

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
 Data File : VX026083.D
 Acq On : 28 Dec 2021 00:13
 Operator : JC/MD
 Sample : PB141699ZHE#01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB141699ZHE#01

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: VX026083.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	57	rVB	99728	98288	3.42%	0.683%
2	1.672	92	96	102	rVB	89904	106729	3.71%	0.742%
3	2.313	195	201	209	rBV	163053	266469	9.27%	1.853%
4	2.386	209	213	225	rVB	15632	30073	1.05%	0.209%
5	2.520	231	235	237	rBV3	1316	1924	0.07%	0.013%
6	2.794	273	280	290	rBV	50690	94162	3.28%	0.655%
7	3.001	312	314	317	rVB2	933	966	0.03%	0.007%
8	3.166	340	341	343	rBV	488	391	0.01%	0.003%
9	3.233	350	352	354	rBV	443	516	0.02%	0.004%
10	3.428	381	384	385	rBV2	709	830	0.03%	0.006%
11	3.526	398	400	402	rVB	658	397	0.01%	0.003%
12	3.587	403	410	414	rVV3	2441	5687	0.20%	0.040%
13	3.666	421	423	426	rBV2	525	508	0.02%	0.004%
14	3.873	455	457	458	rBV	787	668	0.02%	0.005%
15	4.074	488	490	492	rBV	742	573	0.02%	0.004%
16	4.251	517	519	523	rBV2	620	528	0.02%	0.004%
17	4.318	525	530	532	rBV	644	1068	0.04%	0.007%
18	4.349	532	535	538	rBV2	568	593	0.02%	0.004%
19	4.458	545	553	565	rBV	73049	208801	7.27%	1.452%
20	4.861	617	619	621	rVB	744	407	0.01%	0.003%
21	4.897	623	625	629	rVB	954	1063	0.04%	0.007%
22	4.946	629	633	634	rBV2	800	944	0.03%	0.007%
23	5.068	641	653	665	rBV	119020	353445	12.30%	2.458%
24	5.355	695	700	702	rBV2	705	1117	0.04%	0.008%
25	5.550	729	732	733	rBV	360	379	0.01%	0.003%
26	5.970	789	801	817	rVV2	276940	843279	29.35%	5.864%
27	6.239	843	845	847	rVB2	450	394	0.01%	0.003%
28	6.269	847	850	851	rBV2	590	517	0.02%	0.004%
29	6.348	855	863	872	rVV2	13046	34922	1.22%	0.243%
30	6.501	885	888	891	rVB2	495	483	0.02%	0.003%
31	6.763	922	931	945	rBV	198215	508187	17.69%	3.534%
32	7.312	1013	1021	1031	rVB	184624	395747	13.77%	2.752%
33	7.464	1040	1046	1057	rBV2	7424	15523	0.54%	0.108%
34	7.641	1071	1075	1080	rBV	8151	12318	0.43%	0.086%
35	7.799	1094	1101	1114	rBV	1167573	1997159	69.51%	13.888%
36	8.049	1141	1142	1145	rBV	911	820	0.03%	0.006%

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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	8.324	1181	1187	1200	rVV	126245	210963	7.34%	1.467%
38	8.415	1200	1202	1207	rVB3	829	726	0.03%	0.005%
39	8.549	1218	1224	1234	rBV	204001	309297	10.77%	2.151%
40	8.653	1234	1241	1249	rBV	414354	649547	22.61%	4.517%
41	8.811	1262	1267	1272	rVB3	3004	5172	0.18%	0.036%
42	8.872	1272	1277	1281	rVV	4412	7600	0.26%	0.053%
43	8.952	1284	1290	1306	rVB2	114535	168768	5.87%	1.174%
44	9.116	1314	1317	1319	rVB3	464	371	0.01%	0.003%
45	9.250	1333	1339	1343	rBV	56836	85871	2.99%	0.597%
46	9.342	1351	1354	1357	rBV	129042	169756	5.91%	1.180%
47	9.384	1357	1361	1372	rVB	359779	519515	18.08%	3.613%
48	9.488	1372	1378	1388	rBV	2202699	2873165	100.00%	19.979%
49	9.579	1389	1393	1406	rVB	246806	318991	11.10%	2.218%
50	9.915	1443	1448	1458	rBV	1507827	1860736	64.76%	12.939%
51	10.055	1465	1471	1477	rBV	424619	566131	19.70%	3.937%
52	10.238	1499	1501	1504	rVB2	713	746	0.03%	0.005%
53	10.281	1504	1508	1515	rBV5	2144	5376	0.19%	0.037%
54	10.512	1542	1546	1551	rVV2	2926	4182	0.15%	0.029%
55	10.640	1563	1567	1575	rBV	52729	66059	2.30%	0.459%
56	11.012	1625	1628	1629	rBV2	809	710	0.02%	0.005%
57	11.122	1640	1646	1650	rVB4	2355	3872	0.13%	0.027%
58	11.195	1652	1658	1666	rVV	336287	424682	14.78%	2.953%
59	11.323	1674	1679	1688	rVB2	16820	26872	0.94%	0.187%
60	11.451	1697	1700	1703	rBV2	3441	3747	0.13%	0.026%
61	11.719	1742	1744	1745	rBV	591	473	0.02%	0.003%
62	11.750	1745	1749	1752	rVB5	2515	3710	0.13%	0.026%
63	11.890	1770	1772	1774	rVB2	845	748	0.03%	0.005%
64	11.914	1774	1776	1777	rBV	651	660	0.02%	0.005%
65	11.945	1777	1781	1783	rVV3	911	1138	0.04%	0.008%
66	12.024	1789	1794	1800	rBV	418070	505884	17.61%	3.518%
67	12.207	1822	1824	1825	rBV2	513	396	0.01%	0.003%
68	12.219	1825	1826	1829	rVV2	1037	771	0.03%	0.005%
69	12.280	1833	1836	1837	rBV	661	638	0.02%	0.004%
70	12.323	1837	1843	1852	rVB	448323	565855	19.69%	3.935%
71	12.402	1854	1856	1858	rBV	602	687	0.02%	0.005%
72	12.481	1867	1869	1873	rBV3	578	780	0.03%	0.005%
73	12.573	1882	1884	1885	rBV2	786	584	0.02%	0.004%
74	12.622	1889	1892	1895	rBV2	642	881	0.03%	0.006%
75	12.658	1896	1898	1900	rVB2	625	544	0.02%	0.004%
76	12.768	1912	1916	1924	rVB3	6365	8759	0.30%	0.061%

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Integrator: RTE

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Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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 Title : VOC Analysis

77	12.933	1942	1943	1945	rBV	698	594	0.02%	0.004%
78	13.042	1959	1961	1963	rBV3	472	430	0.01%	0.003%
79	13.371	2013	2015	2018	rVB	609	686	0.02%	0.005%
80	13.402	2018	2020	2021	rBV	536	391	0.01%	0.003%
81	13.518	2037	2039	2041	rVV	716	568	0.02%	0.004%
82	13.701	2067	2069	2070	rBV2	844	511	0.02%	0.004%
83	13.914	2103	2104	2107	rVB3	739	435	0.02%	0.003%
84	14.030	2121	2123	2125	rBV	905	1006	0.04%	0.007%
85	14.134	2135	2140	2144	rVB	3719	4736	0.16%	0.033%
86	14.262	2160	2161	2163	rVB	993	661	0.02%	0.005%
87	14.286	2163	2165	2166	rBV	876	605	0.02%	0.004%
88	14.457	2192	2193	2196	rBV2	611	711	0.02%	0.005%
89	14.768	2242	2244	2246	rBV2	1146	840	0.03%	0.006%
90	14.871	2260	2261	2263	rBV	653	501	0.02%	0.003%
91	14.993	2279	2281	2282	rBV	981	718	0.02%	0.005%
92	15.402	2344	2348	2352	rVB3	868	1400	0.05%	0.010%
93	15.469	2357	2359	2360	rBV	736	434	0.02%	0.003%
94	15.572	2374	2376	2379	rBV2	676	850	0.03%	0.006%
95	15.700	2395	2397	2398	rBV	525	375	0.01%	0.003%
96	15.767	2406	2408	2409	rBV	827	669	0.02%	0.005%
97	15.828	2416	2418	2419	rBV	869	493	0.02%	0.003%
98	15.865	2422	2424	2425	rBV2	822	533	0.02%	0.004%
99	16.188	2476	2477	2481	rBV2	835	797	0.03%	0.006%
100	16.572	2538	2540	2543	rBV3	717	653	0.02%	0.005%

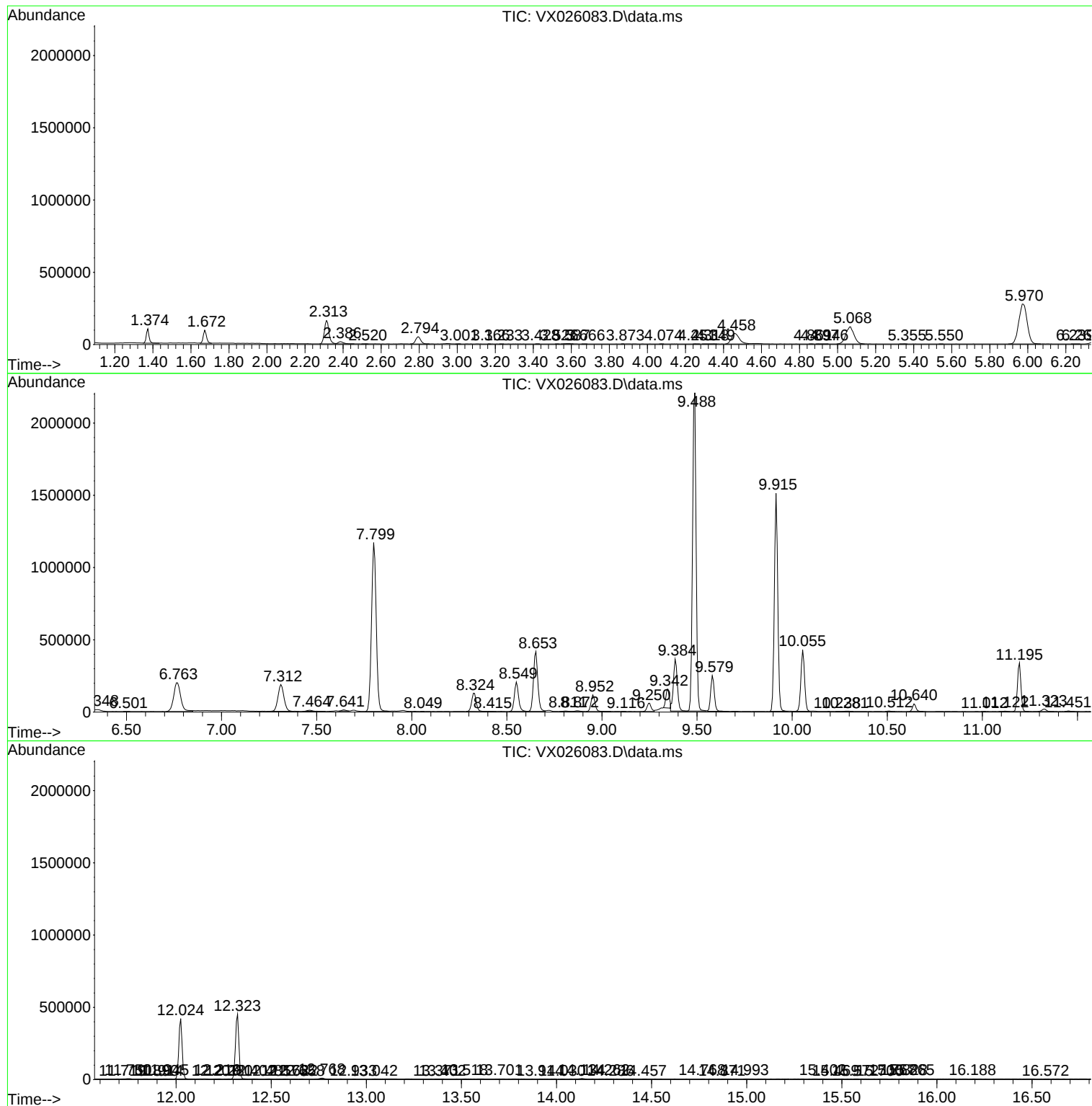
Sum of corrected areas: 14380835

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Instrument :
MSVOA_X
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PB141699ZHE#01

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 : 39 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#01

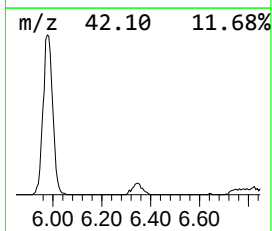
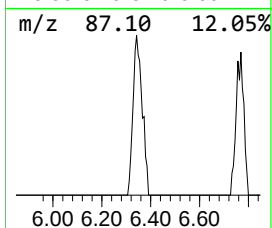
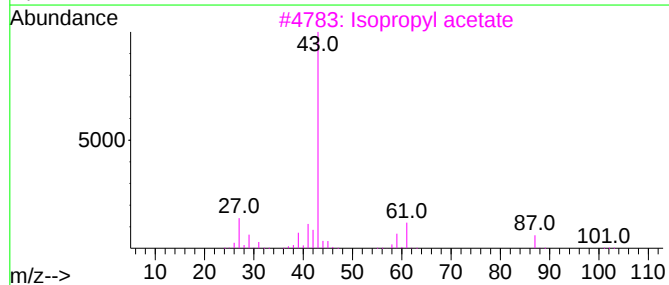
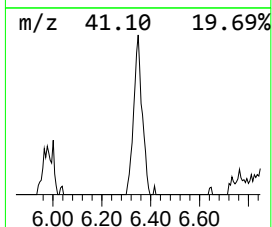
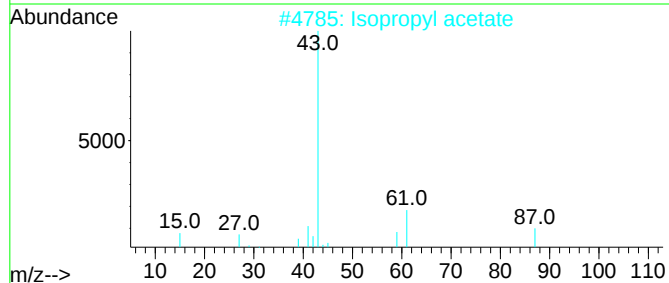
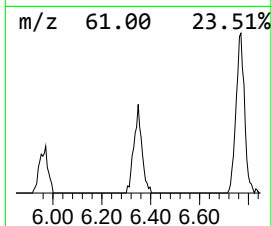
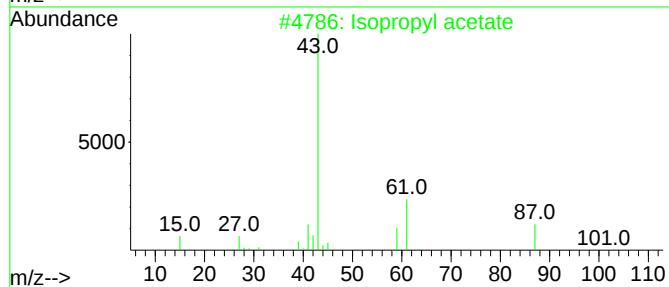
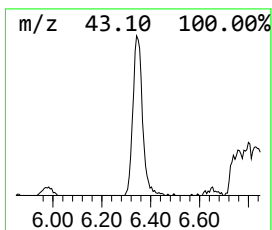
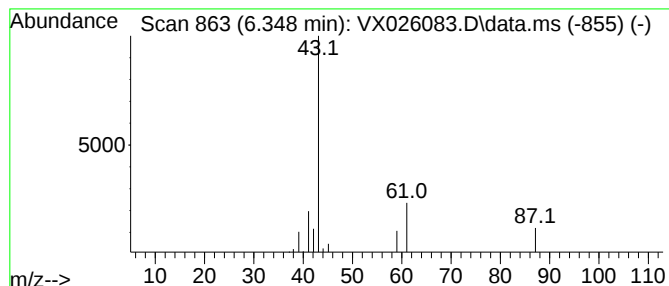
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	3.44 ug/L	34922	1,4-Difluorobenzene	6.769

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	83
3			Isopropyl acetate	102	C5H10O2	000108-21-4	78
4			Isopropyl acetate	102	C5H10O2	000108-21-4	64
5			Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#01

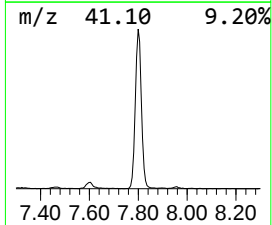
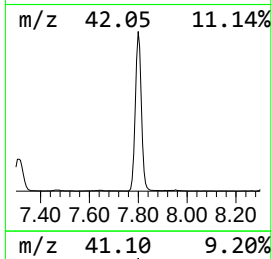
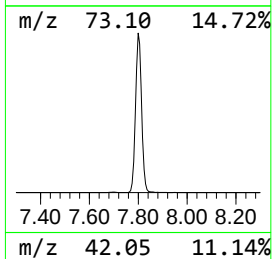
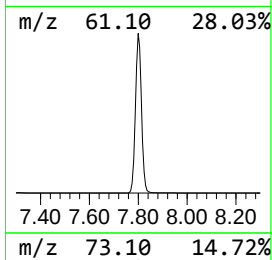
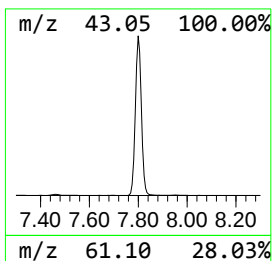
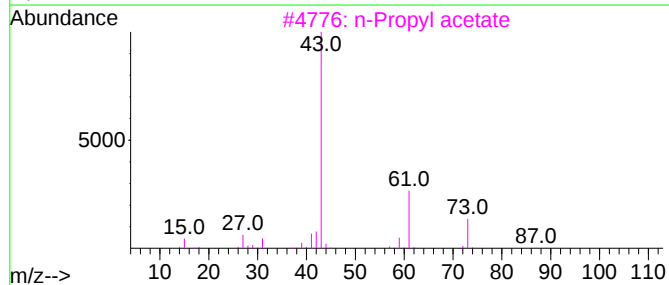
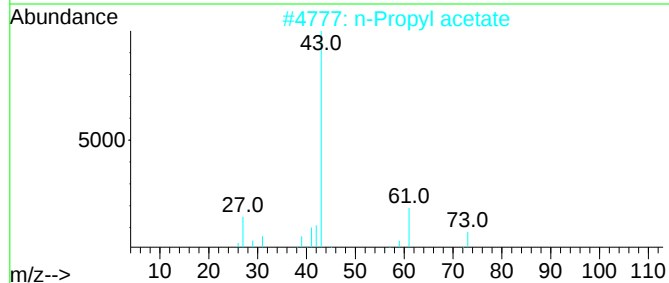
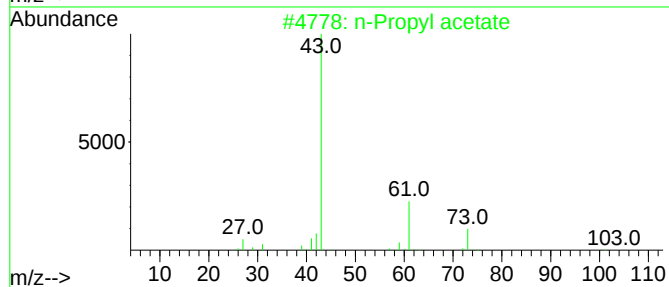
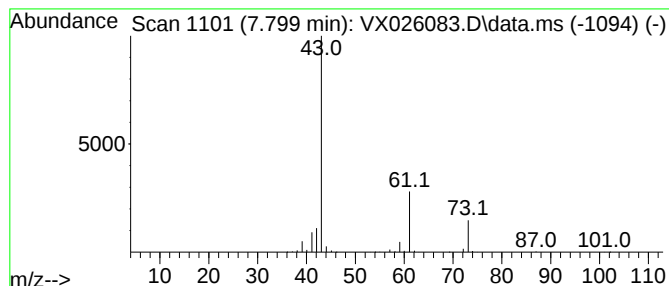
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	196.50 ug/L	1997160	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 : 39 Sample Multiplier: 1

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ClientSampleId :
PB141699ZHE#01

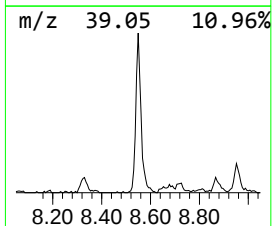
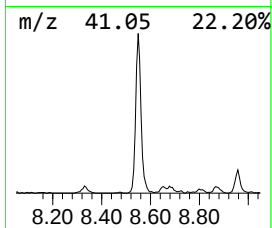
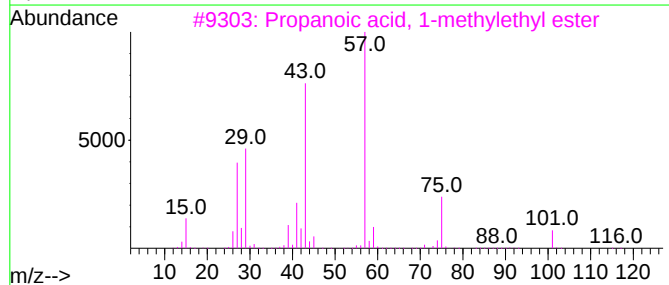
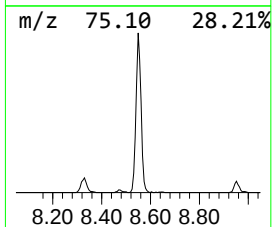
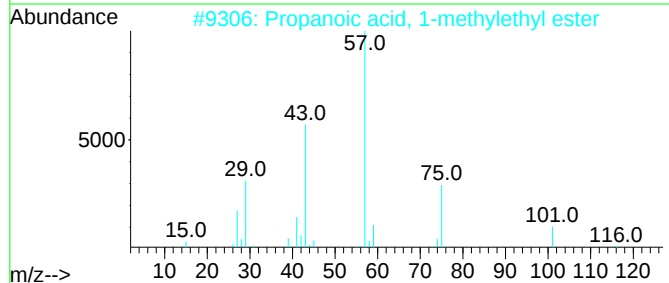
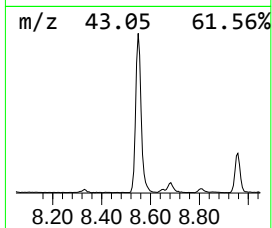
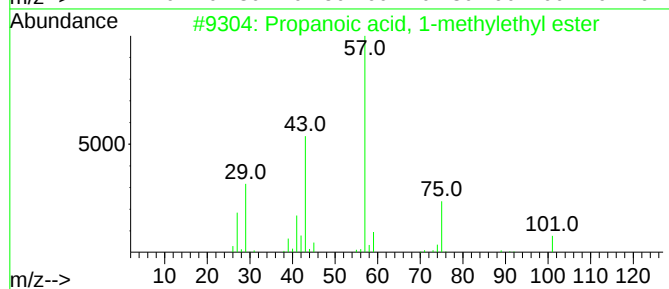
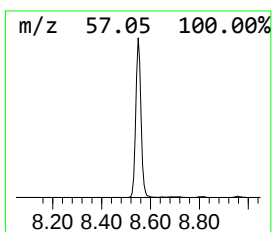
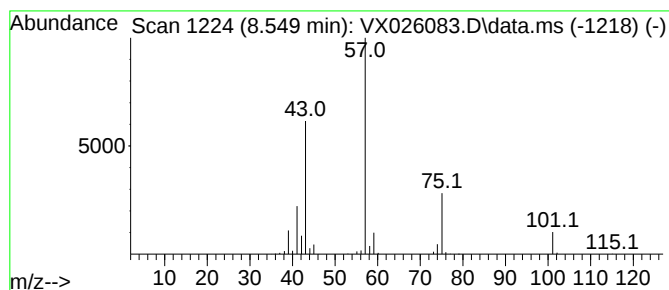
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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	27.32 ug/L	309297	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 : VX026083.D
Acq On : 28 Dec 2021 00:13
Operator : JC/MD
Sample : PB141699ZHE#01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#01

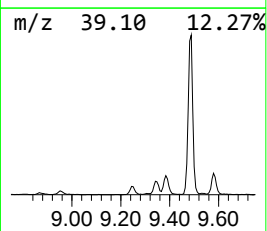
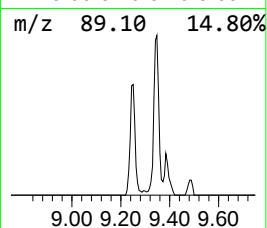
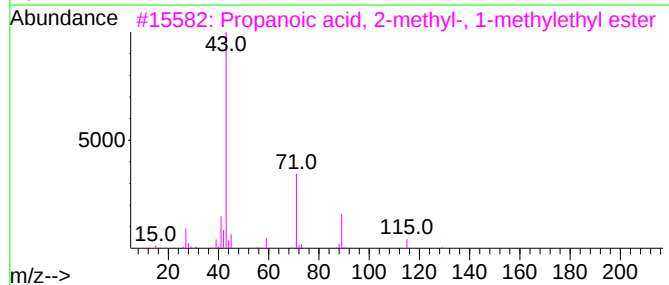
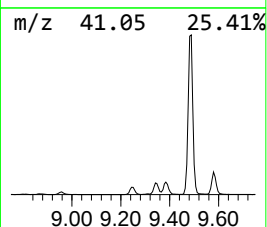
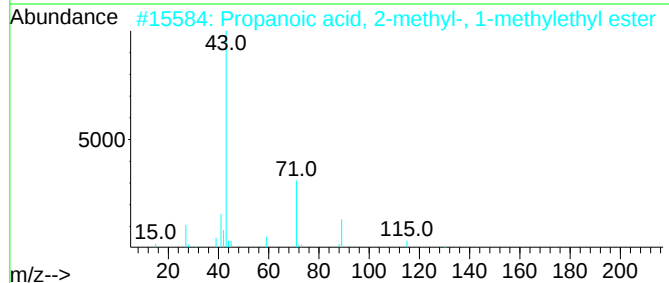
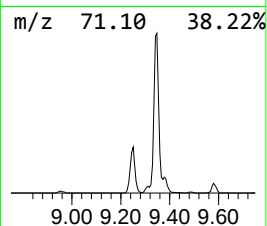
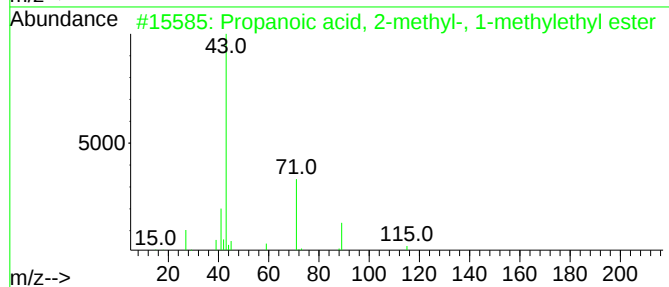
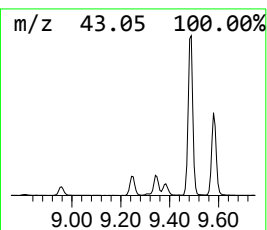
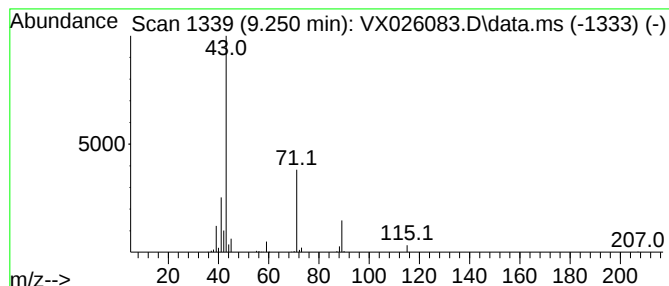
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Quant Title : VOC Analysis

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	7.58 ug/L	85871	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	64
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026083.D
Acq On : 28 Dec 2021 00:13
Operator : JC/MD
Sample : PB141699ZHE#01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#01

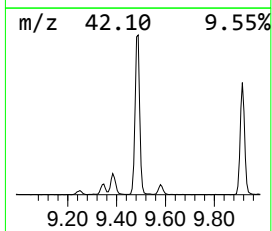
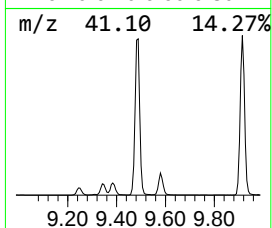
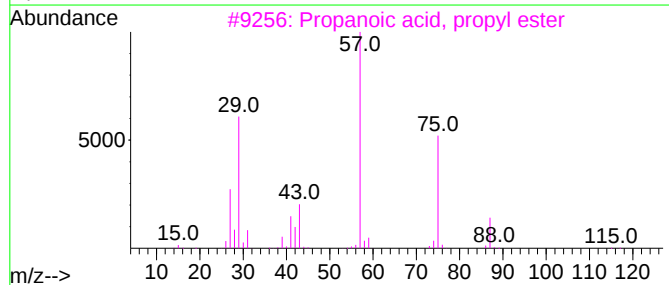
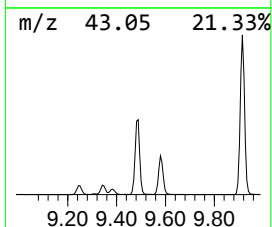
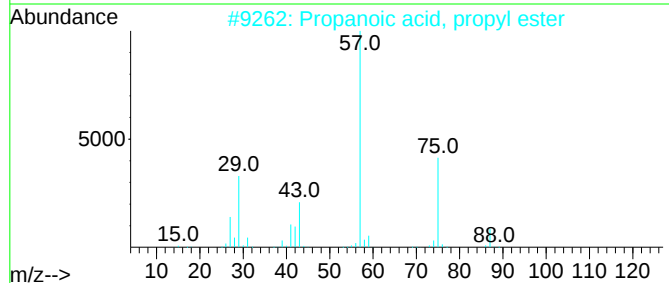
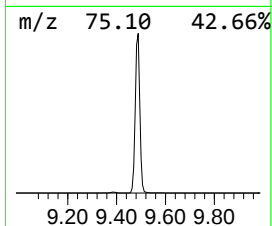
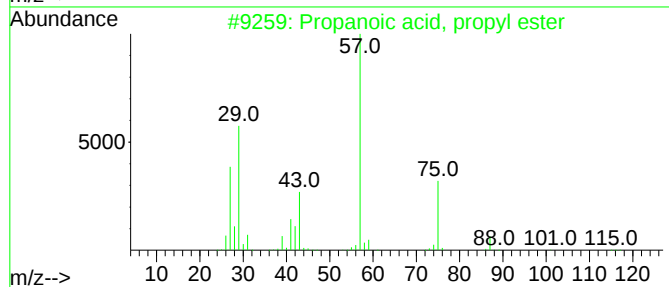
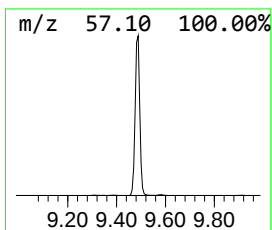
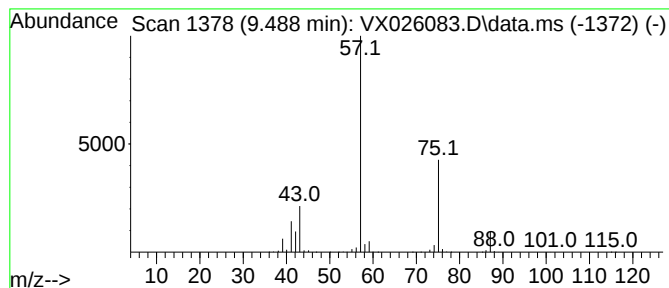
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Quant Title : VOC Analysis

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	253.75 ug/L	2873170	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 : VX026083.D
Acq On : 28 Dec 2021 00:13
Operator : JC/MD
Sample : PB141699ZHE#01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#01

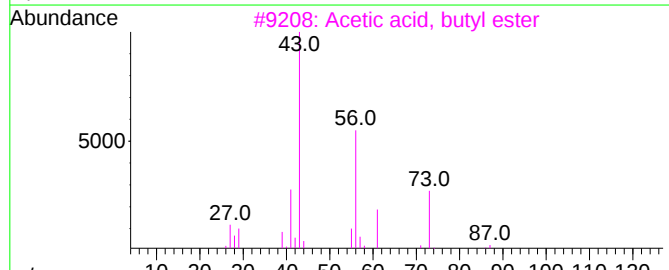
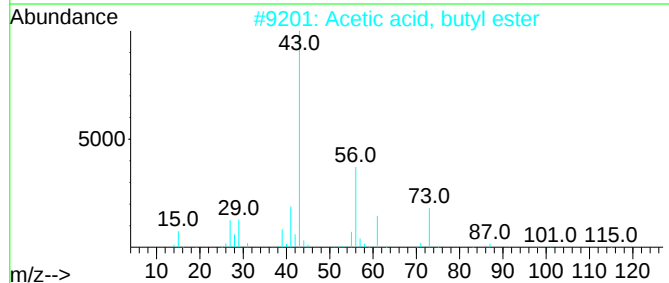
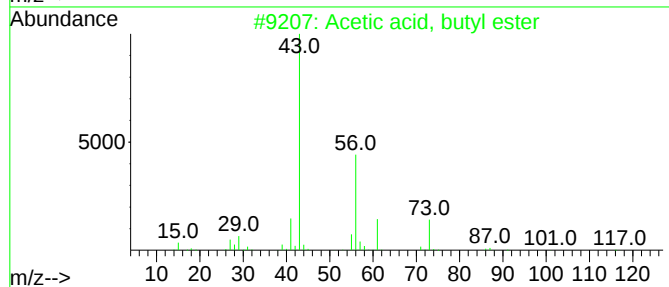
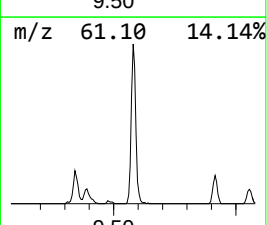
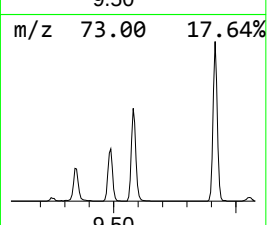
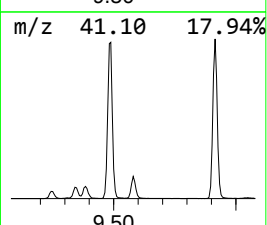
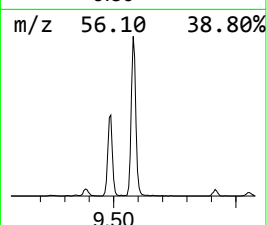
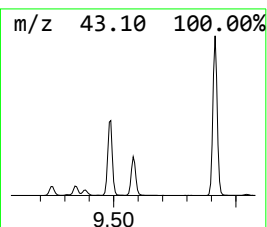
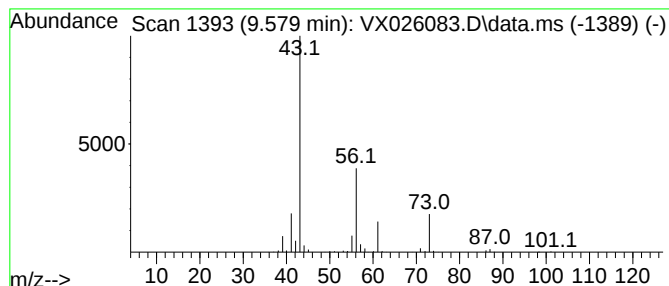
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Quant Title : VOC Analysis

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	28.17 ug/L	318991	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	64
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026083.D
Acq On : 28 Dec 2021 00:13
Operator : JC/MD
Sample : PB141699ZHE#01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#01

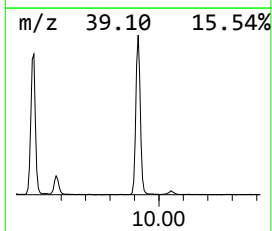
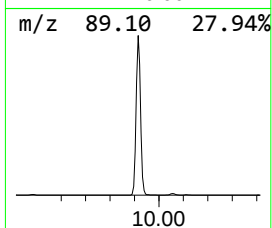
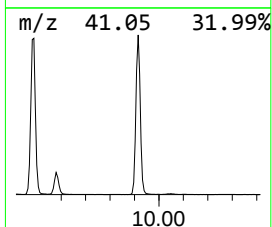
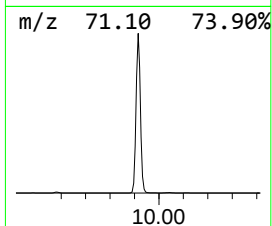
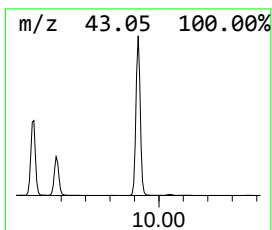
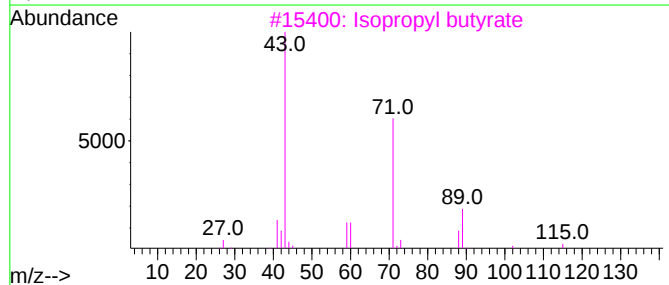
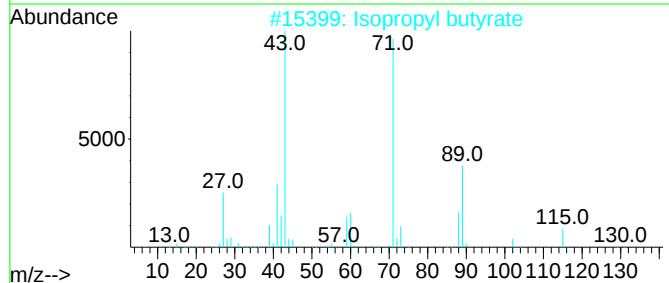
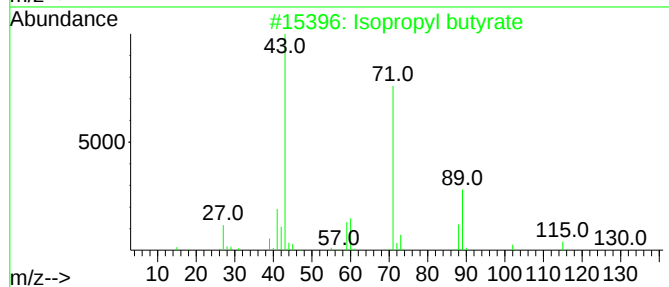
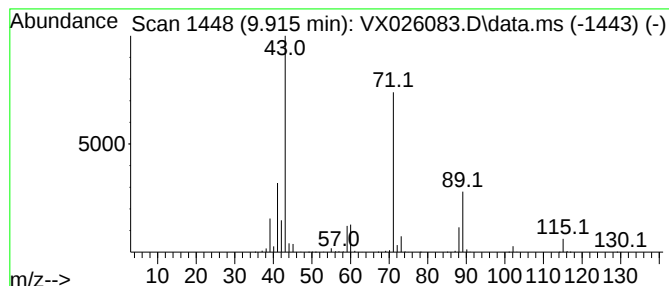
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Quant Title : VOC Analysis

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	164.34 ug/L	1860740	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	94
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 : VX026083.D
Acq On : 28 Dec 2021 00:13
Operator : JC/MD
Sample : PB141699ZHE#01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#01

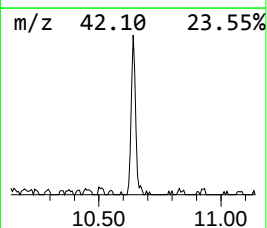
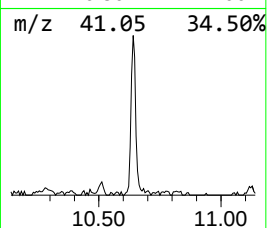
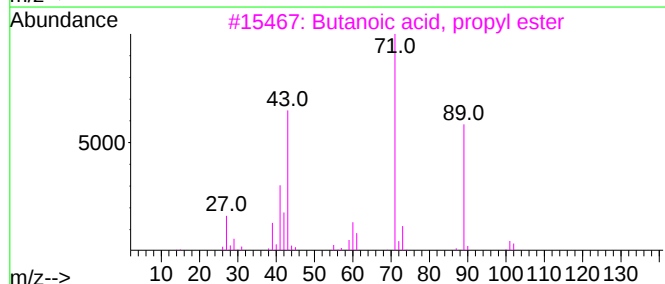
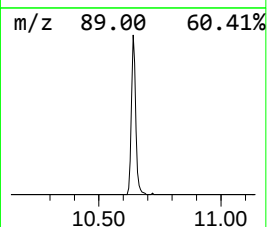
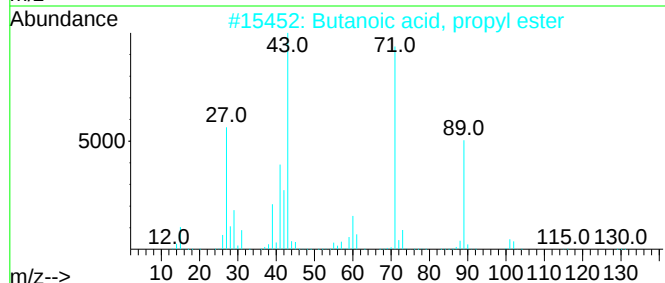
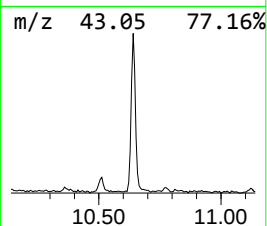
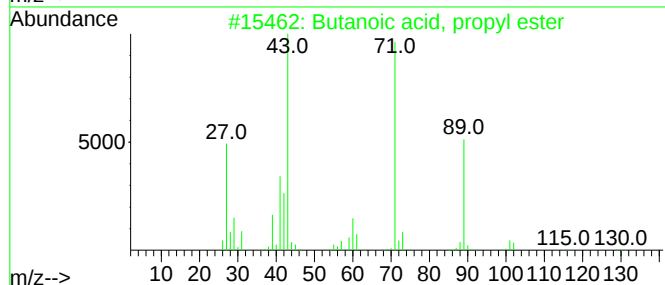
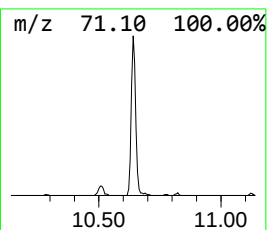
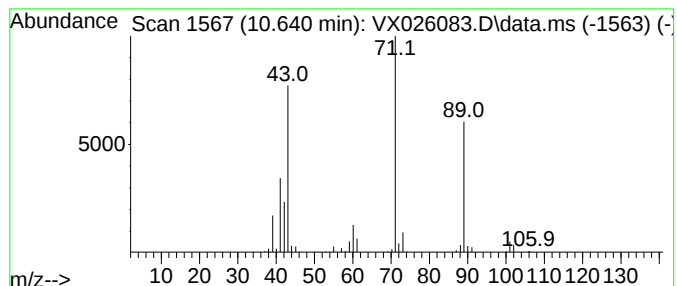
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Quant Title : VOC Analysis

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	5.83 ug/L	66059	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			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	83
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
Data File : VX026083.D
Acq On : 28 Dec 2021 00:13
Operator : JC/MD
Sample : PB141699ZHE#01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB141699ZHE#01

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	3.4	ug/L	34922	1	6.769	508187	50.0
n-Propyl acetate	7.799	196.5	ug/L	1997160	1	6.769	508187	50.0
Propanoic acid,...	8.549	27.3	ug/L	309297	2	10.055	566131	50.0
Propanoic acid,...	9.250	7.6	ug/L	85871	2	10.055	566131	50.0
Propanoic acid,...	9.488	253.8	ug/L	2873170	2	10.055	566131	50.0
Acetic acid, bu...	9.579	28.2	ug/L	318991	2	10.055	566131	50.0
Isopropyl butyrate	9.915	164.3	ug/L	1860740	2	10.055	566131	50.0
Butanoic acid, ...	10.640	5.8	ug/L	66059	2	10.055	566131	50.0