2034960	69.47%	13.918%

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 Title : VOC Analysis

37	8.250	1173	1175	1176	rBV	622	491	0.02%	0.003%
38	8.330	1181	1188	1200	rVB	126378	213992	7.30%	1.464%
39	8.549	1218	1224	1234	rBV	201555	312797	10.68%	2.139%
40	8.653	1234	1241	1249	rBV	421197	678618	23.17%	4.641%
41	8.805	1262	1266	1272	rBV3	3448	5381	0.18%	0.037%
42	8.866	1272	1276	1282	rVB2	4235	7391	0.25%	0.051%
43	8.952	1284	1290	1298	rBV2	113378	167972	5.73%	1.149%
44	9.086	1309	1312	1314	rBV2	950	1026	0.04%	0.007%
45	9.122	1316	1318	1320	rVB	932	605	0.02%	0.004%
46	9.250	1333	1339	1346	rBV	58021	91272	3.12%	0.624%
47	9.311	1346	1349	1350	rVV	10226	12369	0.42%	0.085%
48	9.342	1350	1354	1357	rVV	143075	200678	6.85%	1.373%
49	9.384	1357	1361	1372	rVV	372277	535383	18.28%	3.662%
50	9.482	1372	1377	1388	rVV	2179737	2929444	100.00%	20.036%
51	9.580	1388	1393	1406	rVB	250864	330302	11.28%	2.259%
52	9.915	1442	1448	1463	rBV	1519055	1891367	64.56%	12.936%
53	10.055	1465	1471	1478	rBV	398600	538961	18.40%	3.686%
54	10.409	1527	1529	1531	rVB	1050	617	0.02%	0.004%
55	10.427	1531	1532	1535	rVB	770	539	0.02%	0.004%
56	10.488	1540	1542	1543	rVV	813	680	0.02%	0.005%
57	10.506	1543	1545	1553	rVB	3800	4569	0.16%	0.031%
58	10.640	1563	1567	1579	rVB	54575	69057	2.36%	0.472%
59	10.896	1607	1609	1610	rBV	729	561	0.02%	0.004%
60	11.195	1652	1658	1665	rBV	345479	430001	14.68%	2.941%
61	11.329	1674	1680	1684	rVB2	7446	12034	0.41%	0.082%
62	11.451	1697	1700	1703	rBV2	3824	4627	0.16%	0.032%
63	11.713	1741	1743	1745	rBV	643	535	0.02%	0.004%
64	11.750	1746	1749	1754	rVB2	3301	4416	0.15%	0.030%
65	11.805	1756	1758	1761	rBV2	492	650	0.02%	0.004%
66	11.939	1777	1780	1782	rBV3	1453	1557	0.05%	0.011%
67	11.963	1782	1784	1785	rBV	752	491	0.02%	0.003%
68	12.024	1789	1794	1801	rBV	410483	503984	17.20%	3.447%
69	12.152	1813	1815	1820	rVB2	2186	2507	0.09%	0.017%
70	12.323	1837	1843	1851	rVB	449310	582792	19.89%	3.986%
71	12.475	1866	1868	1869	rBV2	726	512	0.02%	0.004%
72	12.670	1898	1900	1901	rVB2	970	566	0.02%	0.004%
73	12.701	1901	1905	1906	rBV2	590	619	0.02%	0.004%
74	12.719	1906	1908	1909	rVB	794	515	0.02%	0.004%
75	12.768	1909	1916	1921	rBV2	3788	6638	0.23%	0.045%
76	12.975	1949	1950	1955	rVB	569	708	0.02%	0.005%

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 Title : VOC Analysis

77	13.213	1987	1989	1992	rBV2	666	628	0.02%	0.004%
78	13.414	2020	2022	2024	rVB	874	628	0.02%	0.004%
79	13.786	2078	2083	2087	rBV5	904	1801	0.06%	0.012%
80	13.878	2096	2098	2102	rBV2	619	857	0.03%	0.006%
81	13.957	2110	2111	2116	rVB3	785	881	0.03%	0.006%
82	14.067	2127	2129	2130	rBV	674	508	0.02%	0.003%
83	14.134	2137	2140	2147	rVB3	2686	3910	0.13%	0.027%
84	14.213	2151	2153	2156	rVV	517	466	0.02%	0.003%
85	14.243	2156	2158	2161	rVB2	1142	786	0.03%	0.005%
86	14.280	2161	2164	2166	rBV	679	703	0.02%	0.005%
87	14.329	2170	2172	2174	rBV	614	554	0.02%	0.004%
88	14.396	2181	2183	2184	rBV	629	516	0.02%	0.004%
89	14.481	2195	2197	2201	rVB2	754	936	0.03%	0.006%
90	14.652	2223	2225	2228	rBV2	429	566	0.02%	0.004%
91	14.822	2251	2253	2255	rBV2	578	611	0.02%	0.004%
92	14.963	2275	2276	2279	rBV	832	784	0.03%	0.005%
93	15.030	2286	2287	2289	rBV	843	635	0.02%	0.004%
94	15.127	2301	2303	2304	rBV2	585	520	0.02%	0.004%
95	15.237	2319	2321	2324	rVV	552	499	0.02%	0.003%
96	15.530	2367	2369	2372	rBV2	863	915	0.03%	0.006%
97	15.652	2386	2389	2390	rBV2	523	608	0.02%	0.004%
98	16.011	2446	2448	2450	rBV	823	570	0.02%	0.004%
99	16.359	2503	2505	2507	rBV2	749	648	0.02%	0.004%
100	16.658	2552	2554	2555	rBV	558	469	0.02%	0.003%

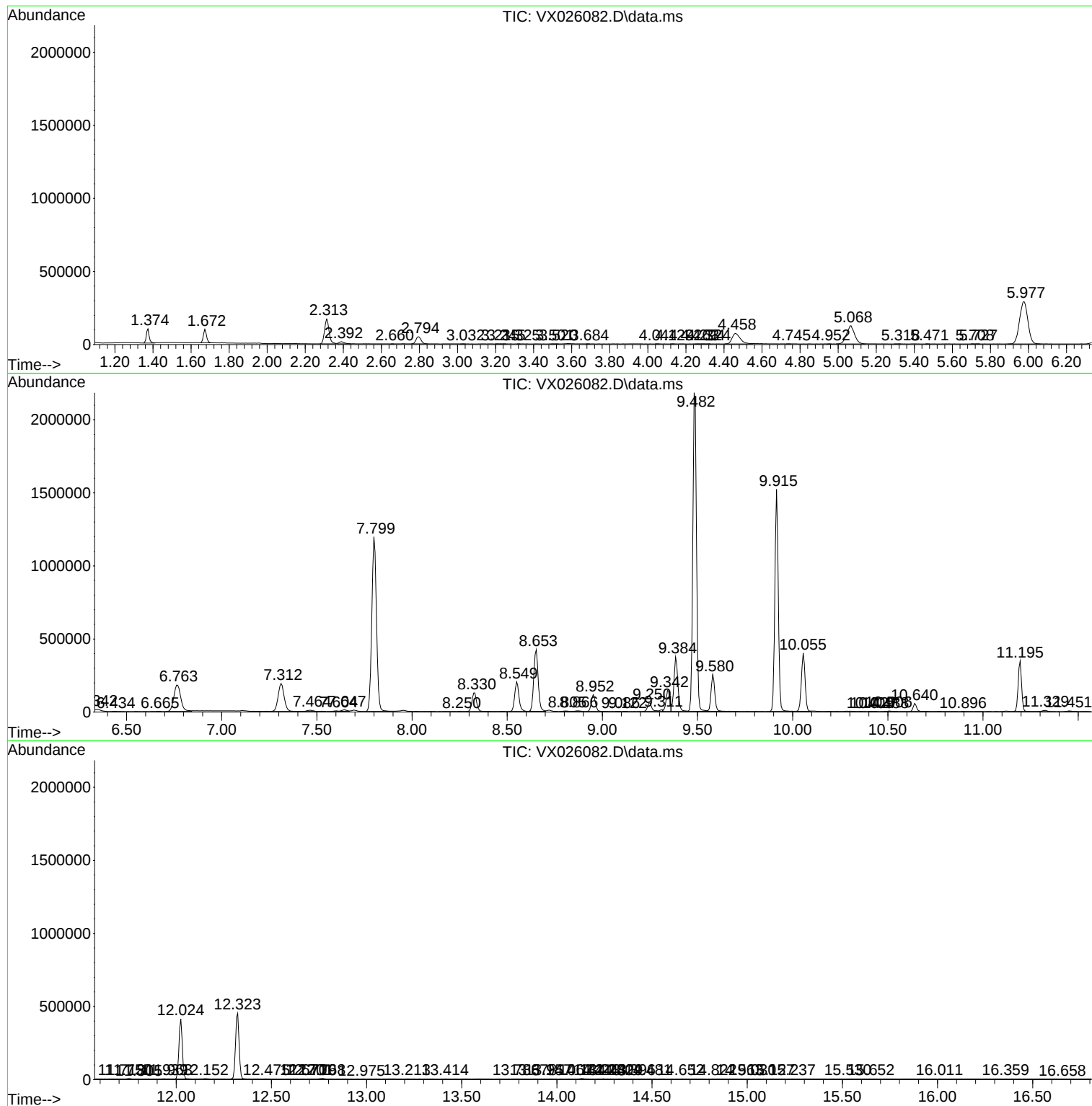
Sum of corrected areas: 14620923

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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 38 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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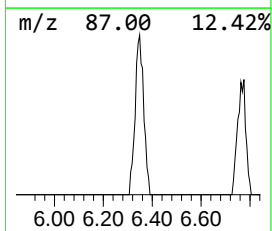
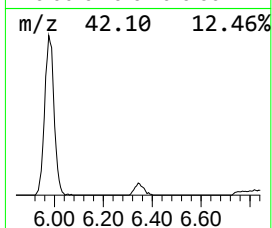
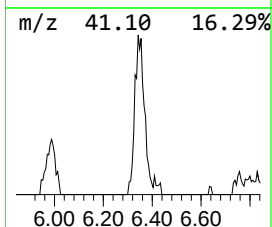
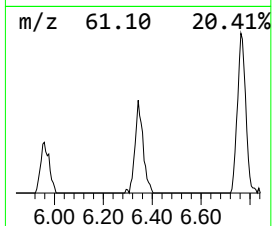
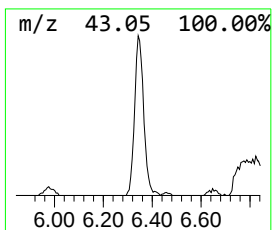
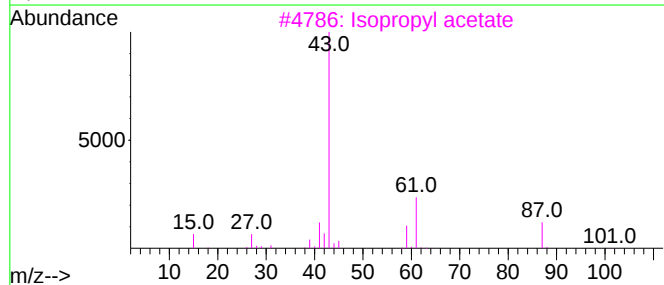
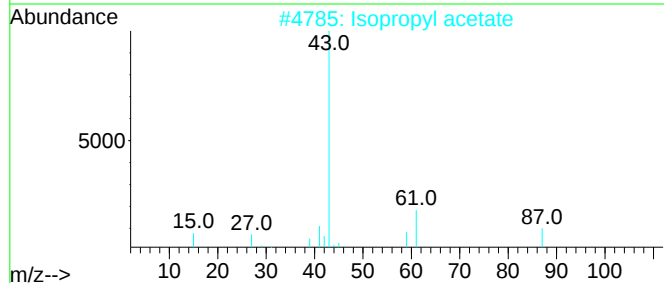
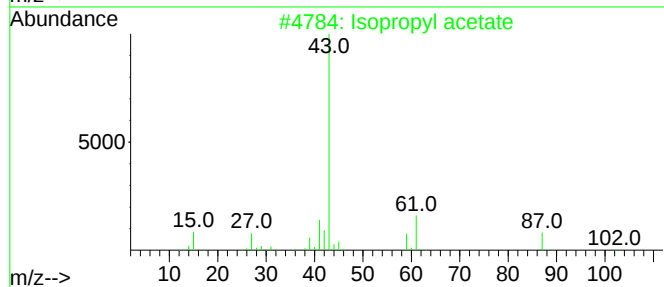
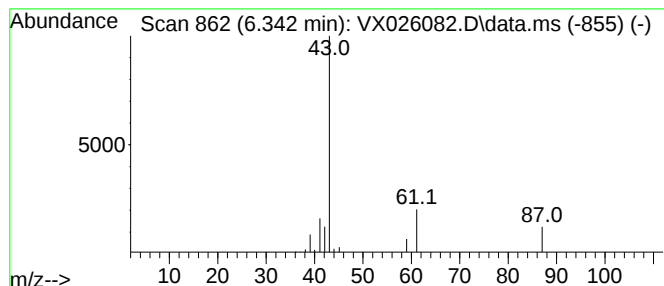
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Isopropyl acetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.342	3.78 ug/L	34536	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl acetate			102	C5H10O2	000108-21-4	74
2	Isopropyl acetate			102	C5H10O2	000108-21-4	43
3	Isopropyl acetate			102	C5H10O2	000108-21-4	38
4	n-Propyl acetate			102	C5H10O2	000109-60-4	9
5	Isopropyl acetate			102	C5H10O2	000108-21-4	9



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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
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ClientSampleId :
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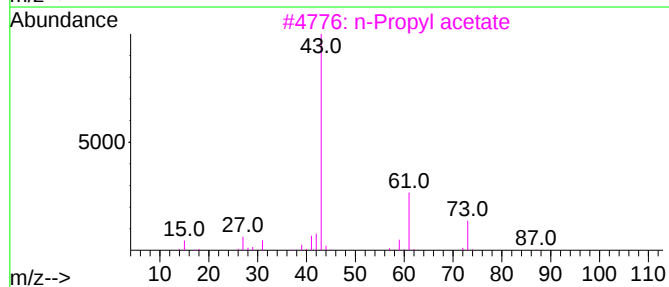
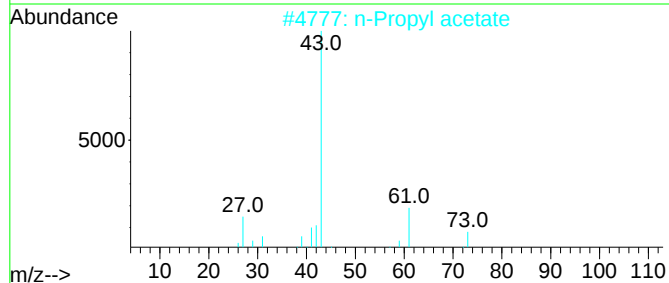
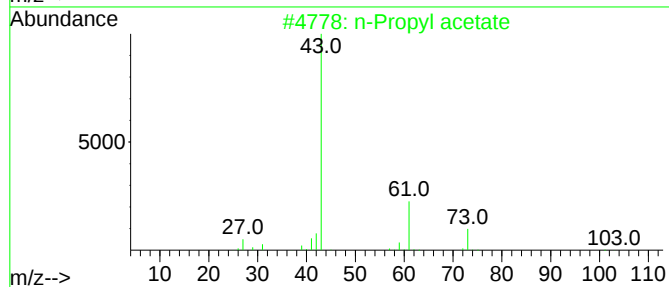
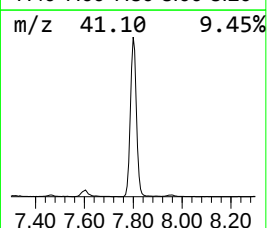
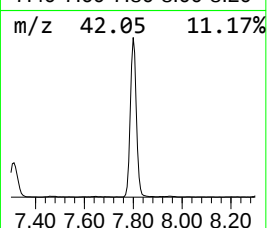
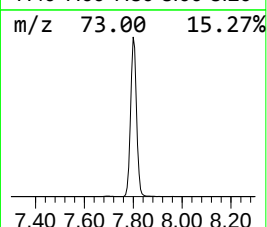
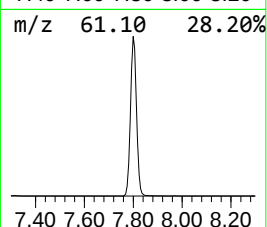
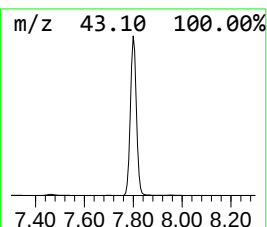
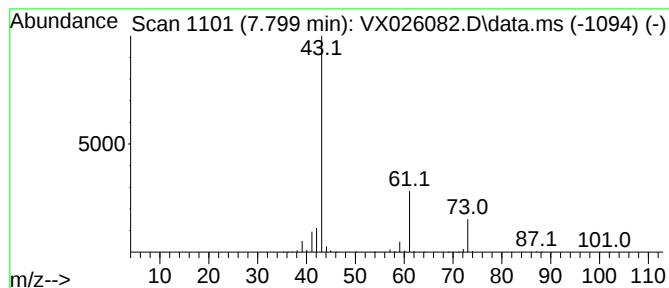
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	222.76 ug/L	2034960	1,4-Difluorobenzene	6.769

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



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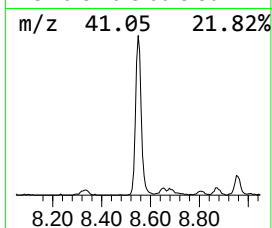
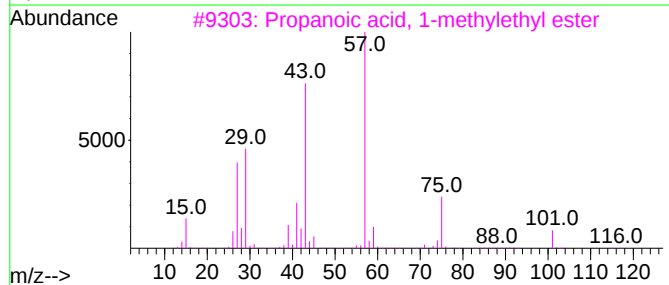
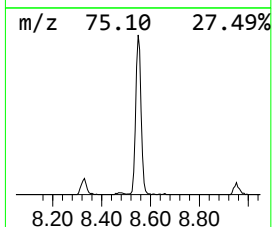
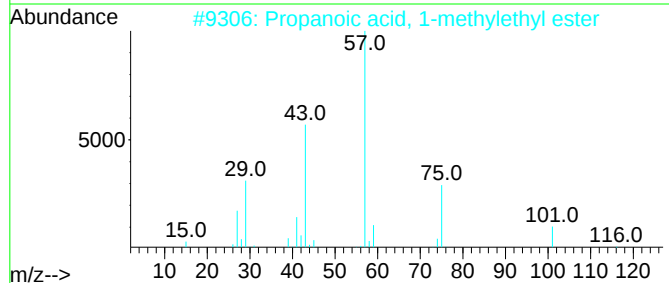
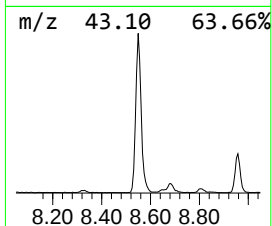
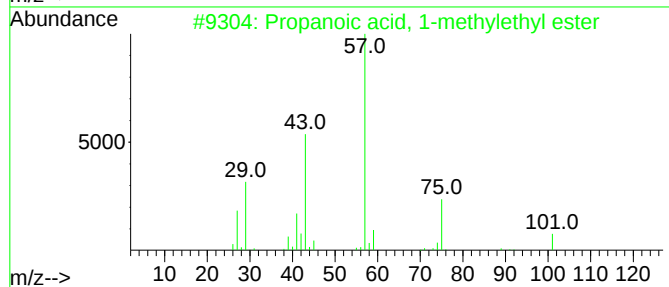
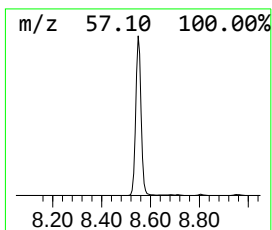
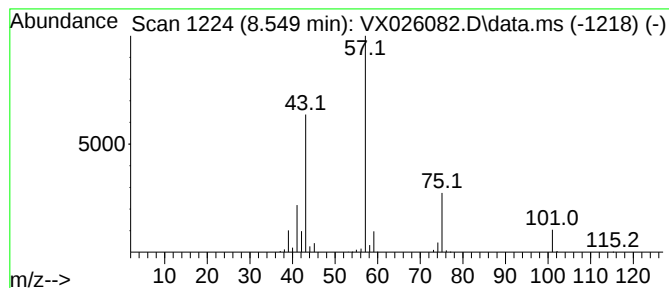
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	29.02 ug/L	312797	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45



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Acq On : 27 Dec 2021 23:50
Operator : JC/MD
Sample : PB141699TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB699

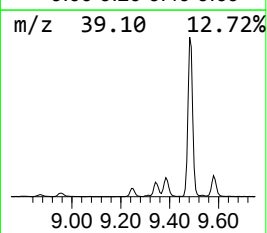
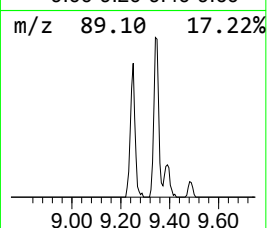
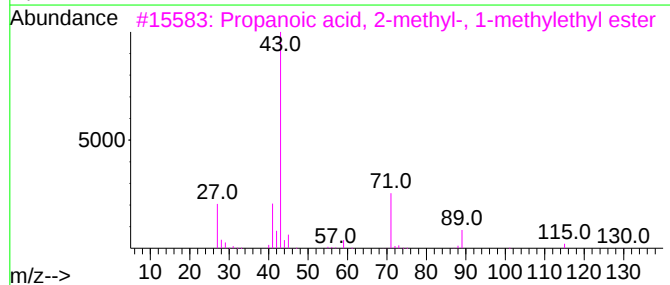
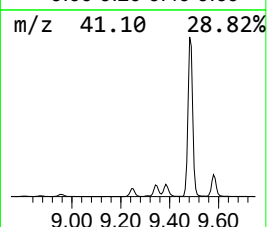
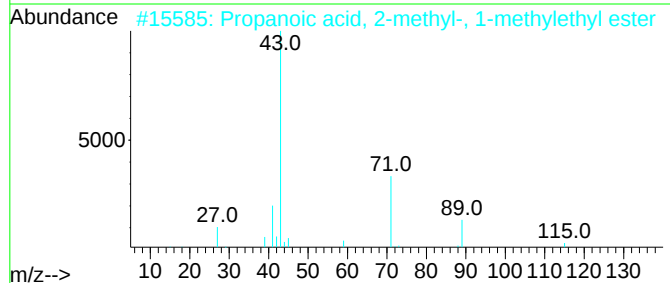
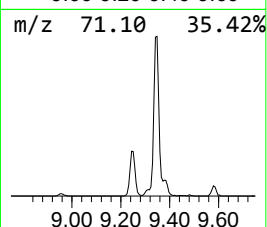
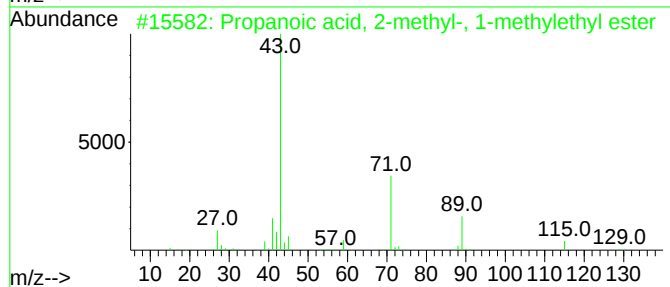
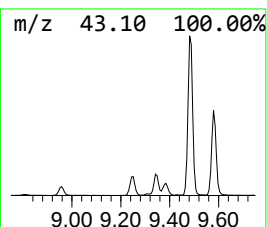
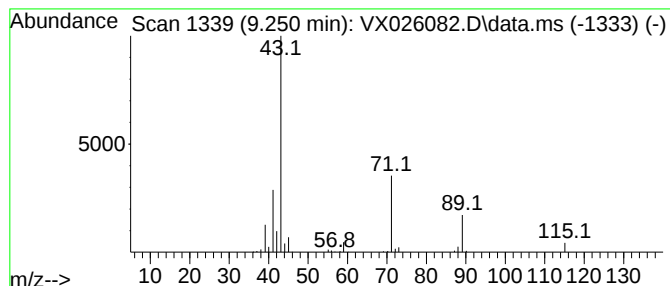
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Quant Title : VOC Analysis

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

Peak Number 7 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.250	8.47 ug/L	91272	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	90
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-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026082.D
Acq On : 27 Dec 2021 23:50
Operator : JC/MD
Sample : PB141699TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB699

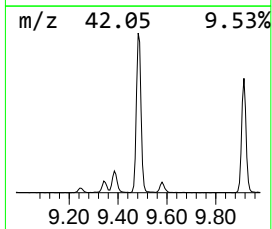
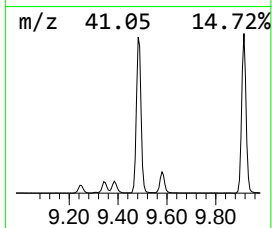
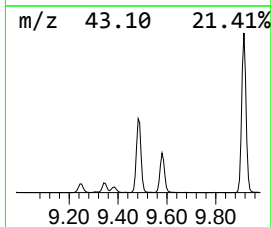
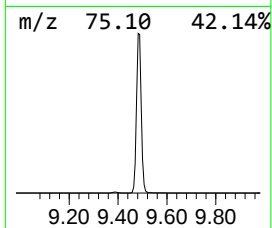
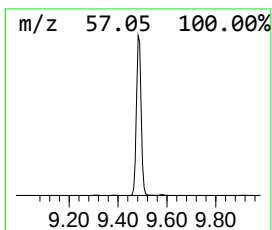
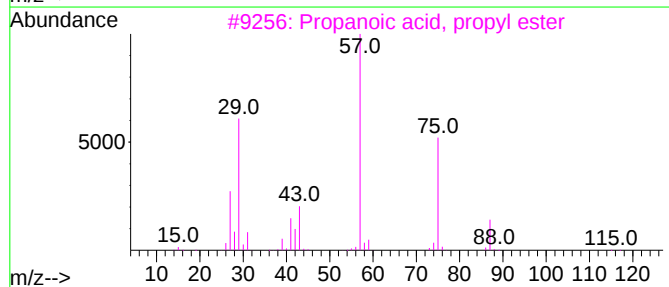
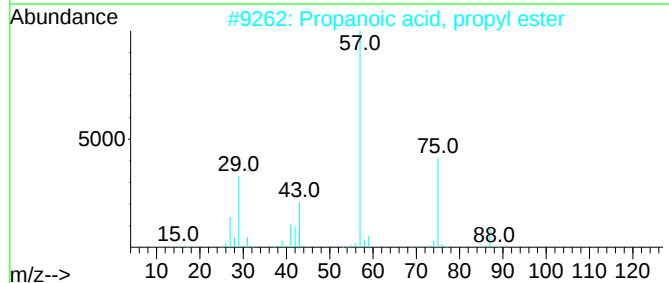
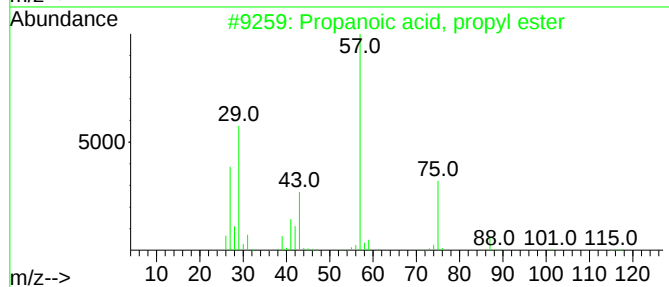
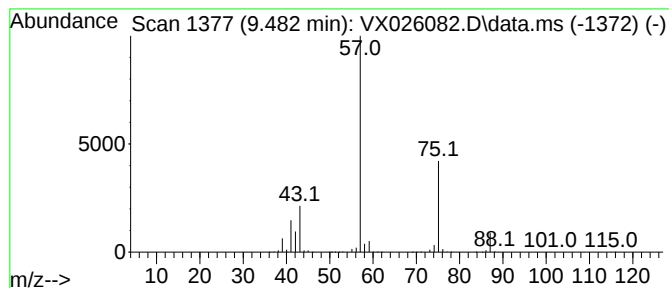
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Quant Title : VOC Analysis

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

Peak Number 8 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	271.77 ug/L	2929440	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026082.D
Acq On : 27 Dec 2021 23:50
Operator : JC/MD
Sample : PB141699TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB699

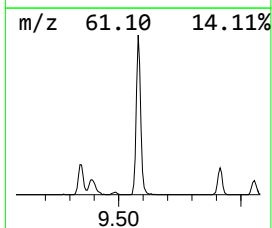
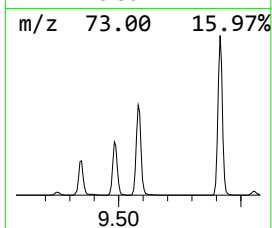
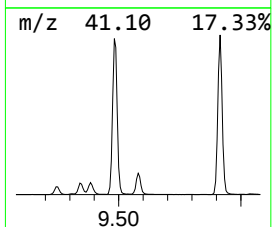
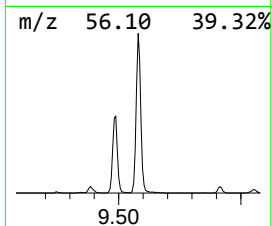
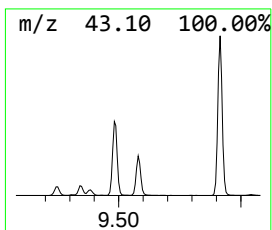
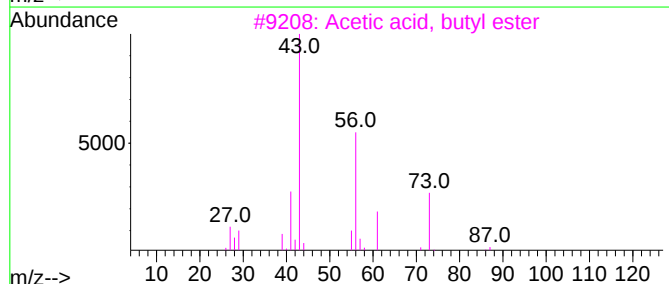
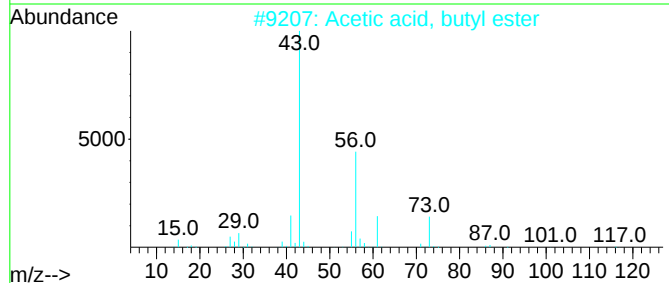
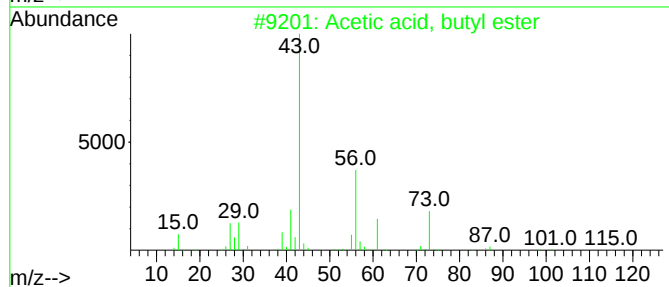
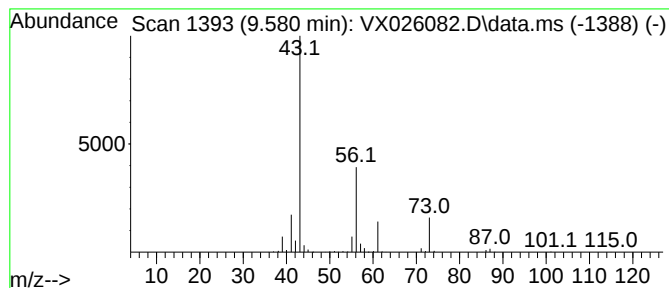
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Quant Title : VOC Analysis

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

Peak Number 9 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	30.64 ug/L	330302	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026082.D
Acq On : 27 Dec 2021 23:50
Operator : JC/MD
Sample : PB141699TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB699

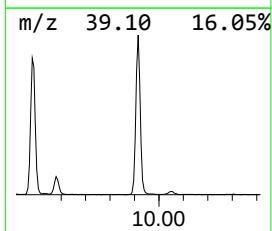
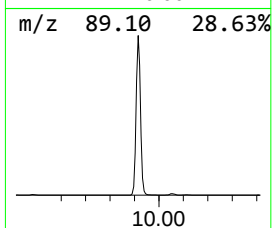
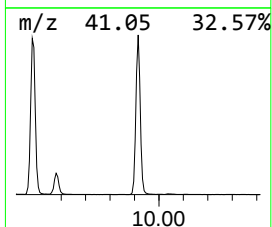
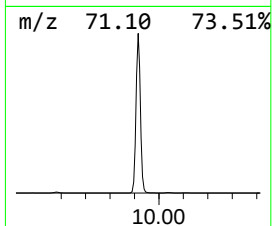
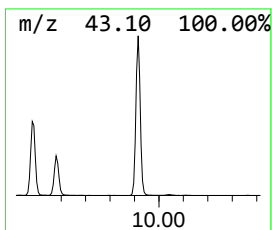
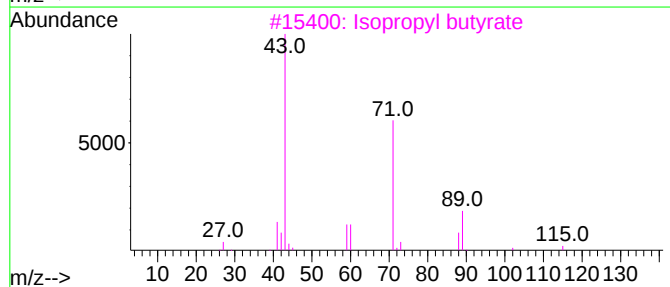
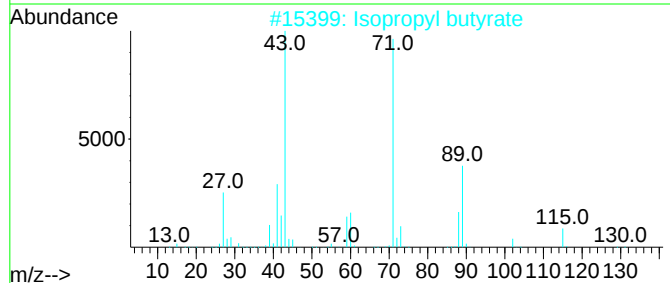
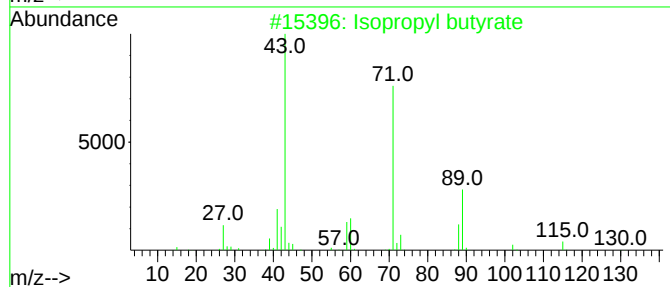
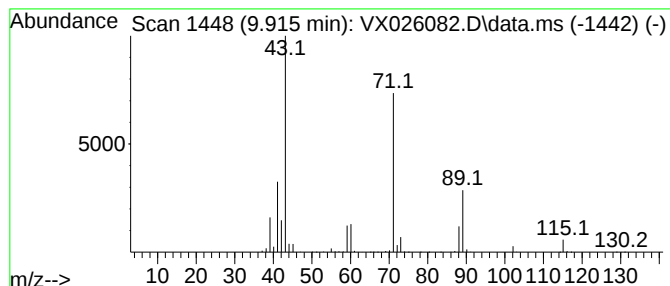
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Quant Title : VOC Analysis

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

Peak Number 10 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	175.46 ug/L	1891370	Chlorobenzene-d5	10.055

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	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026082.D
Acq On : 27 Dec 2021 23:50
Operator : JC/MD
Sample : PB141699TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB699

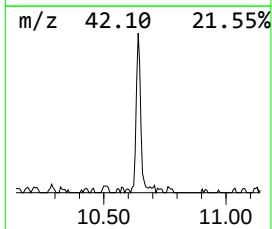
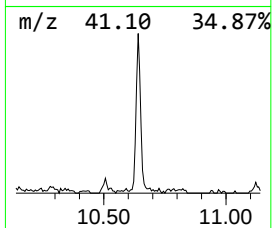
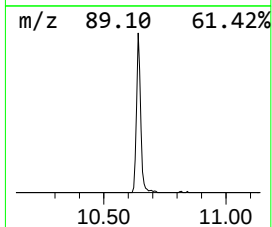
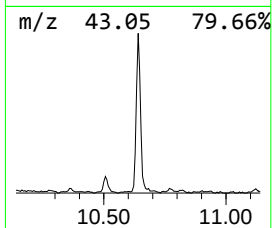
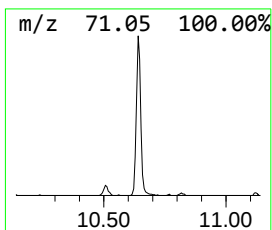
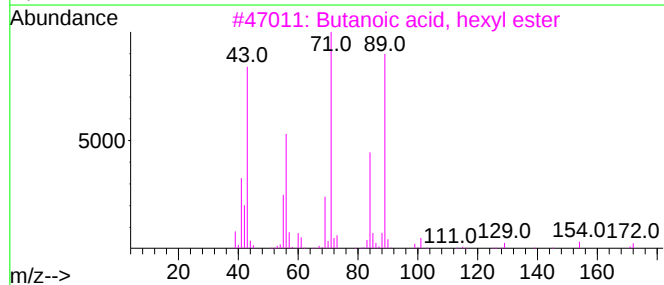
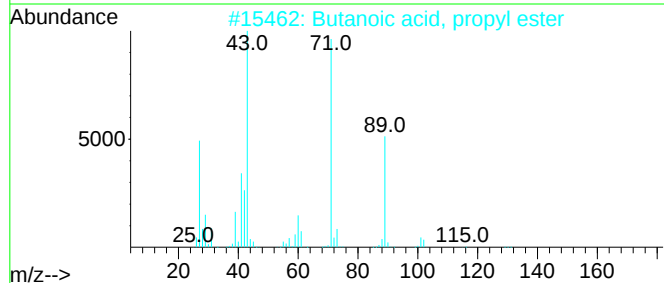
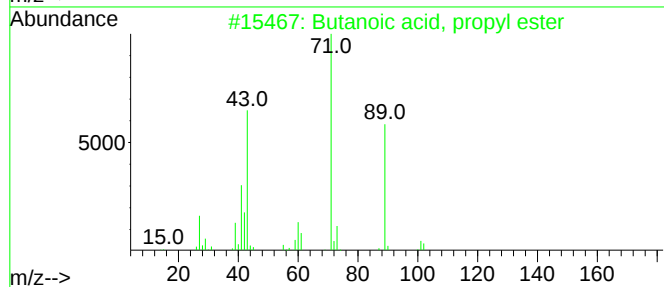
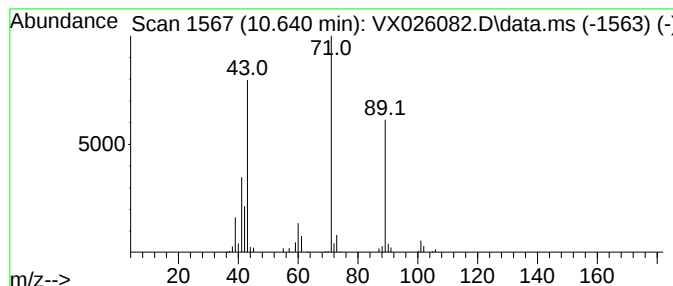
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Quant Title : VOC Analysis

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

Peak Number 11 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	6.41 ug/L	69057	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	83
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	83
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	83
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026082.D
Acq On : 27 Dec 2021 23:50
Operator : JC/MD
Sample : PB141699TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB699

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122321WMA.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
Isopropyl acetate	6.342	3.8	ug/L	34536	1	6.769	456755	50.0
n-Propyl acetate	7.799	222.8	ug/L	2034960	1	6.769	456755	50.0
Propanoic acid,...	8.549	29.0	ug/L	312797	2	10.055	538961	50.0
Propanoic acid,...	9.250	8.5	ug/L	91272	2	10.055	538961	50.0
Propanoic acid,...	9.482	271.8	ug/L	2929440	2	10.055	538961	50.0
Acetic acid, bu...	9.580	30.6	ug/L	330302	2	10.055	538961	50.0
Isopropyl butyrate	9.915	175.5	ug/L	1891370	2	10.055	538961	50.0
Butanoic acid, ...	10.640	6.4	ug/L	69057	2	10.055	538961	50.0