

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
 Data File : VX026087.D
 Acq On : 28 Dec 2021 01:45
 Operator : JC/MD
 Sample : PB141699ZHE#05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB141699ZHE#05

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: VX026087.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	54	rVB	89704	93854	3.31%	0.657%
2	1.672	92	96	107	rVB	89551	104955	3.70%	0.735%
3	2.313	195	201	209	rBV	165630	266069	9.39%	1.863%
4	2.386	209	213	223	rVB	17358	30969	1.09%	0.217%
5	2.794	273	280	291	rVB	52539	94886	3.35%	0.665%
6	2.941	301	304	305	rBV	1473	1382	0.05%	0.010%
7	3.081	325	327	329	rBV	492	431	0.02%	0.003%
8	3.221	348	350	352	rBV2	559	593	0.02%	0.004%
9	3.440	383	386	387	rBV	898	939	0.03%	0.007%
10	3.581	403	409	418	rVB5	3957	9929	0.35%	0.070%
11	3.751	435	437	440	rBV	487	568	0.02%	0.004%
12	3.879	456	458	459	rBV2	627	398	0.01%	0.003%
13	4.117	494	497	499	rBV2	588	597	0.02%	0.004%
14	4.233	515	516	518	rBV2	381	381	0.01%	0.003%
15	4.459	542	553	568	rBV	71652	211688	7.47%	1.482%
16	4.788	605	607	609	rVB	414	414	0.01%	0.003%
17	5.062	638	652	665	rBV	114484	353741	12.48%	2.477%
18	5.611	740	742	744	rBV	747	707	0.02%	0.005%
19	5.970	787	801	816	rBV2	277708	840082	29.65%	5.883%
20	6.105	822	823	826	rBV3	617	467	0.02%	0.003%
21	6.178	834	835	839	rVB	645	428	0.02%	0.003%
22	6.220	839	842	844	rBV2	502	561	0.02%	0.004%
23	6.245	844	846	847	rBV	755	504	0.02%	0.004%
24	6.348	856	863	872	rVB2	13841	34052	1.20%	0.238%
25	6.470	881	883	886	rBV	431	509	0.02%	0.004%
26	6.550	894	896	898	rBV2	406	504	0.02%	0.004%
27	6.629	907	909	910	rBV2	455	395	0.01%	0.003%
28	6.647	910	912	913	rVB	880	429	0.02%	0.003%
29	6.763	922	931	942	rBV	202407	510454	18.01%	3.575%
30	7.312	1013	1021	1031	rBV	184404	395779	13.97%	2.772%
31	7.464	1041	1046	1052	rVB2	7700	14955	0.53%	0.105%
32	7.604	1063	1069	1071	rBV	3476	6401	0.23%	0.045%
33	7.641	1072	1075	1080	rVB	8222	13453	0.47%	0.094%
34	7.799	1094	1101	1116	rBV	1171203	1969911	69.52%	13.796%
35	8.324	1181	1187	1197	rVB	123239	207264	7.31%	1.452%
36	8.549	1218	1224	1234	rBV	205227	305481	10.78%	2.139%

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Integrator: RTE

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 Title : VOC Analysis

37	8.653	1234	1241	1249	rBV	416469	651852	23.01%	4.565%
38	8.811	1263	1267	1271	rVB5	3195	5195	0.18%	0.036%
39	8.872	1272	1277	1284	rVB3	4670	7466	0.26%	0.052%
40	8.952	1284	1290	1298	rBV2	112308	164883	5.82%	1.155%
41	9.147	1320	1322	1323	rBV2	596	501	0.02%	0.004%
42	9.244	1333	1338	1342	rBV	56750	83486	2.95%	0.585%
43	9.342	1350	1354	1357	rBV	134719	177048	6.25%	1.240%
44	9.385	1357	1361	1372	rVB	348401	503870	17.78%	3.529%
45	9.482	1372	1377	1385	rBV	2169499	2833499	100.00%	19.844%
46	9.580	1388	1393	1405	rVB	248563	317559	11.21%	2.224%
47	9.915	1443	1448	1461	rVB	1458371	1838667	64.89%	12.877%
48	10.055	1465	1471	1477	rBV	425374	572358	20.20%	4.008%
49	10.506	1542	1545	1551	rVB2	3102	4071	0.14%	0.029%
50	10.640	1562	1567	1574	rBV	53974	68082	2.40%	0.477%
51	10.817	1593	1596	1598	rBV3	1023	1126	0.04%	0.008%
52	11.018	1628	1629	1634	rVB	659	649	0.02%	0.005%
53	11.073	1636	1638	1640	rBV	410	428	0.02%	0.003%
54	11.122	1643	1646	1652	rVB3	2053	2591	0.09%	0.018%
55	11.195	1652	1658	1665	rBV	328411	426759	15.06%	2.989%
56	11.323	1674	1679	1685	rVB3	11029	19098	0.67%	0.134%
57	11.409	1691	1693	1696	rVB2	688	497	0.02%	0.003%
58	11.457	1696	1701	1707	rBV2	8152	12625	0.45%	0.088%
59	11.610	1723	1726	1729	rBV2	827	1047	0.04%	0.007%
60	11.713	1740	1743	1745	rBV3	514	579	0.02%	0.004%
61	11.750	1746	1749	1756	rVV4	2669	4068	0.14%	0.028%
62	11.817	1758	1760	1762	rVV3	605	600	0.02%	0.004%
63	11.872	1766	1769	1770	rVB	429	380	0.01%	0.003%
64	11.933	1776	1779	1782	rVB	1597	1534	0.05%	0.011%
65	12.024	1788	1794	1802	rBV	410144	510722	18.02%	3.577%
66	12.146	1812	1814	1818	rVB3	1412	1449	0.05%	0.010%
67	12.225	1823	1827	1831	rVB3	1212	2019	0.07%	0.014%
68	12.262	1831	1833	1835	rBV	722	496	0.02%	0.003%
69	12.323	1837	1843	1851	rVB	432255	560247	19.77%	3.924%
70	12.427	1858	1860	1864	rVB	1056	964	0.03%	0.007%
71	12.524	1874	1876	1879	rBV	569	636	0.02%	0.004%
72	12.579	1884	1885	1887	rBV2	564	416	0.01%	0.003%
73	12.597	1887	1888	1890	rVB	783	447	0.02%	0.003%
74	12.634	1892	1894	1895	rVB	725	406	0.01%	0.003%
75	12.768	1912	1916	1919	rBV	4923	6186	0.22%	0.043%
76	13.048	1959	1962	1964	rBV	897	1101	0.04%	0.008%

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Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	13.219	1988	1990	1994	rVB4	1095	1232	0.04%	0.009%
78	13.329	2007	2008	2010	rVB	793	550	0.02%	0.004%
79	13.372	2012	2015	2018	rBV2	510	860	0.03%	0.006%
80	13.451	2026	2028	2031	rBV2	436	489	0.02%	0.003%
81	13.689	2064	2067	2069	rBV	711	848	0.03%	0.006%
82	13.780	2080	2082	2087	rVB3	901	938	0.03%	0.007%
83	14.048	2123	2126	2128	rVV2	430	539	0.02%	0.004%
84	14.091	2131	2133	2135	rBV	792	584	0.02%	0.004%
85	14.128	2136	2139	2144	rVB	2620	3836	0.14%	0.027%
86	14.274	2161	2163	2167	rBV	612	721	0.03%	0.005%
87	14.371	2176	2179	2182	rVB2	598	842	0.03%	0.006%
88	14.396	2182	2183	2186	rBV	660	521	0.02%	0.004%
89	14.457	2192	2193	2197	rVB2	653	722	0.03%	0.005%
90	14.518	2202	2203	2206	rVV	533	380	0.01%	0.003%
91	14.597	2214	2216	2219	rBV3	622	783	0.03%	0.005%
92	14.652	2224	2225	2227	rBV	559	536	0.02%	0.004%
93	14.762	2241	2243	2246	rBV2	560	653	0.02%	0.005%
94	14.792	2246	2248	2250	rVB2	693	486	0.02%	0.003%
95	14.810	2250	2251	2253	rBV	673	522	0.02%	0.004%
96	15.268	2324	2326	2329	rVB	749	640	0.02%	0.004%
97	15.816	2414	2416	2418	rBV	572	632	0.02%	0.004%
98	15.914	2429	2432	2433	rBV	675	749	0.03%	0.005%
99	16.066	2454	2457	2459	rBV2	814	841	0.03%	0.006%
100	16.761	2570	2571	2573	rVB	1074	560	0.02%	0.004%

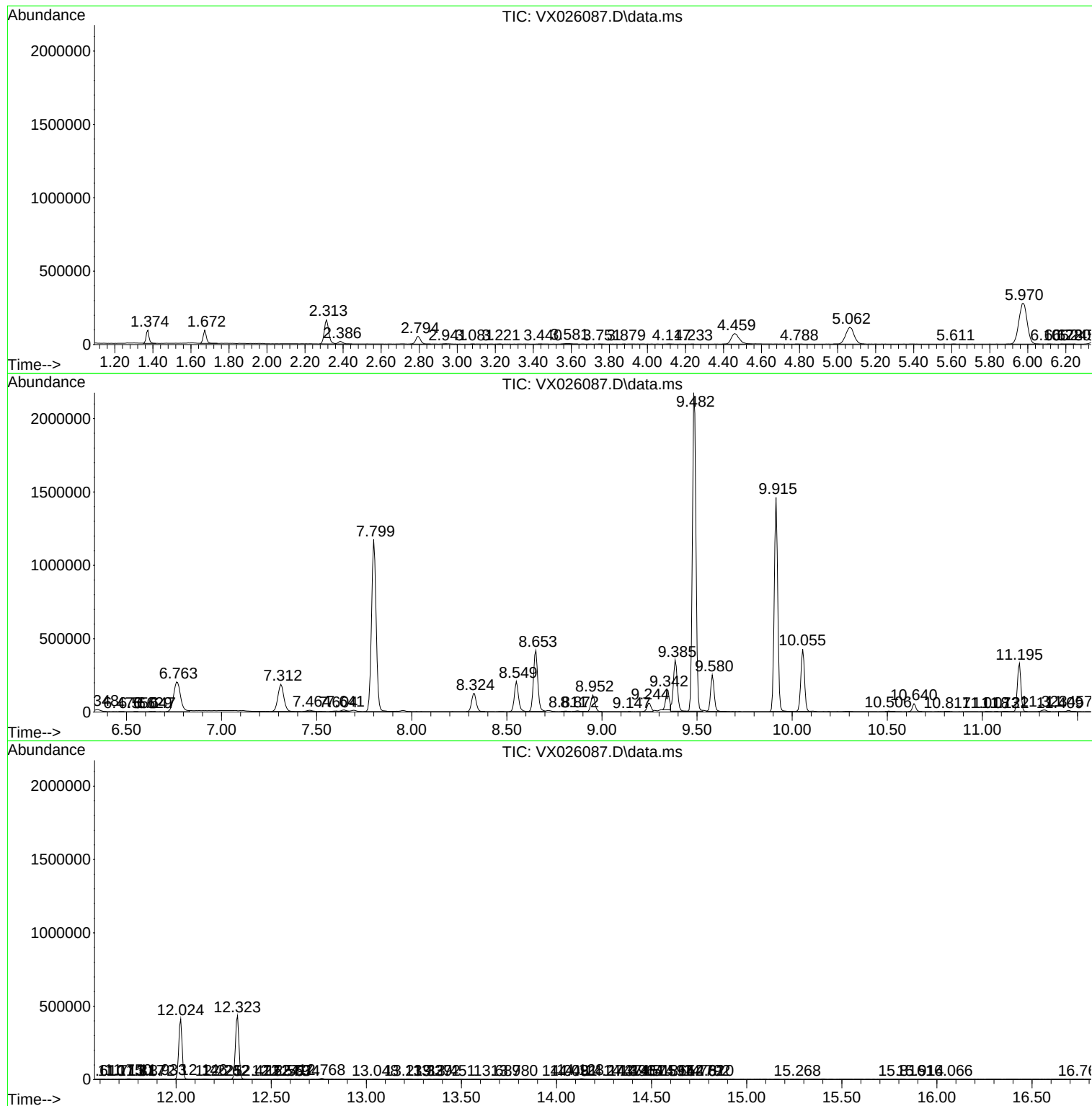
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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



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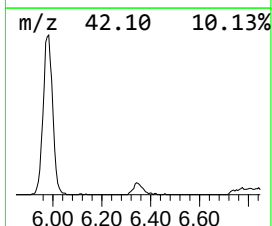
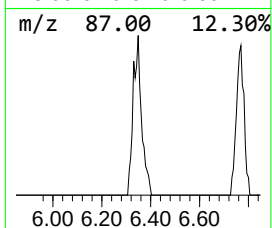
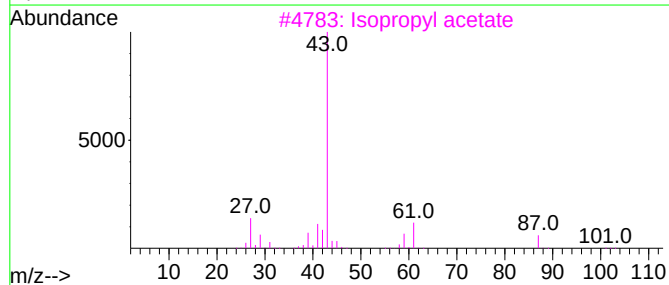
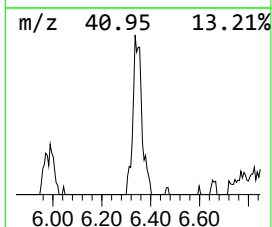
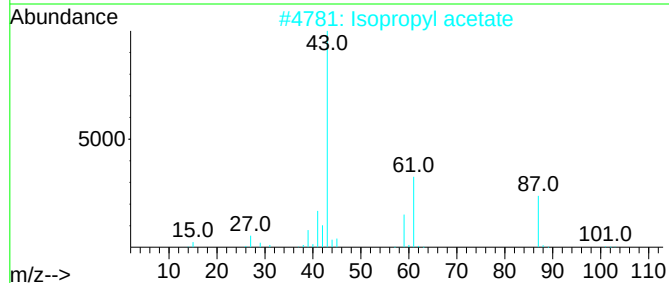
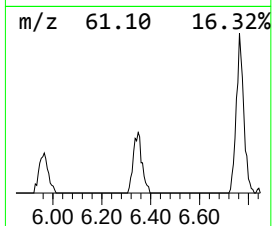
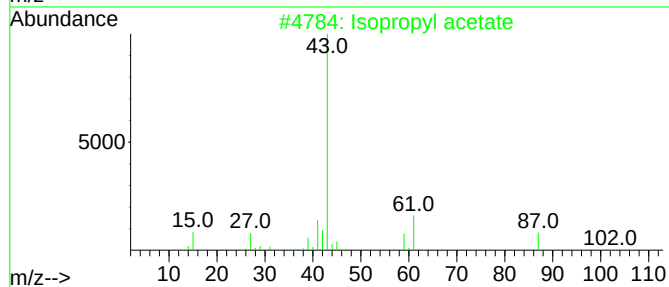
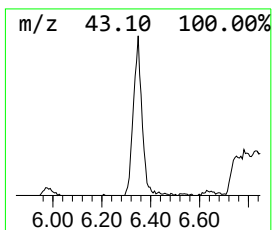
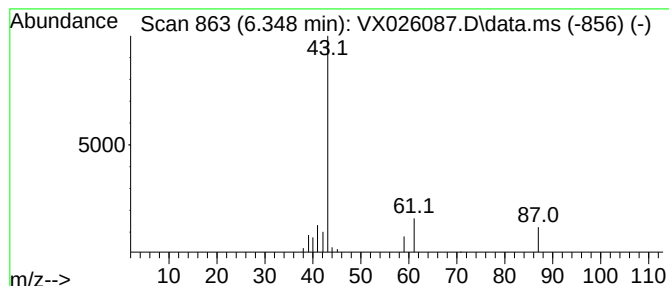
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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.
6.348	3.34 ug/L	34052	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	56
3			Isopropyl acetate	102	C5H10O2	000108-21-4	40
4			Isopropyl acetate	102	C5H10O2	000108-21-4	9
5			Isopropyl acetate	102	C5H10O2	000108-21-4	9



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#05

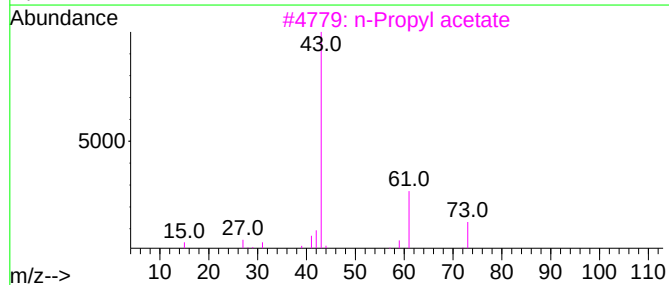
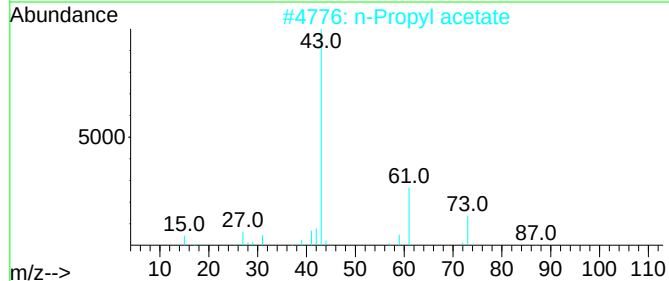
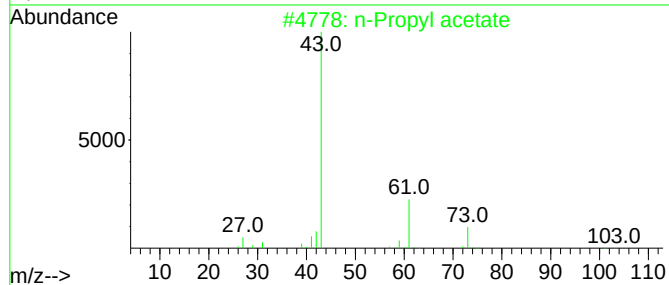
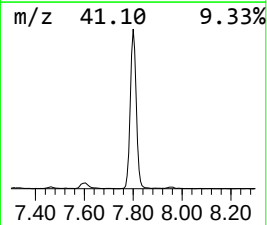
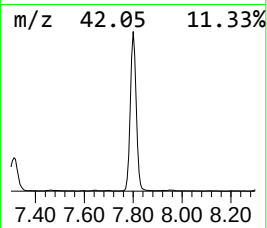
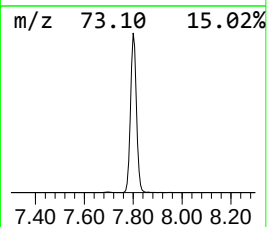
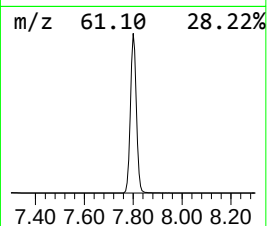
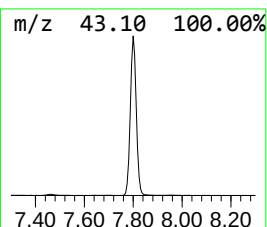
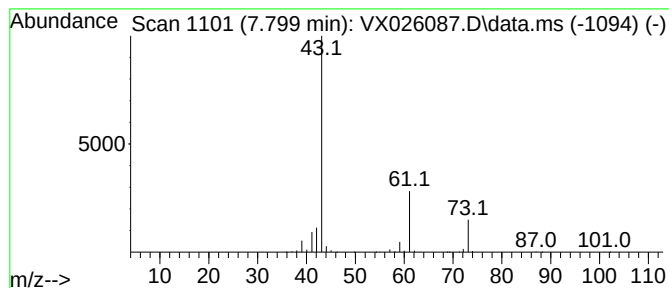
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	192.96 ug/L	1969910	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	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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ClientSampleId :
PB141699ZHE#05

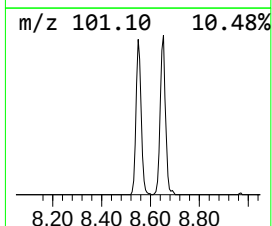
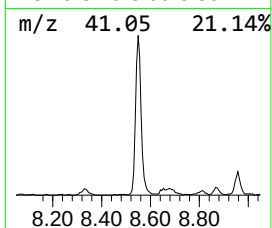
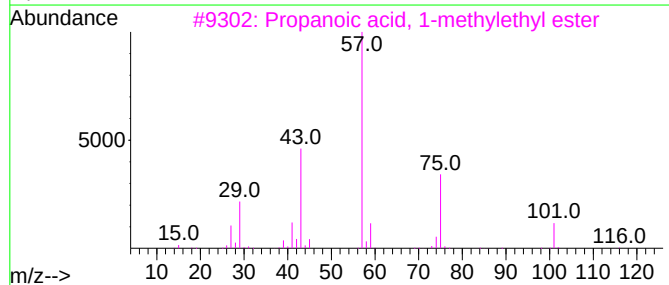
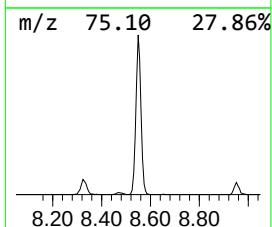
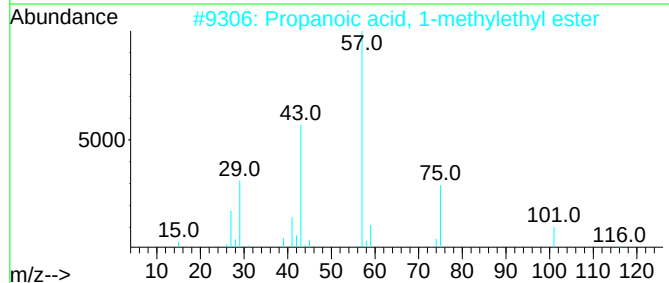
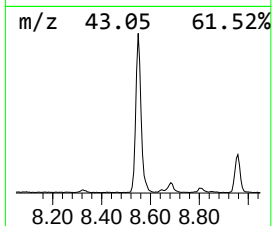
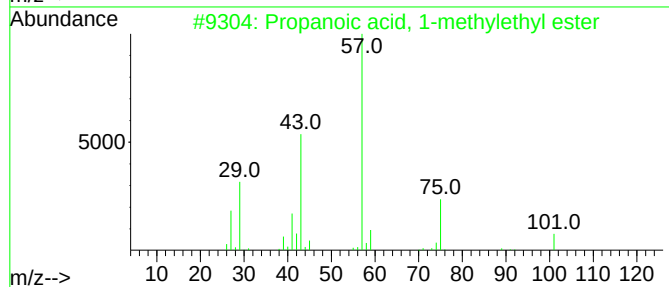
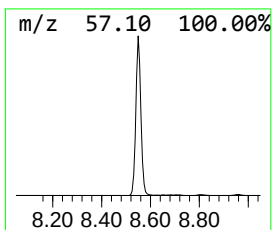
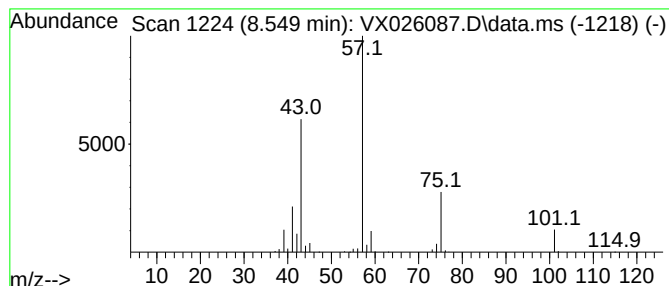
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	26.69 ug/L	305481	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	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026087.D
Acq On : 28 Dec 2021 01:45
Operator : JC/MD
Sample : PB141699ZHE#05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#05

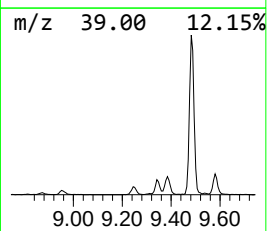
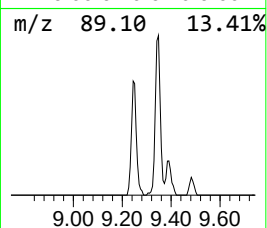
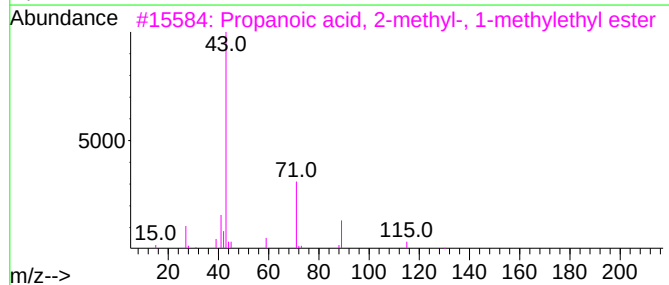
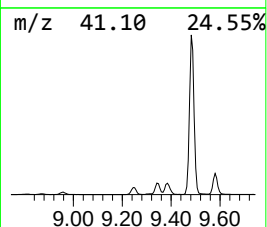
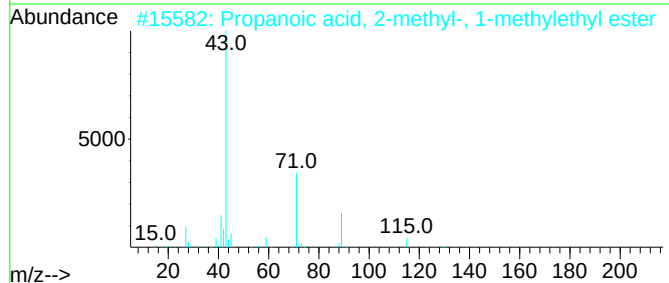
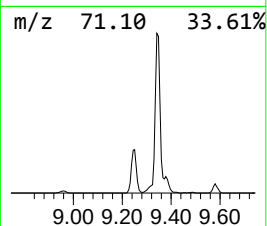
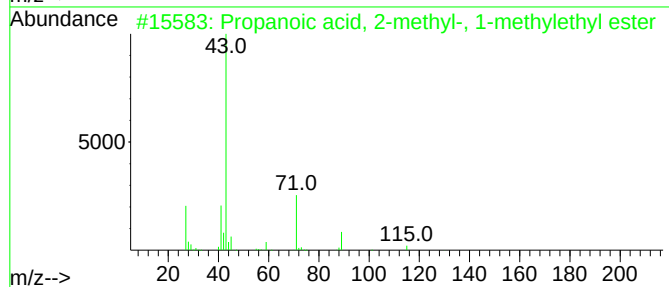
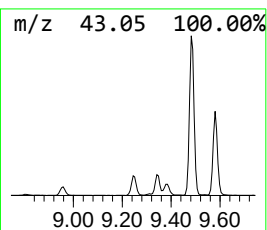
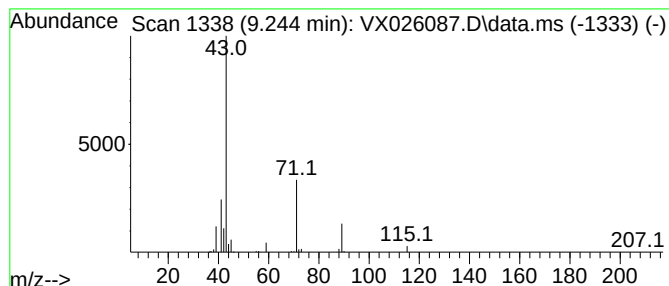
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Quant Title : VOC Analysis

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	83486	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	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026087.D
Acq On : 28 Dec 2021 01:45
Operator : JC/MD
Sample : PB141699ZHE#05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#05

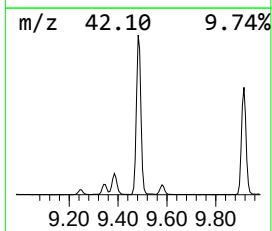
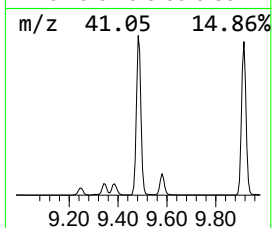
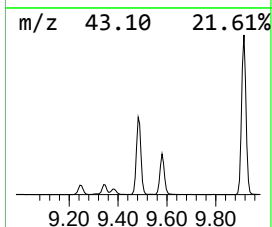
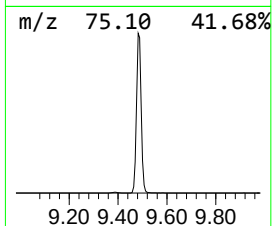
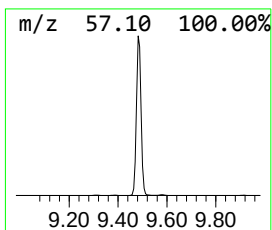
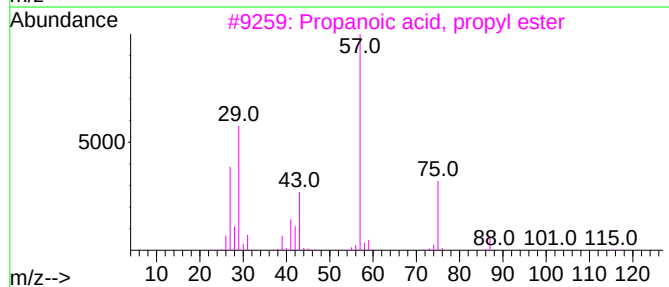
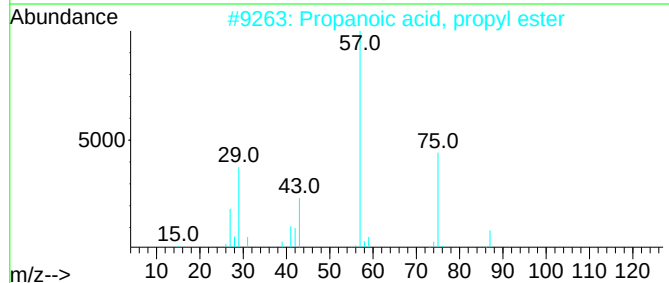
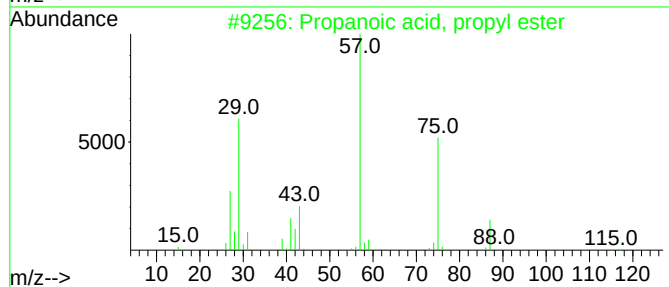
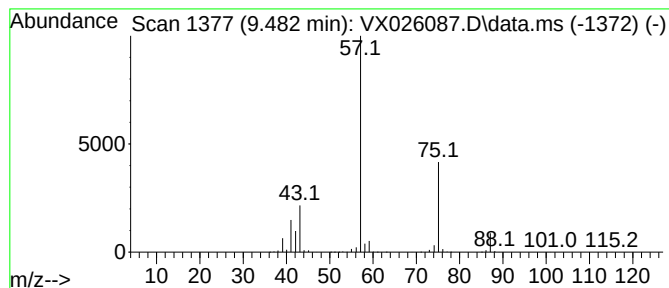
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Quant Title : VOC Analysis

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	247.53 ug/L	2833500	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 : VX026087.D
Acq On : 28 Dec 2021 01:45
Operator : JC/MD
Sample : PB141699ZHE#05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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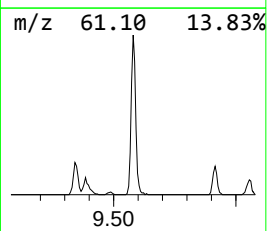
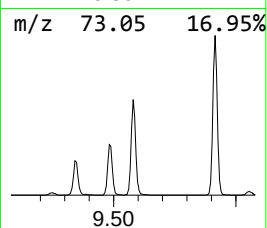
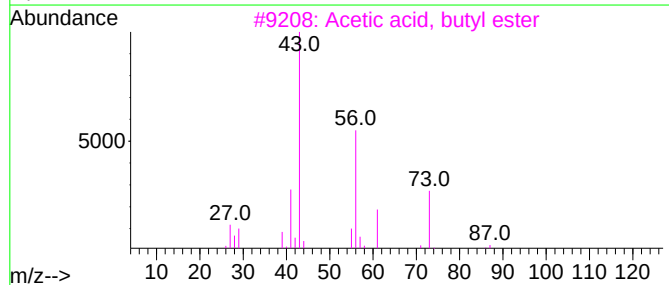
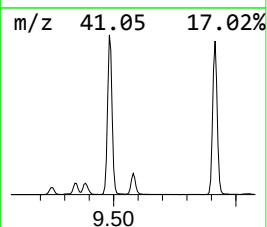
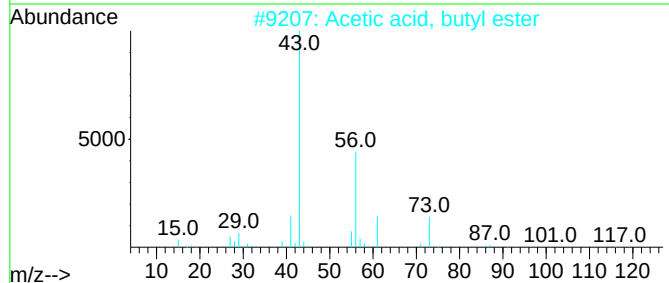
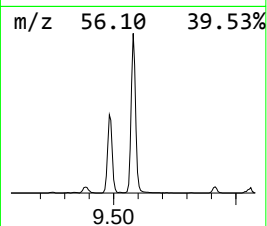
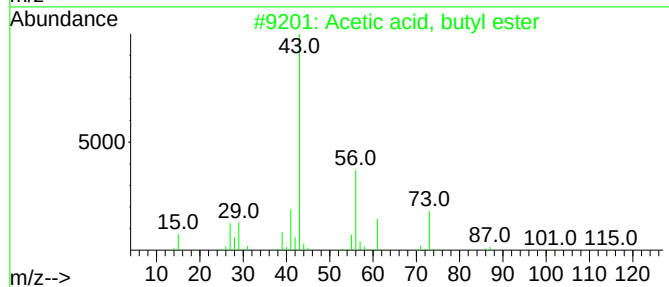
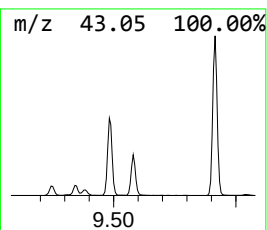
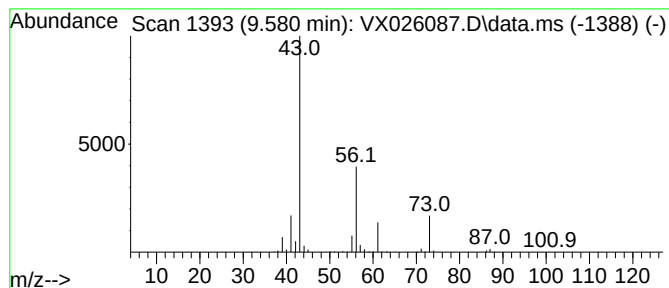
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Quant Title : VOC Analysis

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	27.74 ug/L	317559	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	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026087.D
Acq On : 28 Dec 2021 01:45
Operator : JC/MD
Sample : PB141699ZHE#05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#05

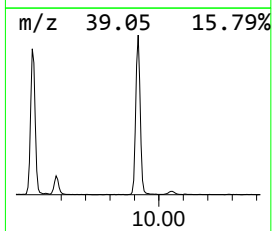
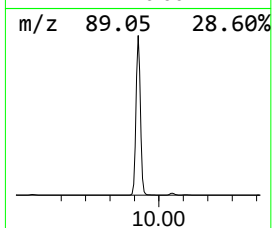
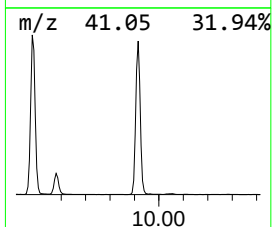
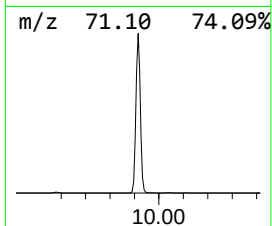
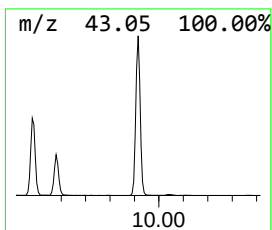
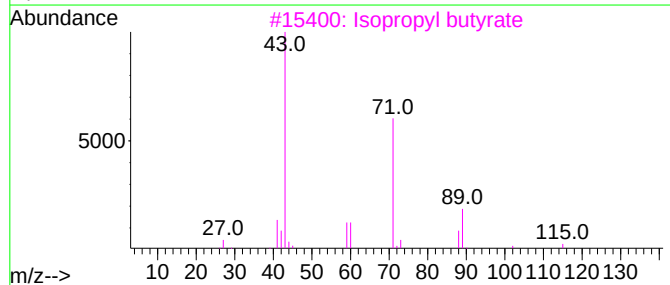
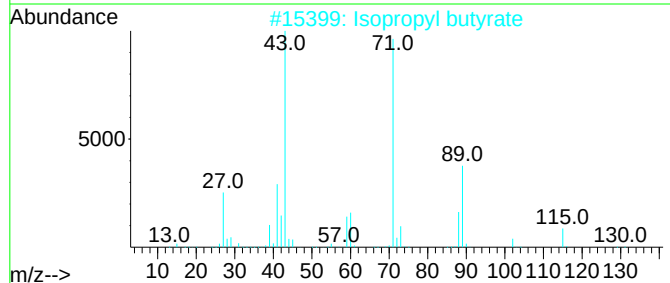
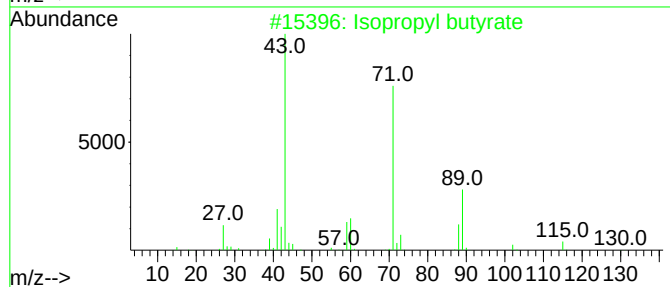
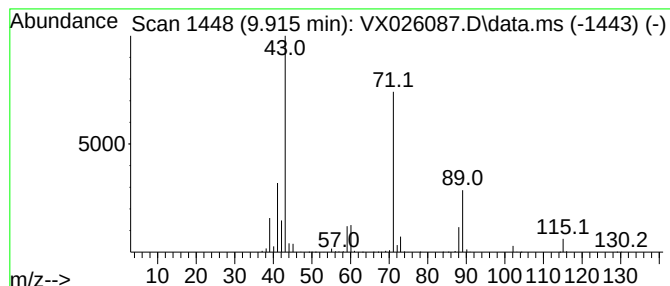
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Quant Title : VOC Analysis

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	160.62 ug/L	1838670	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	95
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 : VX026087.D
Acq On : 28 Dec 2021 01:45
Operator : JC/MD
Sample : PB141699ZHE#05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB141699ZHE#05

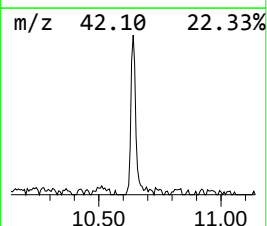
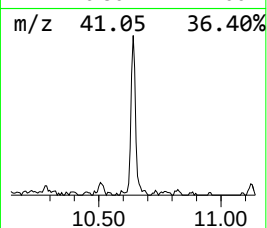
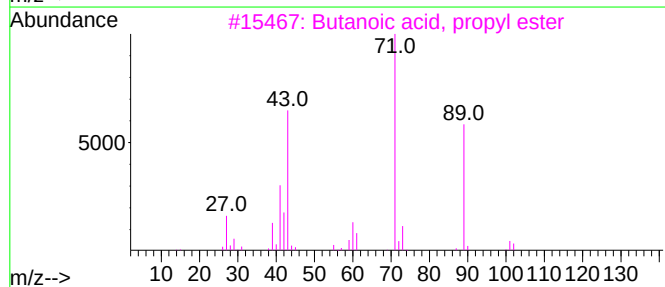
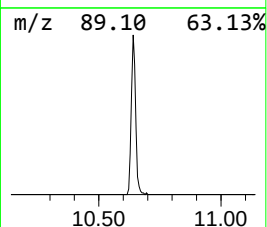
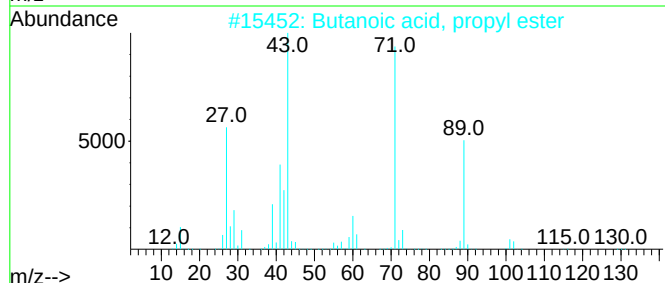
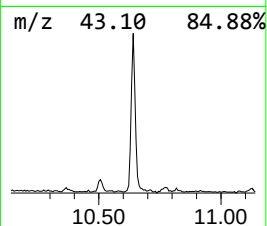
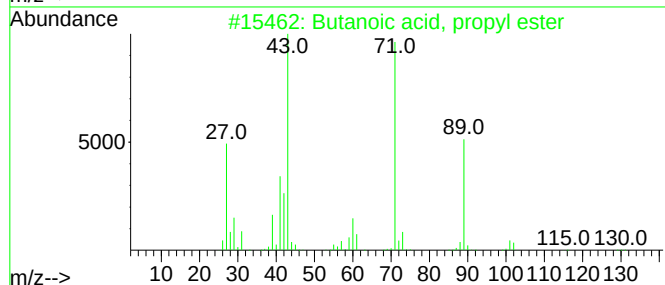
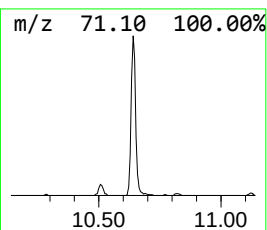
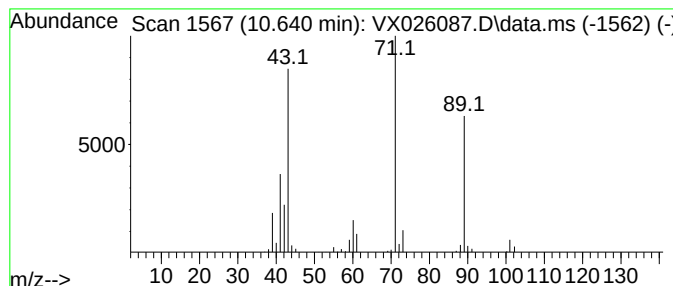
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Quant Title : VOC Analysis

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	5.95 ug/L	68082	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	90
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026087.D
Acq On : 28 Dec 2021 01:45
Operator : JC/MD
Sample : PB141699ZHE#05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#05

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	6.348	3.3	ug/L	34052	1	6.769	510454	50.0
n-Propyl acetate	7.799	193.0	ug/L	1969910	1	6.769	510454	50.0
Propanoic acid,...	8.549	26.7	ug/L	305481	2	10.055	572358	50.0
Propanoic acid,...	9.244	7.3	ug/L	83486	2	10.055	572358	50.0
Propanoic acid,...	9.482	247.5	ug/L	2833500	2	10.055	572358	50.0
Acetic acid, bu...	9.580	27.7	ug/L	317559	2	10.055	572358	50.0
Isopropyl butyrate	9.915	160.6	ug/L	1838670	2	10.055	572358	50.0
Butanoic acid, ...	10.640	6.0	ug/L	68082	2	10.055	572358	50.0