

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
 Data File : VX026084.D
 Acq On : 28 Dec 2021 00:36
 Operator : JC/MD
 Sample : PB141699ZHE#02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB141699ZHE#02

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\SFAMXML122321WMA.M
 Title : VOC Analysis

Signal : TIC: VX026084.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	99157	103938	3.64%	0.713%
2	1.672	92	96	103	rVB	93520	111133	3.90%	0.762%
3	2.312	195	201	209	rBV	169314	275857	9.67%	1.892%
4	2.386	209	213	222	rVB	17977	30572	1.07%	0.210%
5	2.794	274	280	288	rVB	52559	92193	3.23%	0.632%
6	2.946	301	305	314	rVB2	4750	10800	0.38%	0.074%
7	3.270	354	358	360	rBV2	490	543	0.02%	0.004%
8	3.367	373	374	376	rBV	702	532	0.02%	0.004%
9	3.440	384	386	387	rBV2	636	615	0.02%	0.004%
10	3.581	403	409	418	rBV3	4389	9041	0.32%	0.062%
11	3.709	428	430	437	rBB2	713	887	0.03%	0.006%
12	3.763	437	439	440	rBV	800	395	0.01%	0.003%
13	3.830	448	450	452	rBV	576	488	0.02%	0.003%
14	4.355	534	536	538	rBV2	492	480	0.02%	0.003%
15	4.458	545	553	566	rBV	77303	223992	7.85%	1.536%
16	4.818	610	612	614	rVB	925	671	0.02%	0.005%
17	4.849	614	617	618	rBV2	687	707	0.02%	0.005%
18	4.964	632	636	637	rBV	583	594	0.02%	0.004%
19	5.062	640	652	668	rVV	117526	366108	12.83%	2.511%
20	5.330	694	696	697	rBV2	642	475	0.02%	0.003%
21	5.348	697	699	702	rVV	699	608	0.02%	0.004%
22	5.391	702	706	709	rVB	767	1118	0.04%	0.008%
23	5.422	709	711	713	rBV2	620	625	0.02%	0.004%
24	5.446	713	715	717	rVV	611	481	0.02%	0.003%
25	5.470	717	719	722	rVB	579	555	0.02%	0.004%
26	5.507	722	725	726	rBV2	444	466	0.02%	0.003%
27	5.544	729	731	733	rVV2	538	454	0.02%	0.003%
28	5.580	733	737	741	rVV3	598	985	0.03%	0.007%
29	5.635	745	746	748	rBV	687	652	0.02%	0.004%
30	5.757	765	766	768	rBV	431	381	0.01%	0.003%
31	5.976	787	802	818	rBV2	292401	882148	30.92%	6.051%
32	6.178	833	835	839	rBV	449	583	0.02%	0.004%
33	6.342	855	862	872	rVV2	13627	36545	1.28%	0.251%
34	6.428	875	876	878	rVV	584	545	0.02%	0.004%
35	6.470	881	883	886	rVB	646	571	0.02%	0.004%
36	6.531	892	893	896	rVB2	722	606	0.02%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Stop Thrs : 0

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 Title : VOC Analysis

37	6.568	898	899	903	rBV2	610	680	0.02%	0.005%
38	6.604	903	905	907	rBV	719	753	0.03%	0.005%
39	6.769	920	932	946	rBV	197431	504670	17.69%	3.461%
40	7.312	1013	1021	1035	rVB	192733	419240	14.70%	2.876%
41	7.464	1041	1046	1052	rVB	7103	14360	0.50%	0.098%
42	7.604	1064	1069	1071	rBV2	3312	5852	0.21%	0.040%
43	7.641	1072	1075	1080	rVV	9329	16408	0.58%	0.113%
44	7.690	1080	1083	1093	rVB2	8107	15593	0.55%	0.107%
45	7.799	1094	1101	1113	rBV	1169608	1977706	69.33%	13.565%
46	8.104	1149	1151	1153	rVB2	893	538	0.02%	0.004%
47	8.177	1161	1163	1165	rBV3	776	836	0.03%	0.006%
48	8.324	1181	1187	1197	rBV	130954	216059	7.57%	1.482%
49	8.458	1207	1209	1210	rBV2	1127	1065	0.04%	0.007%
50	8.549	1218	1224	1234	rBV	194081	306255	10.74%	2.101%
51	8.653	1234	1241	1249	rBV	430251	679460	23.82%	4.660%
52	8.805	1263	1266	1271	rVB4	3429	4592	0.16%	0.031%
53	8.866	1274	1276	1282	rVB2	4086	5819	0.20%	0.040%
54	8.952	1285	1290	1297	rBV2	115515	169819	5.95%	1.165%
55	9.153	1321	1323	1326	rBV2	635	789	0.03%	0.005%
56	9.250	1333	1339	1343	rBV	55751	86734	3.04%	0.595%
57	9.342	1350	1354	1357	rBV	133583	177817	6.23%	1.220%
58	9.384	1357	1361	1372	rVB	383607	549880	19.28%	3.772%
59	9.488	1372	1378	1388	rBV	2105565	2852688	100.00%	19.566%
60	9.579	1388	1393	1410	rVB	246426	322693	11.31%	2.213%
61	9.805	1428	1430	1431	rBV	828	483	0.02%	0.003%
62	9.915	1443	1448	1458	rBV	1489166	1825026	63.98%	12.518%
63	10.055	1465	1471	1478	rBV	423197	562579	19.72%	3.859%
64	10.195	1491	1494	1495	rBV2	795	851	0.03%	0.006%
65	10.281	1505	1508	1509	rBV2	1926	1774	0.06%	0.012%
66	10.506	1541	1545	1550	rVB2	3210	4378	0.15%	0.030%
67	10.640	1563	1567	1573	rBV	52266	65399	2.29%	0.449%
68	11.122	1643	1646	1650	rVB3	2768	3148	0.11%	0.022%
69	11.195	1652	1658	1665	rVV	353252	446733	15.66%	3.064%
70	11.323	1674	1679	1686	rVB2	17702	28949	1.01%	0.199%
71	11.451	1696	1700	1704	rBV2	8648	11691	0.41%	0.080%
72	11.549	1714	1716	1718	rBV2	895	933	0.03%	0.006%
73	11.750	1747	1749	1753	rVB2	2506	2634	0.09%	0.018%
74	11.890	1768	1772	1773	rBV2	882	954	0.03%	0.007%
75	11.933	1777	1779	1783	rVV2	1287	1643	0.06%	0.011%
76	11.969	1783	1785	1789	rVV3	959	1128	0.04%	0.008%

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Integrator: RTE

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Stop Thrs : 0

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Peak separation: 5

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 Title : VOC Analysis

77	12.024	1789	1794	1806	rVB	419431	508243	17.82%	3.486%
78	12.323	1835	1843	1854	rBV	472408	595509	20.88%	4.085%
79	12.426	1857	1860	1863	rBV3	757	1196	0.04%	0.008%
80	12.573	1882	1884	1885	rBV2	568	413	0.01%	0.003%
81	12.628	1891	1893	1896	rBV2	535	843	0.03%	0.006%
82	12.658	1896	1898	1903	rVV3	1031	1594	0.06%	0.011%
83	12.768	1912	1916	1921	rVB	6766	9016	0.32%	0.062%
84	12.933	1940	1943	1944	rVB2	767	632	0.02%	0.004%
85	13.329	2006	2008	2009	rBV	610	477	0.02%	0.003%
86	13.378	2014	2016	2018	rBV2	612	739	0.03%	0.005%
87	13.865	2093	2096	2097	rBV	427	573	0.02%	0.004%
88	13.902	2100	2102	2106	rVV	966	859	0.03%	0.006%
89	14.134	2135	2140	2144	rBV2	3784	6668	0.23%	0.046%
90	14.292	2164	2166	2169	rBV	577	714	0.03%	0.005%
91	14.365	2176	2178	2180	rBV	535	427	0.01%	0.003%
92	14.414	2182	2186	2187	rVV2	530	493	0.02%	0.003%
93	14.755	2239	2242	2243	rBV2	771	861	0.03%	0.006%
94	14.889	2261	2264	2265	rBV3	878	855	0.03%	0.006%
95	15.286	2326	2329	2331	rBV	592	657	0.02%	0.005%
96	15.584	2377	2378	2380	rBV	684	572	0.02%	0.004%
97	15.603	2380	2381	2383	rVV	941	670	0.02%	0.005%
98	15.938	2435	2436	2437	rBV	935	472	0.02%	0.003%
99	16.377	2506	2508	2509	rBV	807	616	0.02%	0.004%
100	16.749	2567	2569	2572	rBV	706	639	0.02%	0.004%

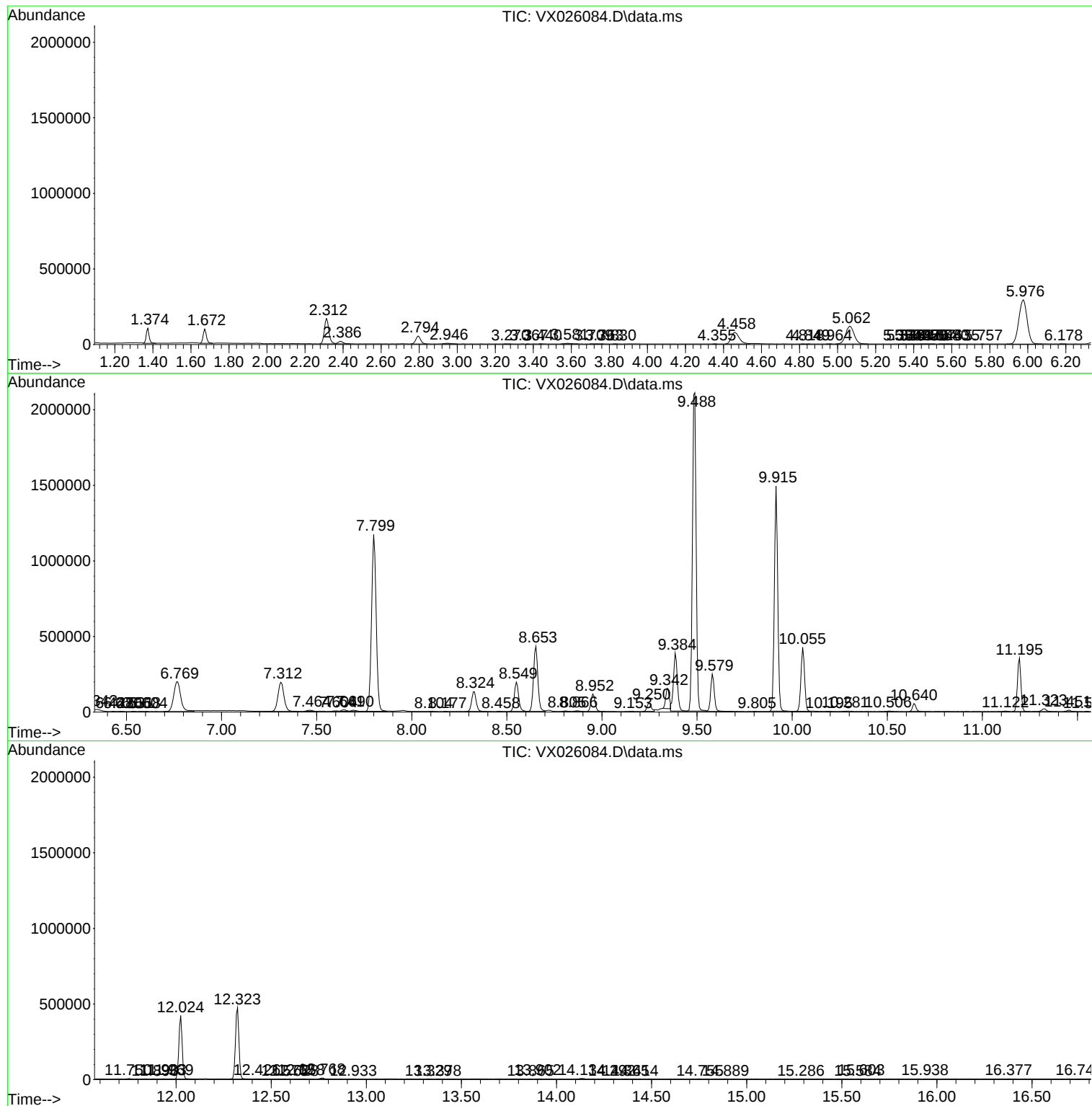
Sum of corrected areas: 14579691

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Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#02

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 : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#02

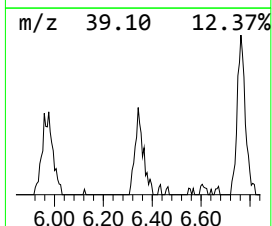
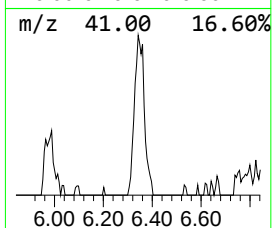
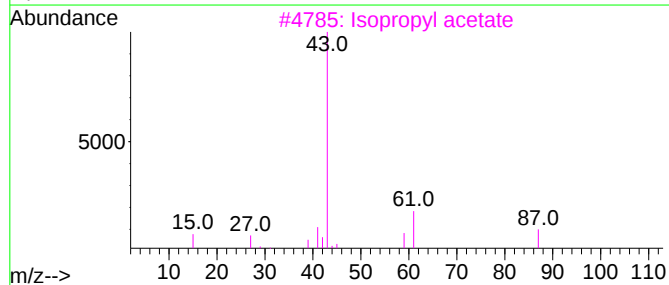
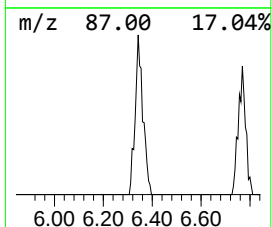
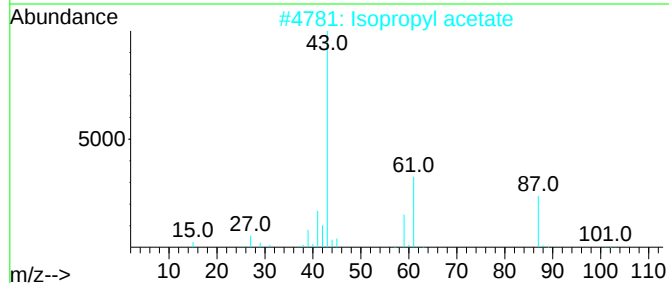
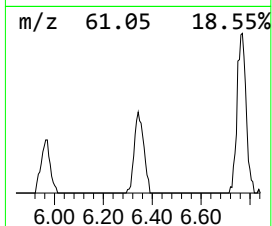
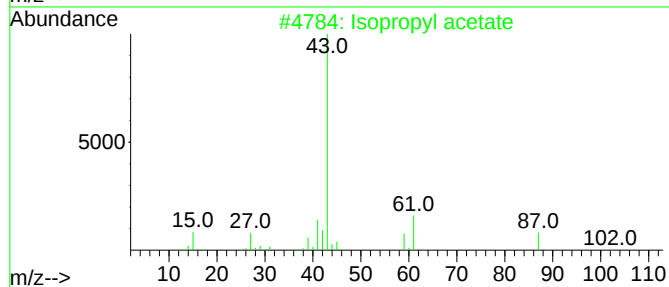
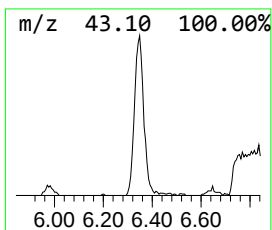
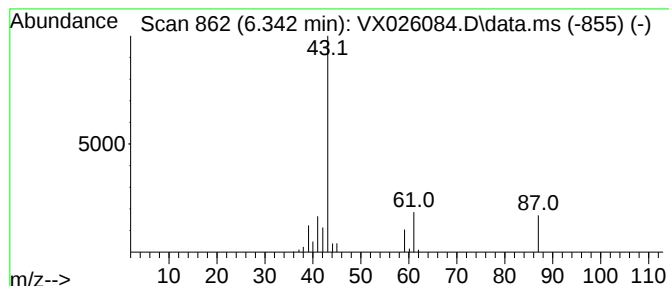
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	3.62 ug/L	36545	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl acetate	102	C5H10O2	000108-21-4	64
2			Isopropyl acetate	102	C5H10O2	000108-21-4	64
3			Isopropyl acetate	102	C5H10O2	000108-21-4	38
4			Isopropyl acetate	102	C5H10O2	000108-21-4	38
5			Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB141699ZHE#02

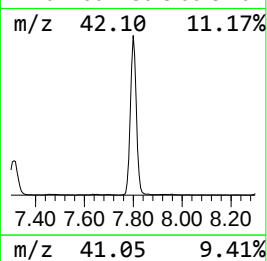
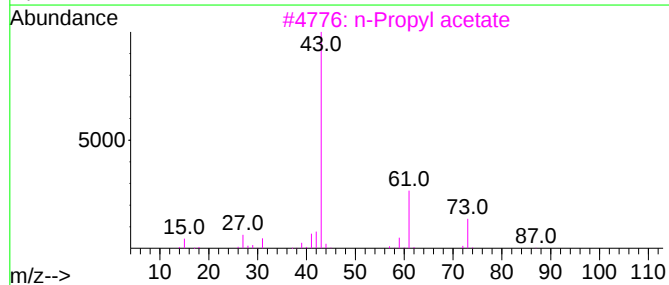
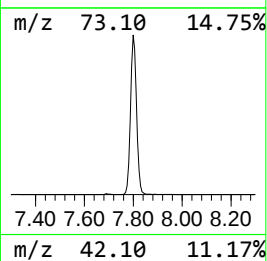
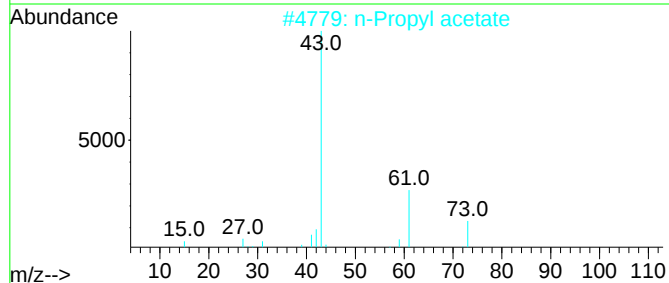
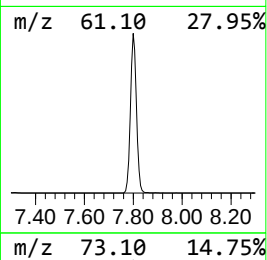
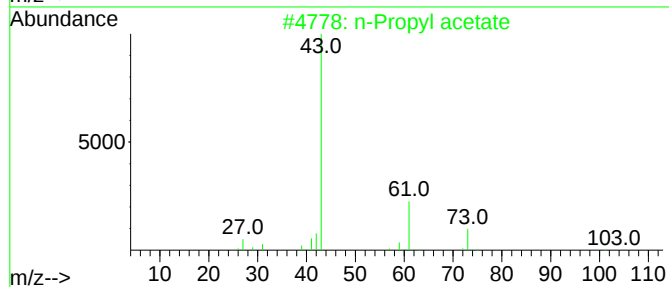
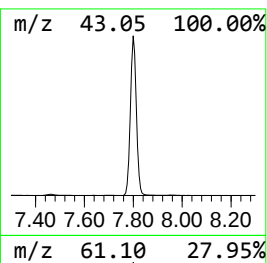
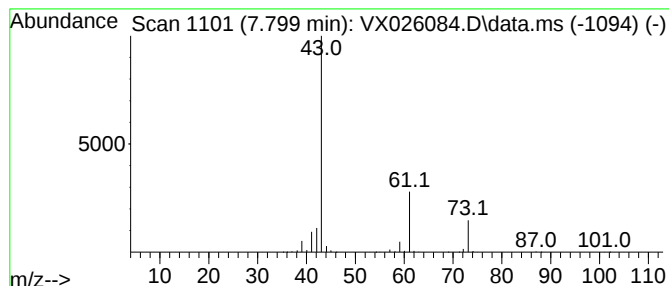
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	195.94 ug/L	1977710	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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ALS Vial : 40 Sample Multiplier: 1

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ClientSampleId :
PB141699ZHE#02

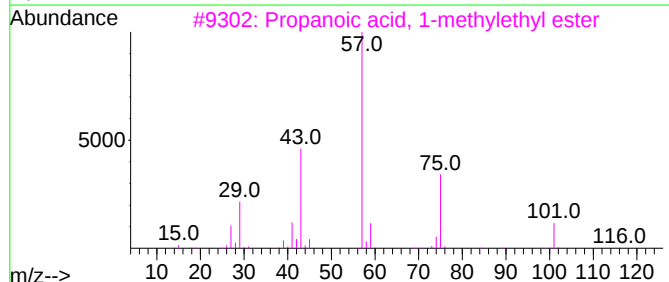
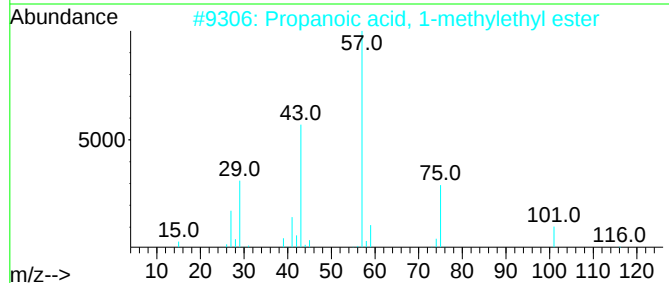
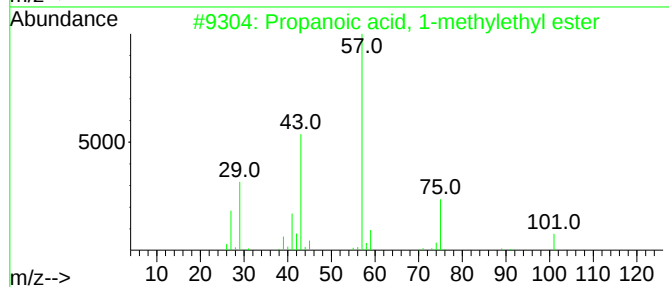
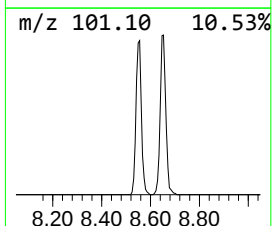
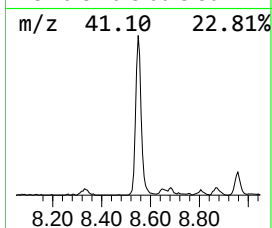
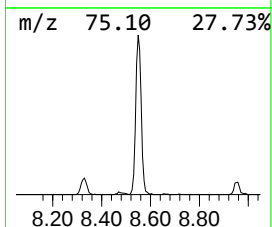
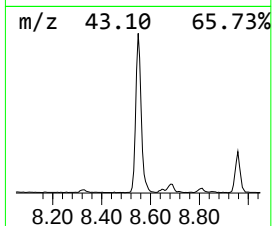
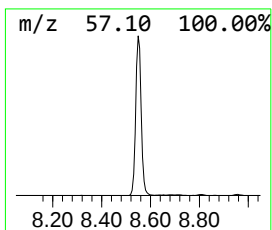
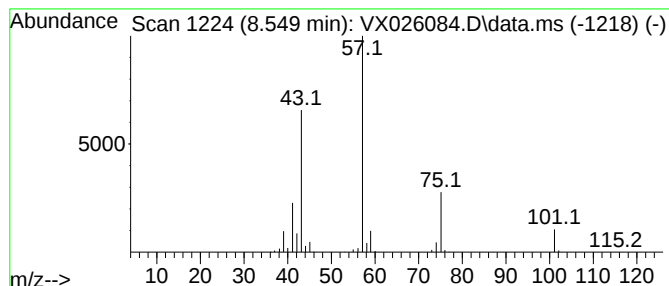
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	27.22 ug/L	306255	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	64
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42



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Acq On : 28 Dec 2021 00:36
Operator : JC/MD
Sample : PB141699ZHE#02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#02

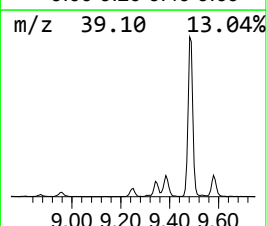
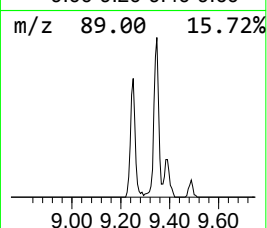
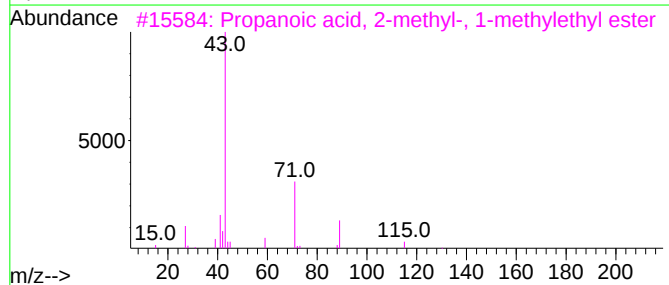
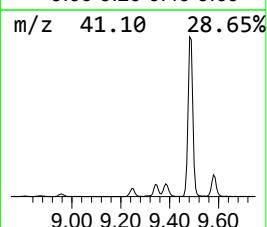
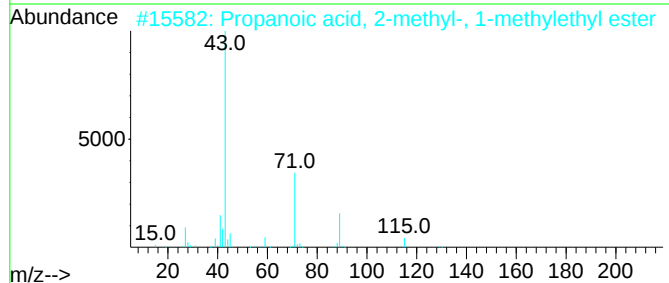
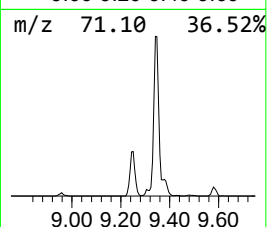
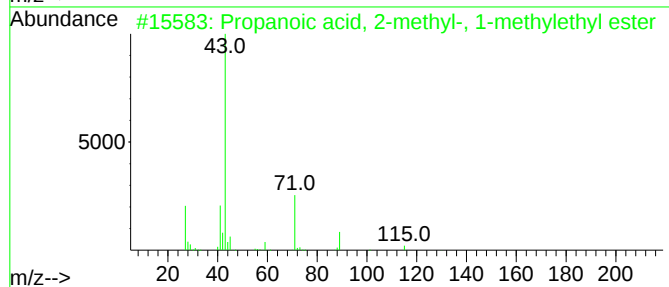
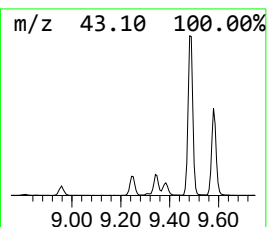
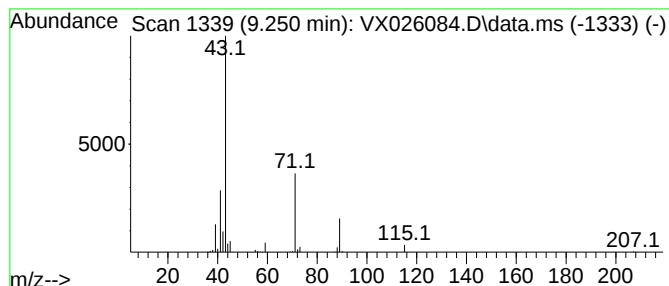
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Quant Title : VOC Analysis

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	7.71 ug/L	86734	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	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026084.D
Acq On : 28 Dec 2021 00:36
Operator : JC/MD
Sample : PB141699ZHE#02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#02

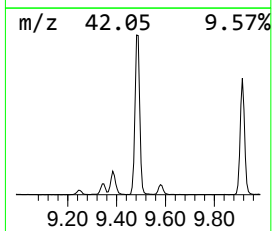
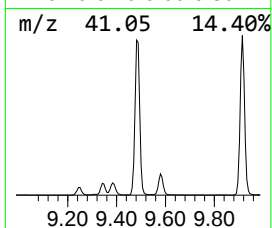
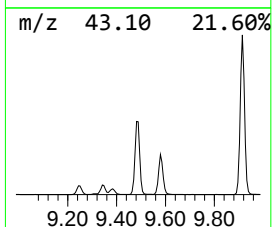
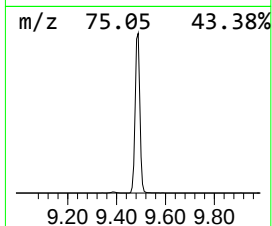
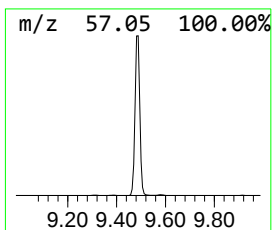
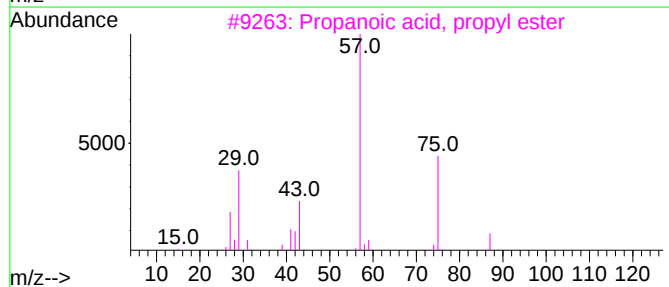
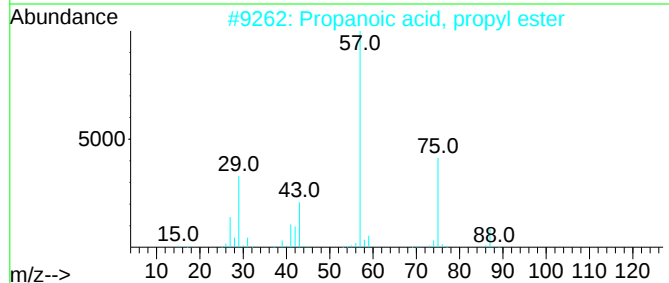
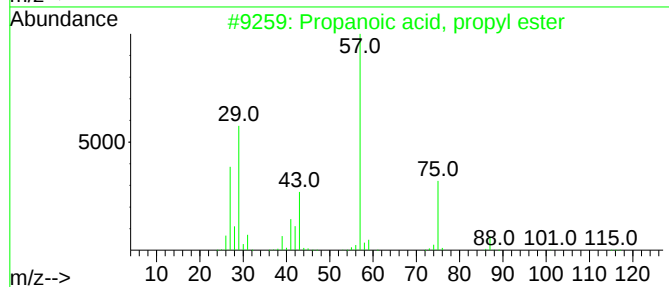
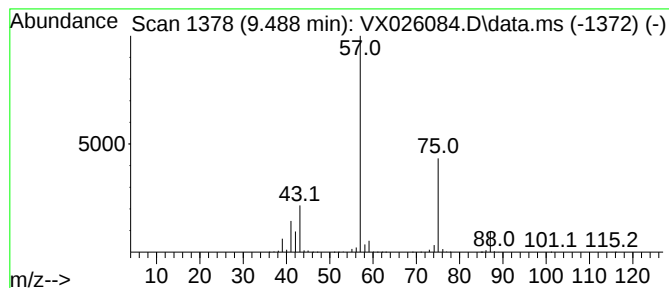
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Quant Title : VOC Analysis

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.
9.488	253.54 ug/L	2852690	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	78
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026084.D
Acq On : 28 Dec 2021 00:36
Operator : JC/MD
Sample : PB141699ZHE#02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#02

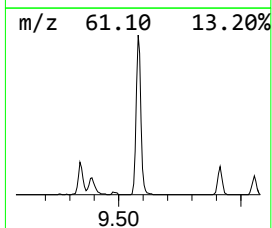
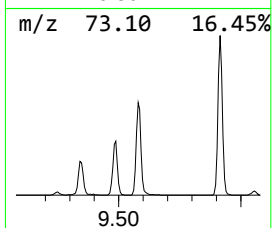
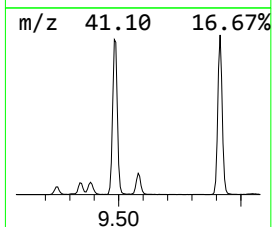
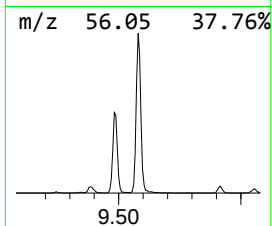
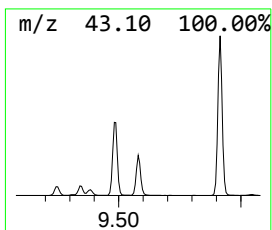
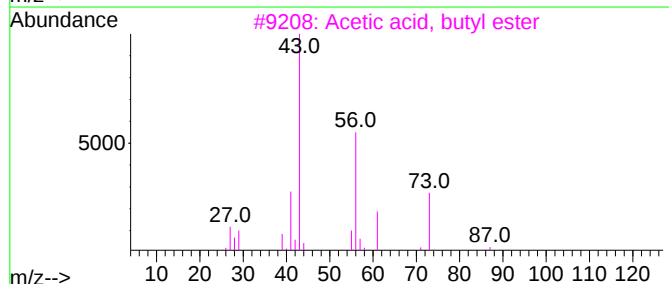
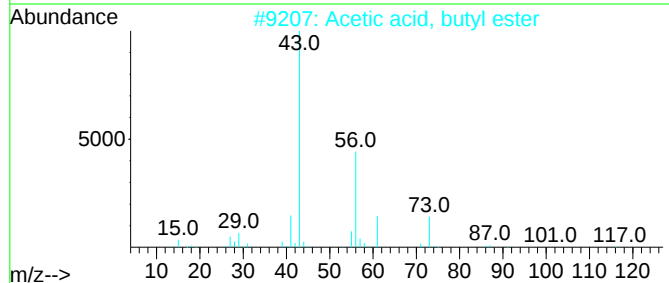
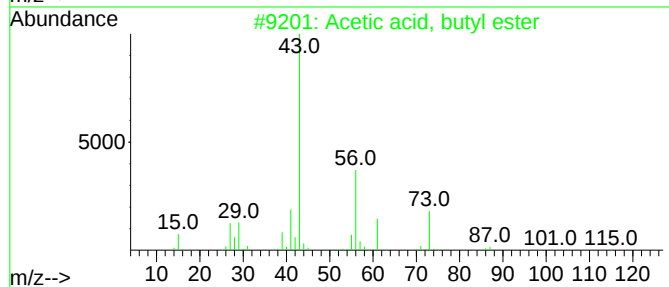
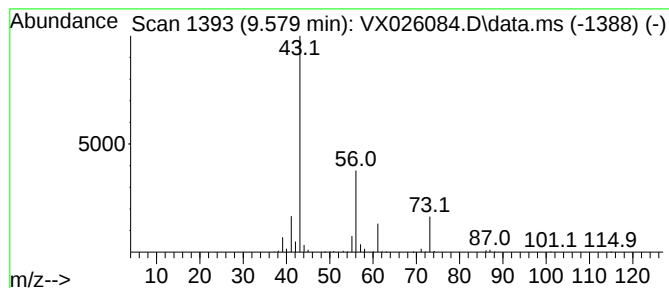
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Quant Title : VOC Analysis

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	28.68 ug/L	322693	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	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	59
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
5			Isobutyl acetate	116	C6H12O2	000110-19-0	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026084.D
Acq On : 28 Dec 2021 00:36
Operator : JC/MD
Sample : PB141699ZHE#02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#02

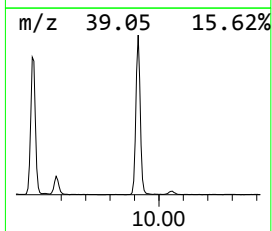
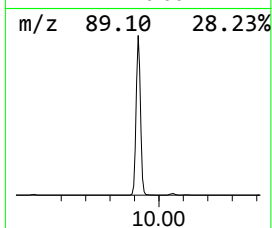
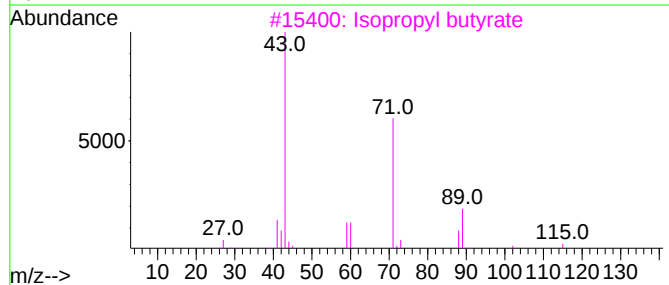
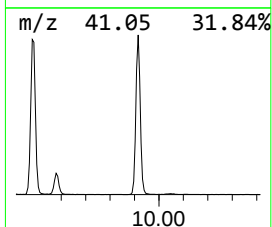
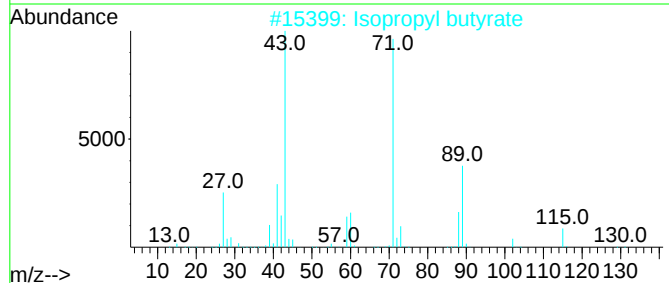
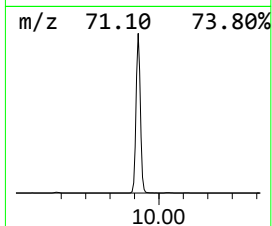
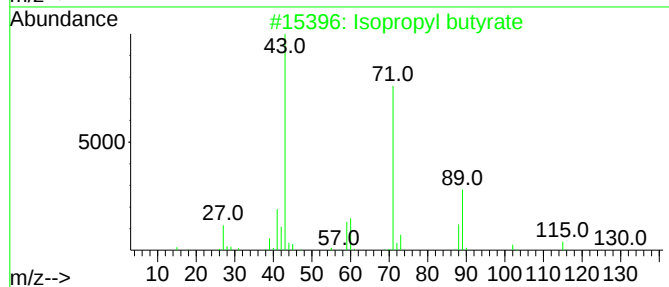
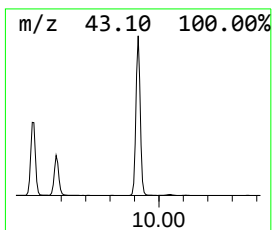
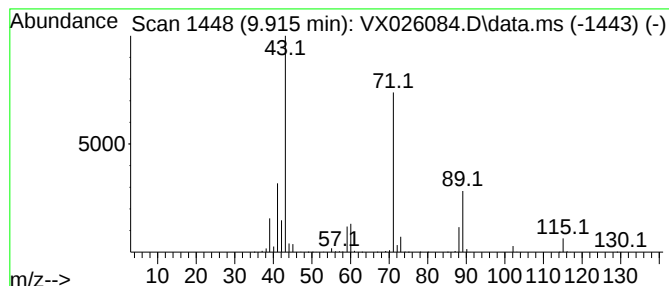
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Quant Title : VOC Analysis

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	162.20 ug/L	1825030	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 : VX026084.D
Acq On : 28 Dec 2021 00:36
Operator : JC/MD
Sample : PB141699ZHE#02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#02

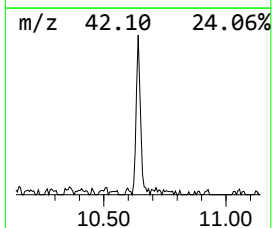
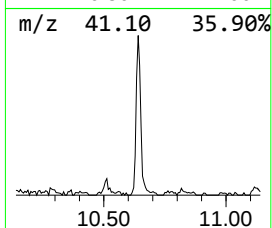
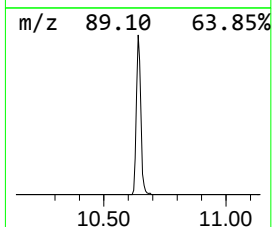
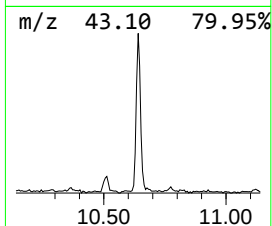
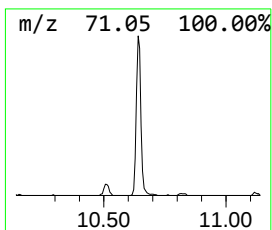
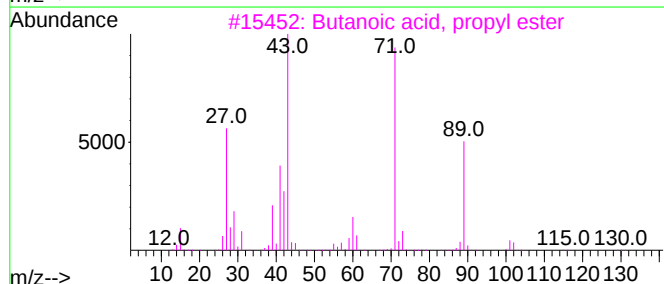
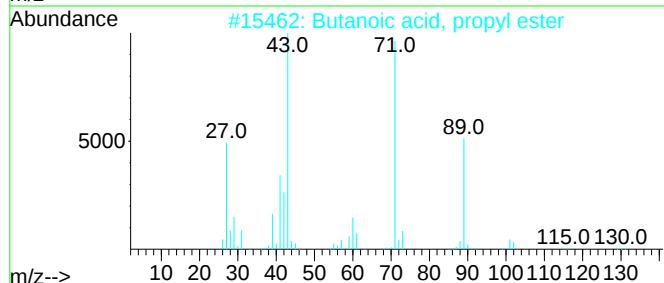
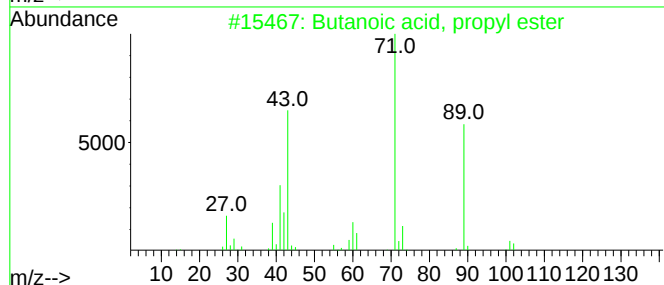
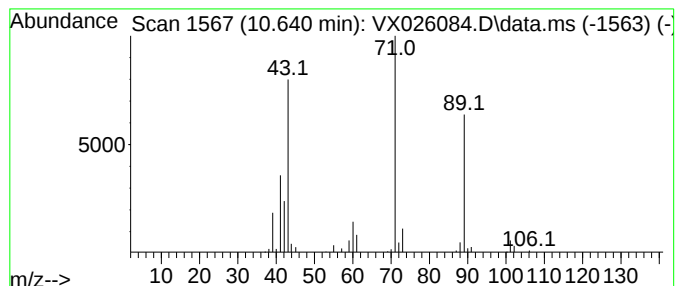
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Quant Title : VOC Analysis

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	5.81 ug/L	65399	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	90
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026084.D
Acq On : 28 Dec 2021 00:36
Operator : JC/MD
Sample : PB141699ZHE#02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#02

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	3.6	ug/L	36545	1	6.769	504670	50.0
n-Propyl acetate	7.799	195.9	ug/L	1977710	1	6.769	504670	50.0
Propanoic acid,...	8.549	27.2	ug/L	306255	2	10.055	562579	50.0
Propanoic acid,...	9.250	7.7	ug/L	86734	2	10.055	562579	50.0
Propanoic acid,...	9.488	253.5	ug/L	2852690	2	10.055	562579	50.0
Acetic acid, bu...	9.579	28.7	ug/L	322693	2	10.055	562579	50.0
Isopropyl butyrate	9.915	162.2	ug/L	1825030	2	10.055	562579	50.0
Butanoic acid, ...	10.640	5.8	ug/L	65399	2	10.055	562579	50.0