

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
 Data File : VX026086.D
 Acq On : 28 Dec 2021 01:22
 Operator : JC/MD
 Sample : PB141699ZHE#04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB141699ZHE#04

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: VX026086.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	55	rVB	96456	100451	3.52%	0.684%
2	1.672	92	96	103	rVB	93041	107380	3.76%	0.732%
3	2.313	195	201	209	rBV	177040	284761	9.97%	1.940%
4	2.386	209	213	221	rVB	17149	29177	1.02%	0.199%
5	2.477	227	228	231	rBV2	733	732	0.03%	0.005%
6	2.794	274	280	289	rVB	51768	93818	3.28%	0.639%
7	2.922	299	301	302	rBV2	860	777	0.03%	0.005%
8	3.166	339	341	342	rBV2	547	404	0.01%	0.003%
9	3.325	365	367	369	rBV2	738	722	0.03%	0.005%
10	3.446	383	387	390	rBV3	1335	2088	0.07%	0.014%
11	3.581	403	409	418	rBV2	4114	9486	0.33%	0.065%
12	3.751	436	437	439	rBV	551	490	0.02%	0.003%
13	3.916	463	464	465	rBV	762	384	0.01%	0.003%
14	3.989	474	476	479	rVB2	650	598	0.02%	0.004%
15	4.013	479	480	483	rBV2	576	520	0.02%	0.004%
16	4.458	544	553	567	rBV	75562	221176	7.74%	1.507%
17	4.873	619	621	624	rVB2	469	404	0.01%	0.003%
18	4.916	626	628	630	rBV	455	456	0.02%	0.003%
19	5.068	640	653	667	rBV	116131	366054	12.81%	2.494%
20	5.214	675	677	679	rBV	537	466	0.02%	0.003%
21	5.361	699	701	704	rBV	538	659	0.02%	0.004%
22	5.562	732	734	738	rBV2	614	842	0.03%	0.006%
23	5.745	762	764	765	rVB	883	510	0.02%	0.003%
24	5.763	765	767	768	rBV2	910	809	0.03%	0.006%
25	5.818	774	776	781	rBV2	424	898	0.03%	0.006%
26	5.867	781	784	786	rVB2	625	557	0.02%	0.004%
27	5.885	786	787	790	rBV2	485	624	0.02%	0.004%
28	5.976	790	802	815	rVV2	293925	872537	30.54%	5.944%
29	6.105	821	823	826	rBV2	913	817	0.03%	0.006%
30	6.342	851	862	874	rBV2	13839	38918	1.36%	0.265%
31	6.446	877	879	880	rVV	922	650	0.02%	0.004%
32	6.489	884	886	888	rVV3	580	572	0.02%	0.004%
33	6.537	892	894	896	rVB	658	579	0.02%	0.004%
34	6.556	896	897	900	rBV	725	646	0.02%	0.004%
35	6.763	921	931	945	rBV	206770	530425	18.57%	3.613%
36	7.312	1013	1021	1033	rVB	188197	410875	14.38%	2.799%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

37	7.458	1041	1045	1052	rVB	7173	13567	0.47%	0.092%
38	7.641	1072	1075	1080	rVB	8343	12714	0.45%	0.087%
39	7.799	1093	1101	1118	rBV	1177379	1989958	69.65%	13.556%
40	8.324	1180	1187	1196	rBV	132403	219771	7.69%	1.497%
41	8.549	1218	1224	1234	rBV	202274	304535	10.66%	2.075%
42	8.653	1234	1241	1249	rBV	442558	704761	24.67%	4.801%
43	8.866	1272	1276	1283	rBV3	4046	6833	0.24%	0.047%
44	8.952	1285	1290	1298	rVV2	113213	170280	5.96%	1.160%
45	9.244	1333	1338	1343	rBV	56690	86584	3.03%	0.590%
46	9.342	1350	1354	1357	rBV	133224	181552	6.35%	1.237%
47	9.384	1357	1361	1372	rVB	373379	537871	18.83%	3.664%
48	9.482	1372	1377	1388	rBV	2161844	2856959	100.00%	19.463%
49	9.580	1388	1393	1406	rVB	248547	325225	11.38%	2.216%
50	9.915	1442	1448	1461	rBV	1474896	1849661	64.74%	12.601%
51	10.055	1465	1471	1479	rVV	441608	593653	20.78%	4.044%
52	10.281	1505	1508	1511	rBV2	1706	2625	0.09%	0.018%
53	10.506	1542	1545	1552	rVB3	3032	5193	0.18%	0.035%
54	10.640	1562	1567	1576	rBV	54629	68487	2.40%	0.467%
55	10.854	1601	1602	1605	rVB2	753	495	0.02%	0.003%
56	10.988	1622	1624	1625	rBV	524	361	0.01%	0.002%
57	11.122	1643	1646	1650	rVB3	2182	2505	0.09%	0.017%
58	11.195	1652	1658	1664	rBV	338779	444987	15.58%	3.031%
59	11.323	1674	1679	1684	rVB2	13722	21538	0.75%	0.147%
60	11.451	1696	1700	1707	rBV	9353	12210	0.43%	0.083%
61	11.536	1711	1714	1716	rBV3	779	892	0.03%	0.006%
62	11.671	1732	1736	1737	rBV2	671	837	0.03%	0.006%
63	11.750	1746	1749	1754	rBV5	1745	2384	0.08%	0.016%
64	11.841	1761	1764	1767	rBV2	791	870	0.03%	0.006%
65	12.024	1789	1794	1807	rBV	443501	538088	18.83%	3.666%
66	12.213	1823	1825	1826	rBV	707	433	0.02%	0.003%
67	12.323	1837	1843	1849	rBV	468271	605822	21.21%	4.127%
68	12.475	1866	1868	1870	rBV3	700	562	0.02%	0.004%
69	12.536	1877	1878	1881	rBV3	515	510	0.02%	0.003%
70	12.731	1908	1910	1911	rBV	632	637	0.02%	0.004%
71	12.768	1912	1916	1921	rVV2	5711	8212	0.29%	0.056%
72	12.835	1925	1927	1930	rBV	773	655	0.02%	0.004%
73	13.048	1961	1962	1966	rBV3	573	582	0.02%	0.004%
74	13.134	1971	1976	1978	rBV3	1397	2004	0.07%	0.014%
75	13.219	1986	1990	1992	rVB3	860	1170	0.04%	0.008%
76	13.292	1997	2002	2007	rVB2	771	1646	0.06%	0.011%

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Integrator: RTE

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Filtering: 5

Sampling : 1

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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\SFAMXML122321WMA.M
 Title : VOC Analysis

77	13.341	2007	2010	2012	rBV2	565	825	0.03%	0.006%
78	13.561	2044	2046	2048	rVB	828	529	0.02%	0.004%
79	13.579	2048	2049	2050	rBV	1014	533	0.02%	0.004%
80	13.621	2054	2056	2058	rBV2	777	685	0.02%	0.005%
81	13.689	2065	2067	2068	rBV	1391	1187	0.04%	0.008%
82	13.963	2111	2112	2113	rBV	537	344	0.01%	0.002%
83	14.134	2134	2140	2144	rVB2	3483	4685	0.16%	0.032%
84	14.268	2160	2162	2165	rBV2	498	465	0.02%	0.003%
85	14.329	2171	2172	2176	rBV	623	635	0.02%	0.004%
86	14.487	2196	2198	2199	rBV	808	596	0.02%	0.004%
87	14.664	2225	2227	2231	rBV2	713	636	0.02%	0.004%
88	14.902	2264	2266	2267	rBV2	609	352	0.01%	0.002%
89	14.950	2272	2274	2277	rVB2	799	890	0.03%	0.006%
90	14.981	2277	2279	2281	rBV	777	716	0.03%	0.005%
91	15.255	2322	2324	2325	rBV	721	490	0.02%	0.003%
92	15.389	2342	2346	2350	rBV4	1223	2364	0.08%	0.016%
93	15.487	2360	2362	2363	rBV	655	430	0.02%	0.003%
94	15.652	2387	2389	2391	rBV	527	346	0.01%	0.002%
95	15.670	2391	2392	2395	rBV	603	537	0.02%	0.004%
96	16.011	2446	2448	2450	rBV3	527	343	0.01%	0.002%
97	16.097	2458	2462	2464	rBV2	638	789	0.03%	0.005%
98	16.273	2488	2491	2492	rBV	849	823	0.03%	0.006%
99	16.487	2524	2526	2528	rBV2	673	741	0.03%	0.005%
100	16.664	2553	2555	2557	rBV	654	407	0.01%	0.003%

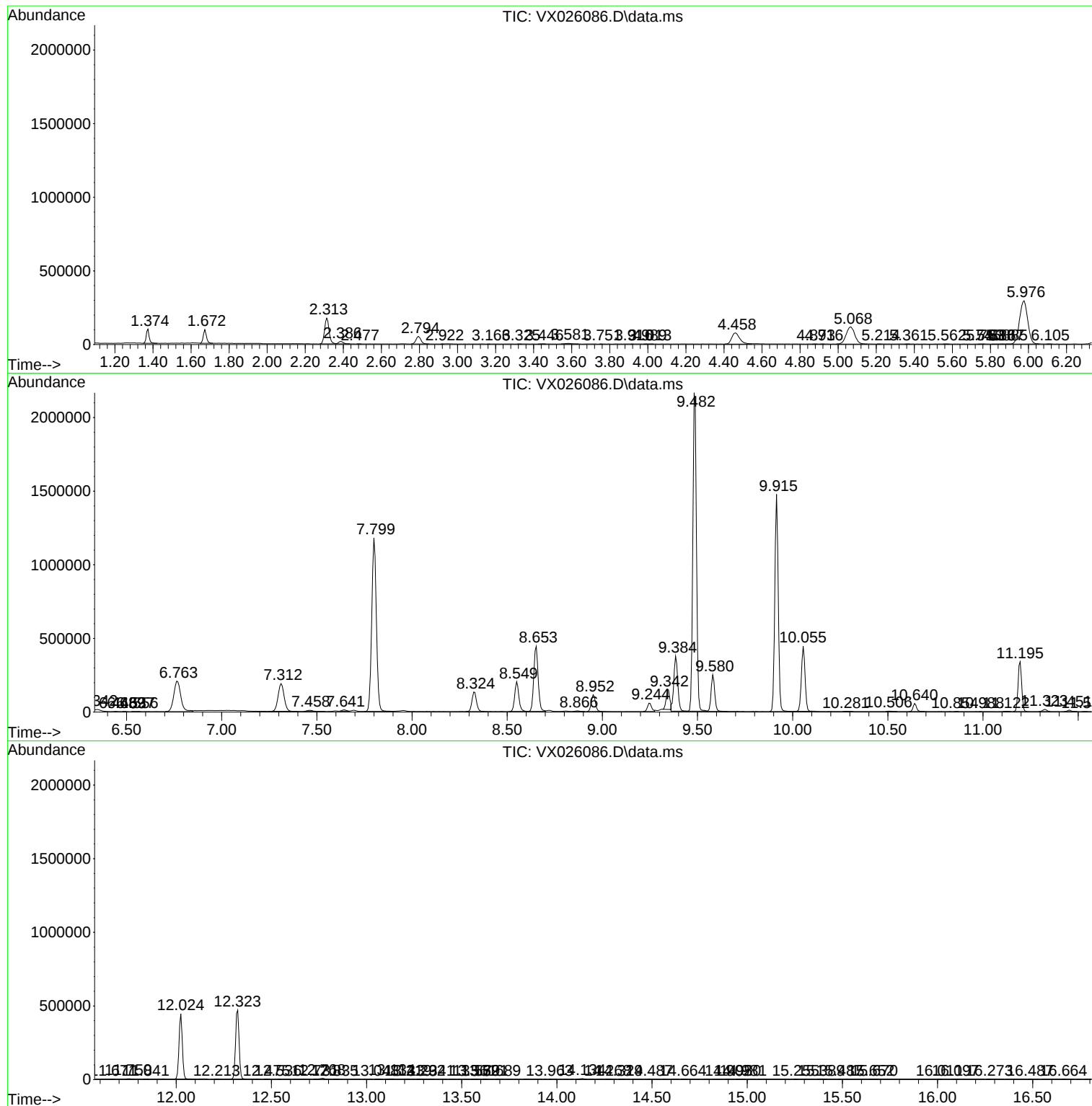
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 42 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB141699ZHE#04

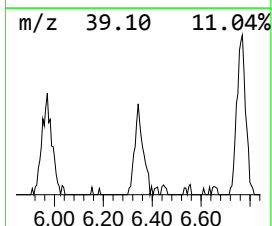
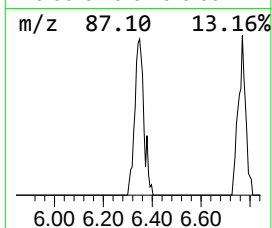
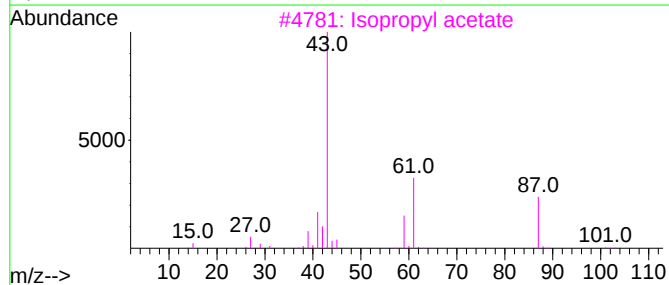
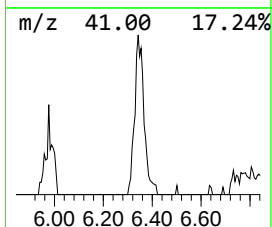
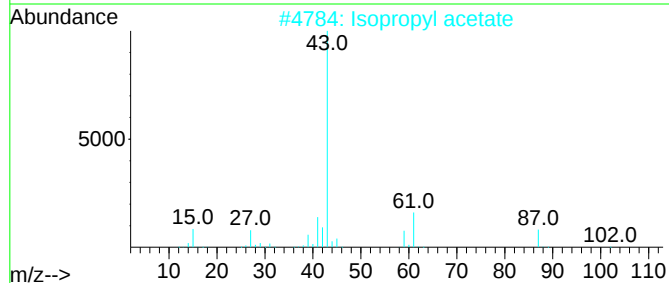
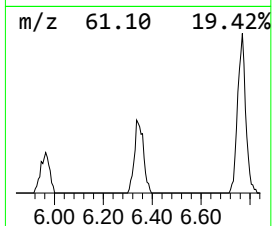
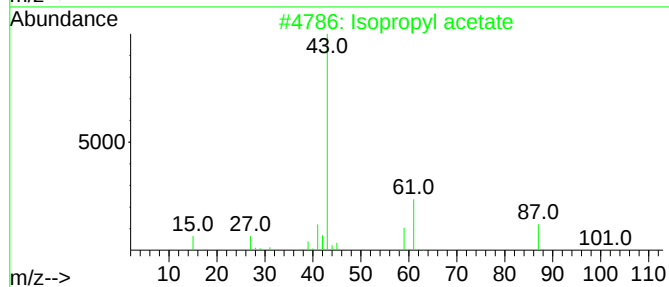
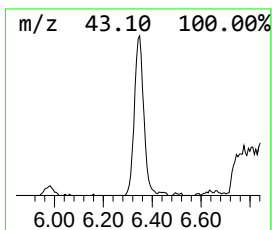
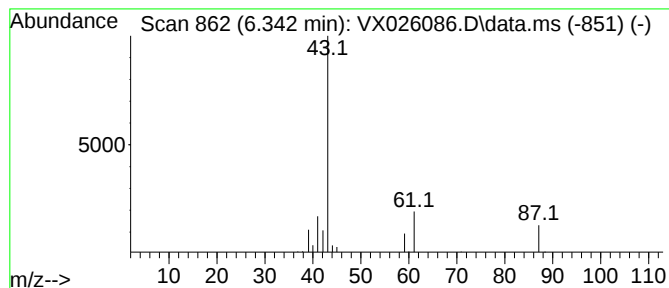
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	3.67 ug/L	38918	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl acetate	102	C5H10O2	000108-21-4	83
2			Isopropyl acetate	102	C5H10O2	000108-21-4	78
3			Isopropyl acetate	102	C5H10O2	000108-21-4	78
4			Isopropyl acetate	102	C5H10O2	000108-21-4	56
5			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	33



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
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PB141699ZHE#04

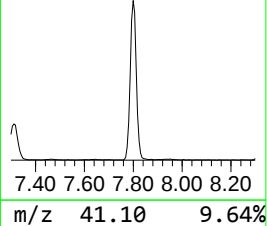
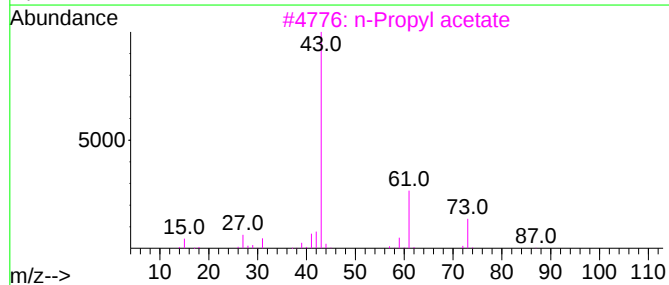
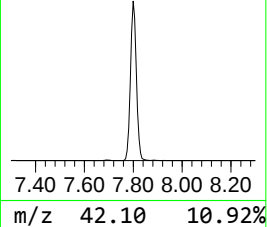
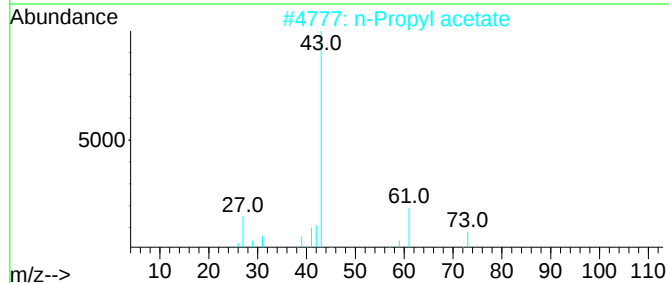
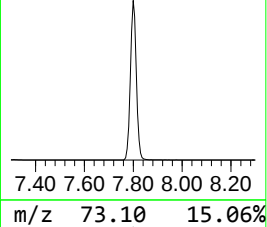
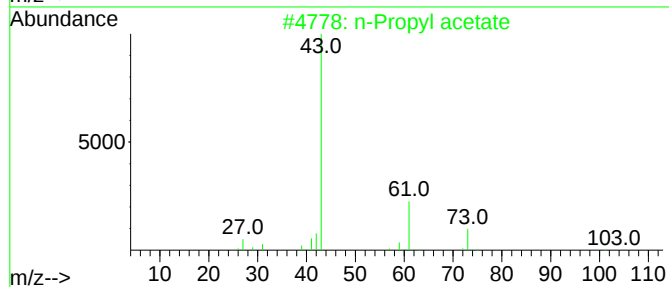
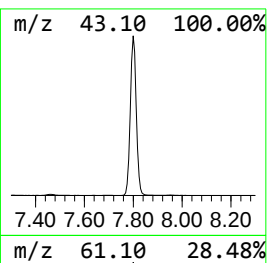
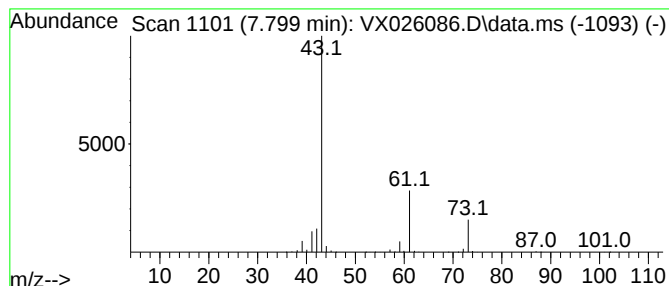
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	187.58 ug/L	1989960	1,4-Difluorobenzene	6.763

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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Instrument :
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ClientSampleId :
PB141699ZHE#04

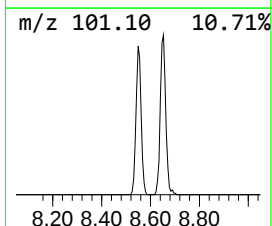
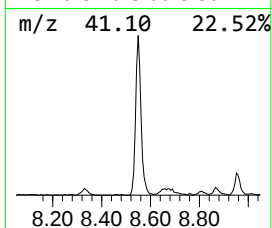
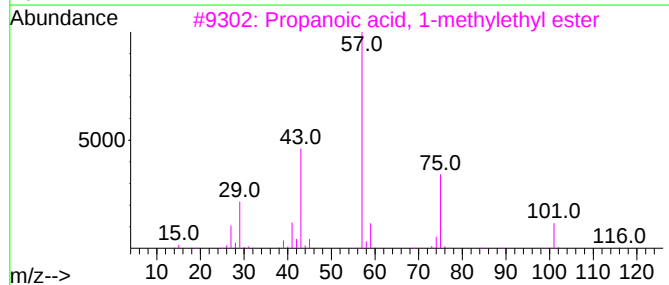
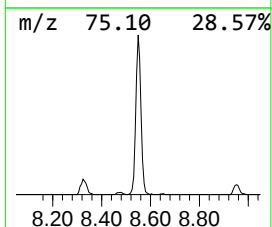
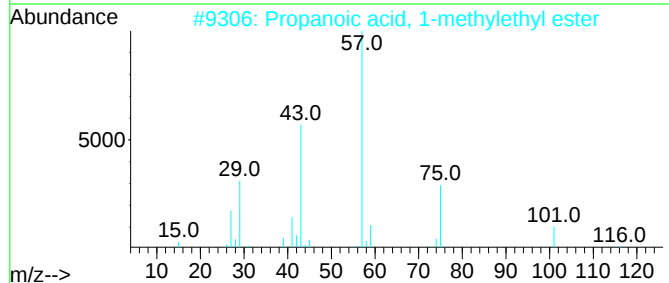
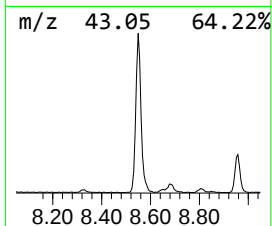
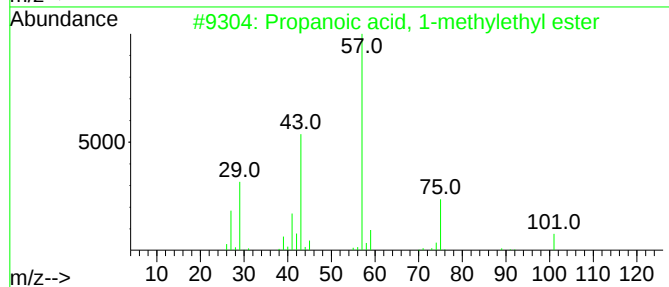
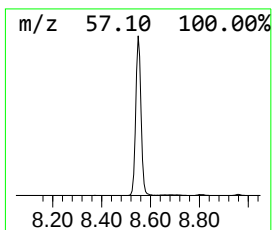
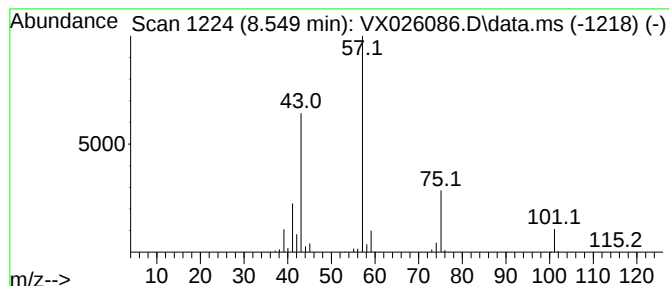
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	25.65 ug/L	304535	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, propyl ester	116	C6H12O2	000106-36-5	50
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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Operator : JC/MD
Sample : PB141699ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#04

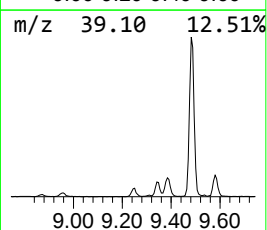
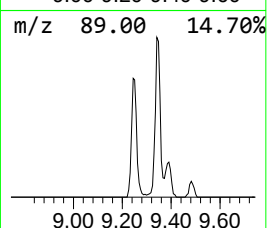
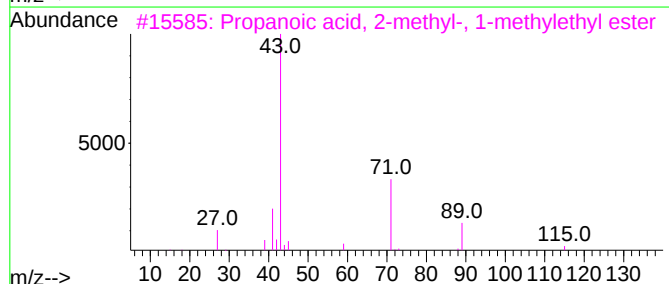
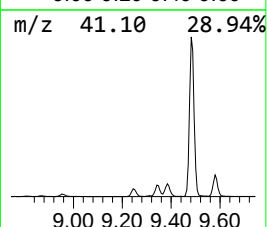
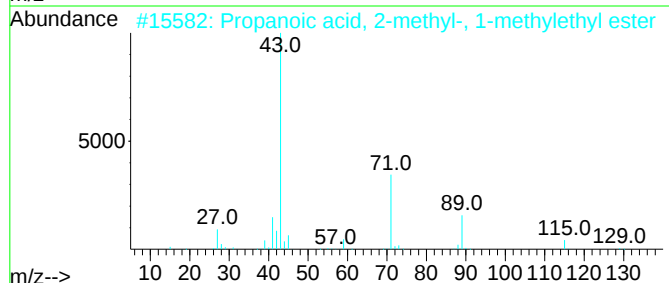
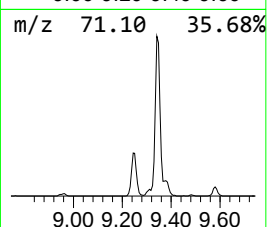
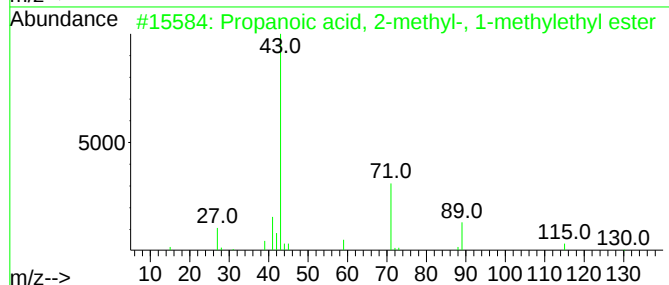
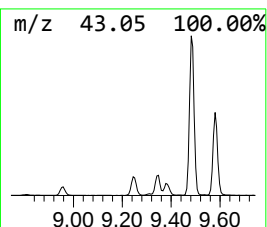
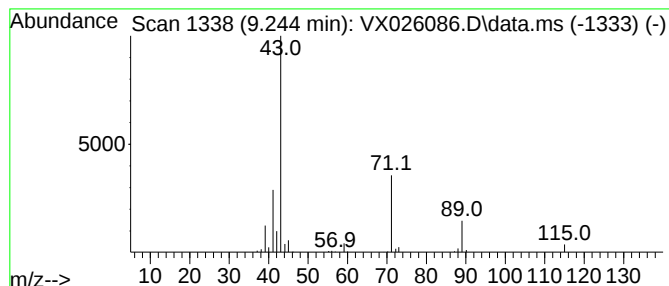
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Quant Title : VOC Analysis

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.
9.244	7.29 ug/L	86584	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	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	78
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 : VX026086.D
Acq On : 28 Dec 2021 01:22
Operator : JC/MD
Sample : PB141699ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#04

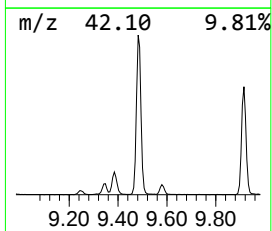
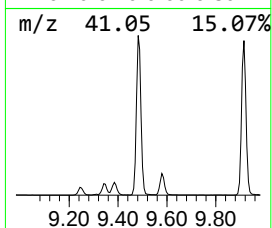
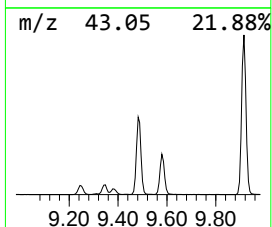
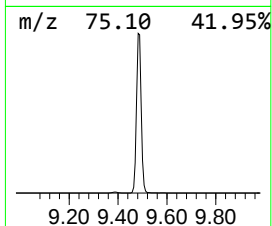
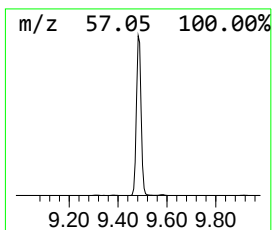
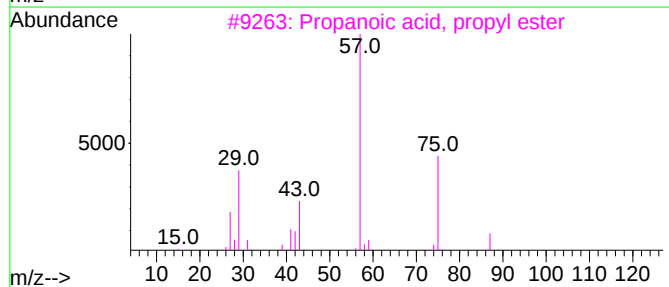
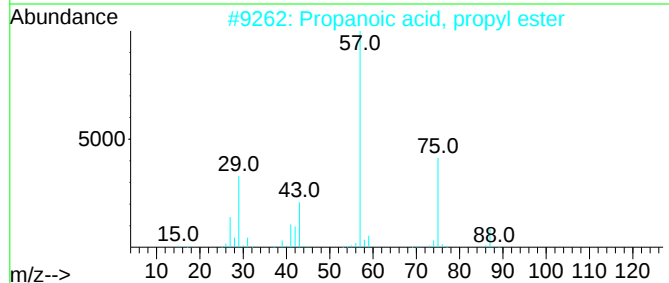
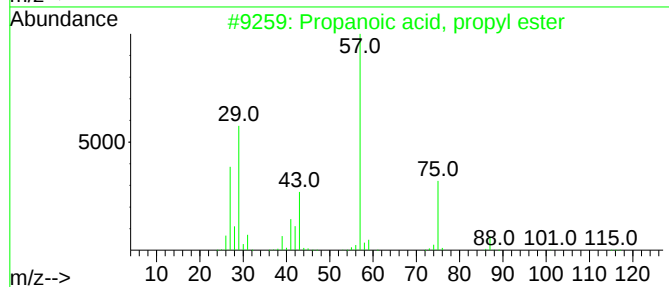
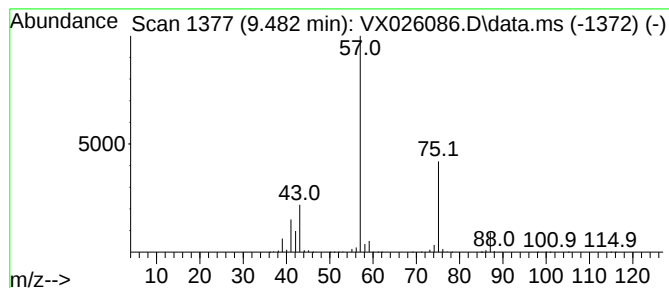
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Quant Title : VOC Analysis

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	240.63 ug/L	2856960	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 : VX026086.D
Acq On : 28 Dec 2021 01:22
Operator : JC/MD
Sample : PB141699ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#04

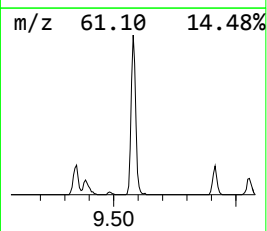
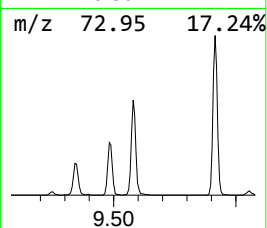
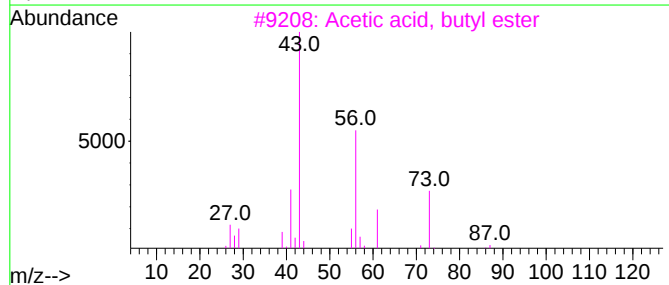
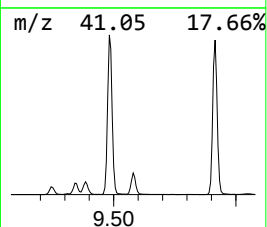
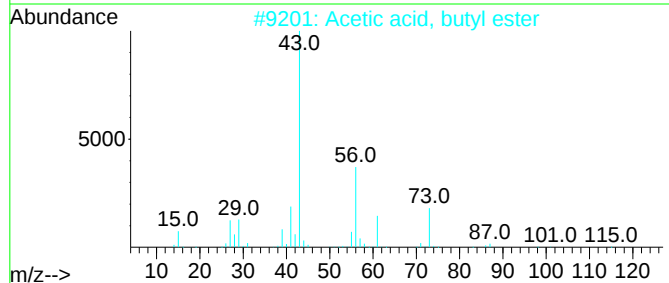
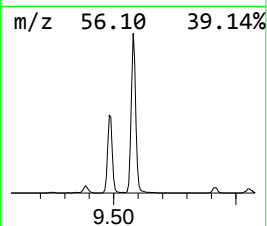
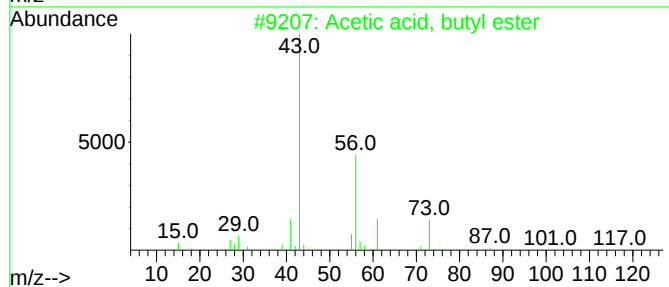
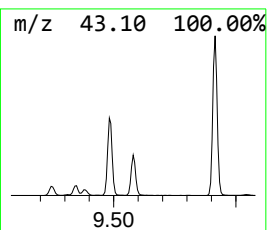
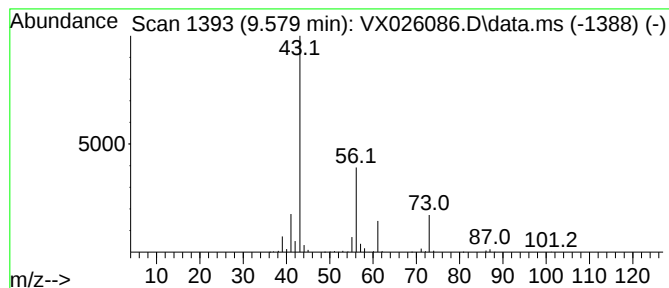
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Quant Title : VOC Analysis

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.
9.579	27.39 ug/L	325225	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 : VX026086.D
Acq On : 28 Dec 2021 01:22
Operator : JC/MD
Sample : PB141699ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#04

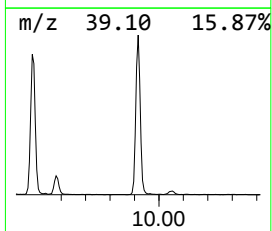
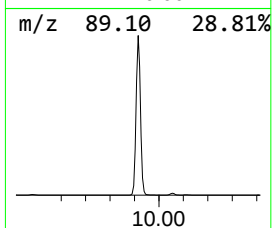
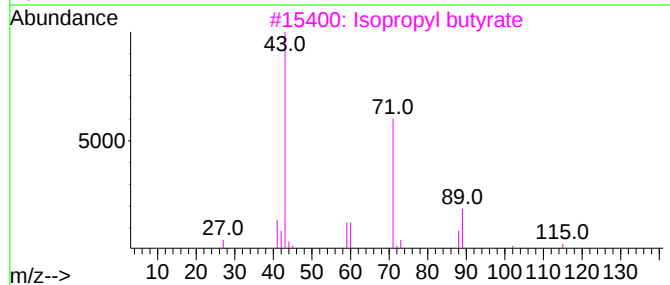
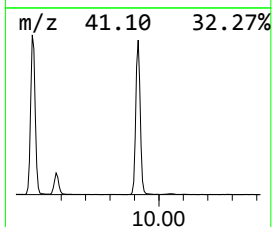
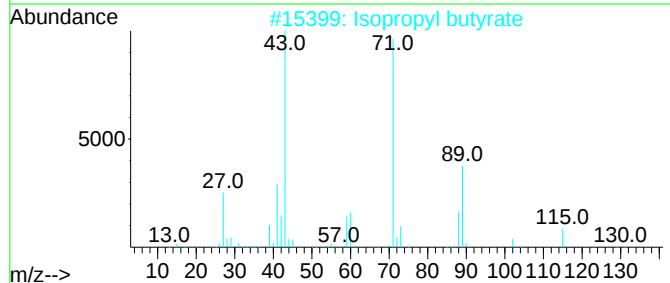
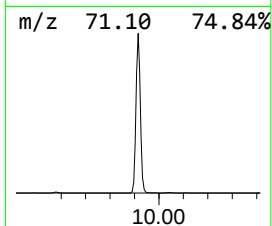
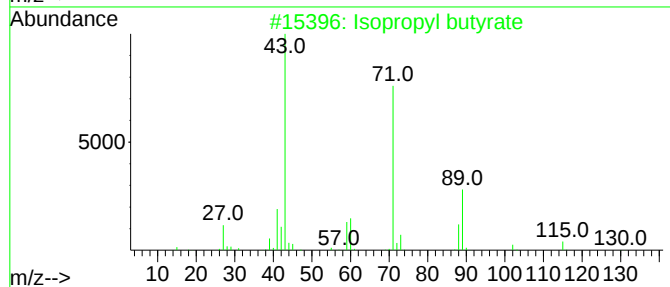
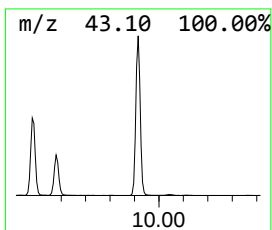
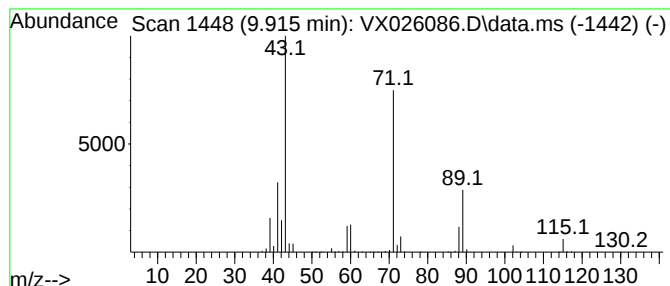
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Quant Title : VOC Analysis

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	155.79 ug/L	1849660	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	91
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	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026086.D
Acq On : 28 Dec 2021 01:22
Operator : JC/MD
Sample : PB141699ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#04

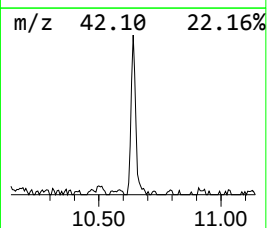
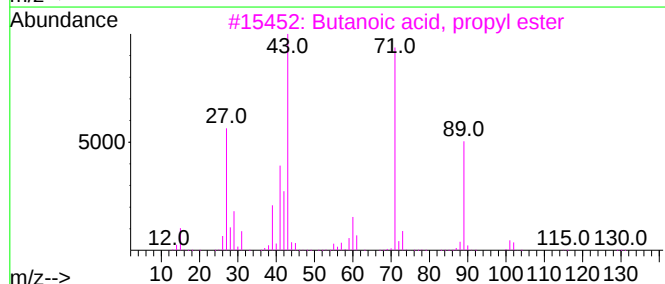
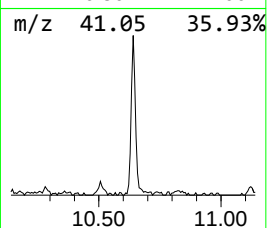
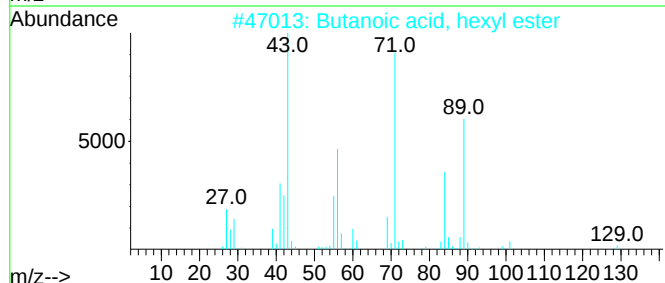
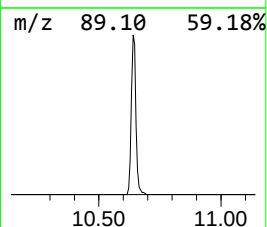
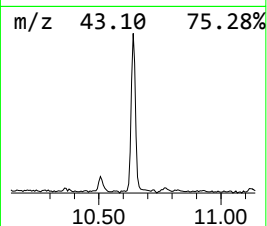
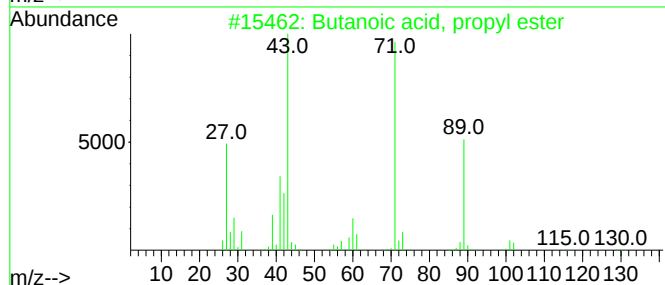
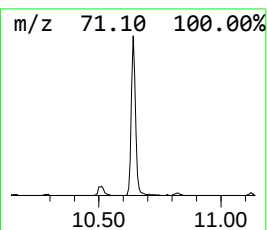
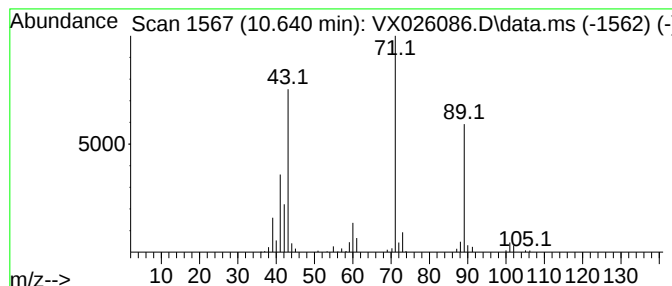
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Quant Title : VOC Analysis

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	5.77 ug/L	68487	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, hexyl ester	172	C10H20O2	002639-63-6	90
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026086.D
Acq On : 28 Dec 2021 01:22
Operator : JC/MD
Sample : PB141699ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#04

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	3.7	ug/L	38918	1	6.763	530425	50.0
n-Propyl acetate	7.799	187.6	ug/L	1989960	1	6.763	530425	50.0
Propanoic acid,...	8.549	25.6	ug/L	304535	2	10.055	593653	50.0
Propanoic acid,...	9.244	7.3	ug/L	86584	2	10.055	593653	50.0
Propanoic acid,...	9.482	240.6	ug/L	2856960	2	10.055	593653	50.0
Acetic acid, bu...	9.579	27.4	ug/L	325225	2	10.055	593653	50.0
Isopropyl butyrate	9.915	155.8	ug/L	1849660	2	10.055	593653	50.0
Butanoic acid, ...	10.640	5.8	ug/L	68487	2	10.055	593653	50.0