

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044341.D
 Acq On : 17 Dec 2024 11:12
 Operator : JC/MD
 Sample : PB165643TB 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VLEB643

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M

Title : VOC Analysis

Signal : TIC: VX044341.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	12	rVB	3413	2644	0.13%	0.018%
2	1.240	21	25	31	rBV	25046	32508	1.60%	0.217%
3	1.368	42	46	56	rBV	115873	127716	6.29%	0.854%
4	1.447	57	59	62	rVV	5683	5143	0.25%	0.034%
5	1.642	88	91	101	rVB	103963	136562	6.72%	0.913%
6	2.294	192	198	208	rVV	184353	283279	13.95%	1.894%
7	2.386	208	213	223	rVB	33627	54317	2.67%	0.363%
8	2.782	273	278	288	rVB4	7397	15578	0.77%	0.104%
9	3.008	314	315	319	rVB	792	526	0.03%	0.004%
10	3.105	329	331	334	rVB2	657	613	0.03%	0.004%
11	3.142	334	337	338	rBV3	392	485	0.02%	0.003%
12	3.184	341	344	346	rBV3	370	515	0.03%	0.003%
13	3.233	350	352	354	rVB2	535	505	0.02%	0.003%
14	3.264	354	357	359	rBV3	730	719	0.04%	0.005%
15	3.312	362	365	366	rBV2	1007	814	0.04%	0.005%
16	3.325	366	367	368	rBV	919	463	0.02%	0.003%
17	3.386	374	377	378	rBV2	632	567	0.03%	0.004%
18	3.428	378	384	390	rVV5	2512	4564	0.22%	0.031%
19	3.575	401	408	421	rVV2	26513	65146	3.21%	0.436%
20	3.709	428	430	433	rVB3	1000	691	0.03%	0.005%
21	4.202	509	511	514	rBV2	472	682	0.03%	0.005%
22	4.398	537	543	545	rBV3	889	1671	0.08%	0.011%
23	4.465	545	554	570	rBV2	72833	220245	10.84%	1.473%
24	4.952	631	634	635	rBV	474	544	0.03%	0.004%
25	5.080	637	655	673	rBV3	346207	1379738	67.94%	9.225%
26	5.294	688	690	694	rBV3	523	595	0.03%	0.004%
27	5.373	701	703	705	rBV3	486	545	0.03%	0.004%
28	5.446	712	715	717	rBV4	564	539	0.03%	0.004%
29	5.532	727	729	731	rBV2	488	583	0.03%	0.004%
30	5.556	731	733	736	rBV3	903	1062	0.05%	0.007%
31	5.629	742	745	748	rBV2	584	742	0.04%	0.005%
32	5.690	751	755	759	rVB3	292	502	0.02%	0.003%
33	5.769	766	768	770	rBV2	575	594	0.03%	0.004%
34	5.836	776	779	781	rBV2	553	477	0.02%	0.003%
35	5.964	789	800	815	rBV2	317357	954022	46.98%	6.379%
36	6.263	848	849	851	rBV	942	562	0.03%	0.004%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
 Title : VOC Analysis

37	6.342	851	862	876	rBV	81860	217551	10.71%	1.455%
38	6.592	902	903	907	rBV2	684	624	0.03%	0.004%
39	6.757	921	930	947	rBV	240492	592446	29.17%	3.961%
40	7.306	1012	1020	1037	rVB	200638	448327	22.08%	2.998%
41	7.641	1070	1075	1081	rBV	39409	72368	3.56%	0.484%
42	7.799	1094	1101	1119	rBV	1180076	2030868	100.00%	13.579%
43	8.196	1164	1166	1168	rVB2	838	689	0.03%	0.005%
44	8.324	1181	1187	1200	rBV	123742	208846	10.28%	1.396%
45	8.549	1218	1224	1234	rBV	242822	383853	18.90%	2.567%
46	8.647	1234	1240	1259	rVB	452226	716874	35.30%	4.793%
47	8.952	1284	1290	1308	rBV	419209	626916	30.87%	4.192%
48	9.244	1332	1338	1345	rBV	321481	461415	22.72%	3.085%
49	9.311	1345	1349	1351	rVV2	28253	41243	2.03%	0.276%
50	9.342	1351	1354	1356	rVV2	48843	68233	3.36%	0.456%
51	9.384	1356	1361	1372	rVV2	435330	725888	35.74%	4.853%
52	9.482	1372	1377	1385	rVV	573122	756782	37.26%	5.060%
53	9.580	1388	1393	1410	rVB	394560	532323	26.21%	3.559%
54	9.811	1426	1431	1436	rBV6	1164	2200	0.11%	0.015%
55	9.915	1442	1448	1463	rBV	977024	1303024	64.16%	8.712%
56	10.055	1464	1471	1478	rBV	479690	699283	34.43%	4.676%
57	10.281	1504	1508	1517	rVB	10312	16362	0.81%	0.109%
58	10.506	1541	1545	1553	rBV	11421	18166	0.89%	0.121%
59	10.640	1562	1567	1581	rVB	69752	93947	4.63%	0.628%
60	10.903	1608	1610	1612	rBV3	768	828	0.04%	0.006%
61	11.055	1634	1635	1640	rBV3	597	717	0.04%	0.005%
62	11.189	1652	1657	1666	rBV	369638	471351	23.21%	3.152%
63	11.427	1693	1696	1699	rBV4	696	965	0.05%	0.006%
64	11.512	1706	1710	1712	rBV3	720	1003	0.05%	0.007%
65	11.616	1725	1727	1730	rBV2	565	603	0.03%	0.004%
66	11.902	1772	1774	1778	rBV3	519	581	0.03%	0.004%
67	11.939	1778	1780	1784	rVB3	429	507	0.02%	0.003%
68	12.018	1788	1793	1805	rBV	432302	567460	27.94%	3.794%
69	12.219	1824	1826	1827	rBV2	827	644	0.03%	0.004%
70	12.317	1837	1842	1851	rBV	450980	575377	28.33%	3.847%
71	12.573	1882	1884	1887	rVB3	717	650	0.03%	0.004%
72	12.603	1887	1889	1891	rBV2	565	631	0.03%	0.004%
73	12.646	1894	1896	1898	rVV2	738	617	0.03%	0.004%
74	12.731	1907	1910	1913	rBV3	668	834	0.04%	0.006%
75	12.774	1913	1917	1918	rBV3	763	870	0.04%	0.006%
76	12.805	1920	1922	1925	rVV3	1183	1232	0.06%	0.008%

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Integrator: RTE

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 Title : VOC Analysis

77	12.908	1938	1939	1943	rVB2	600	627	0.03%	0.004%
78	13.390	2016	2018	2019	rBV	841	490	0.02%	0.003%
79	13.408	2019	2021	2023	rVB	928	715	0.04%	0.005%
80	13.554	2042	2045	2047	rBV3	579	753	0.04%	0.005%
81	13.695	2065	2068	2070	rBV2	720	618	0.03%	0.004%
82	13.896	2099	2101	2102	rBV2	640	492	0.02%	0.003%
83	13.920	2102	2105	2106	rVV3	877	906	0.04%	0.006%
84	14.067	2125	2129	2132	rVB4	571	664	0.03%	0.004%
85	14.097	2132	2134	2135	rBV	760	594	0.03%	0.004%
86	14.237	2156	2157	2161	rVB3	583	598	0.03%	0.004%
87	14.371	2176	2179	2183	rVB2	594	743	0.04%	0.005%
88	14.597	2213	2216	2217	rBV2	576	512	0.03%	0.003%
89	14.646	2221	2224	2229	rVV3	749	1234	0.06%	0.008%
90	14.701	2229	2233	2234	rVB3	760	771	0.04%	0.005%
91	14.798	2247	2249	2253	rVB4	524	578	0.03%	0.004%
92	14.865	2258	2260	2263	rBV4	560	517	0.03%	0.003%
93	14.920	2266	2269	2271	rBV2	559	585	0.03%	0.004%
94	14.987	2279	2280	2282	rBV2	572	519	0.03%	0.003%
95	15.578	2375	2377	2380	rBV4	519	611	0.03%	0.004%
96	15.639	2383	2387	2390	rVB4	654	955	0.05%	0.006%
97	15.914	2431	2432	2435	rVB2	952	680	0.03%	0.005%
98	16.078	2456	2459	2462	rVB3	767	951	0.05%	0.006%
99	16.328	2498	2500	2502	rVB3	795	667	0.03%	0.004%
100	16.688	2556	2559	2560	rBV2	696	700	0.03%	0.005%

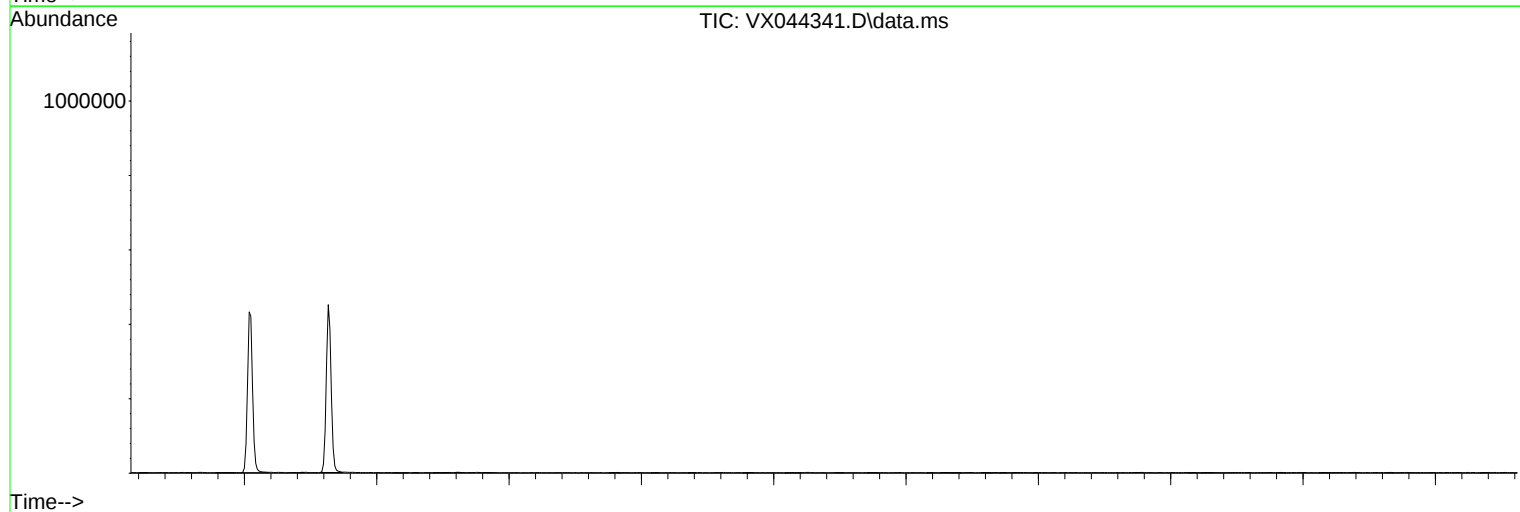
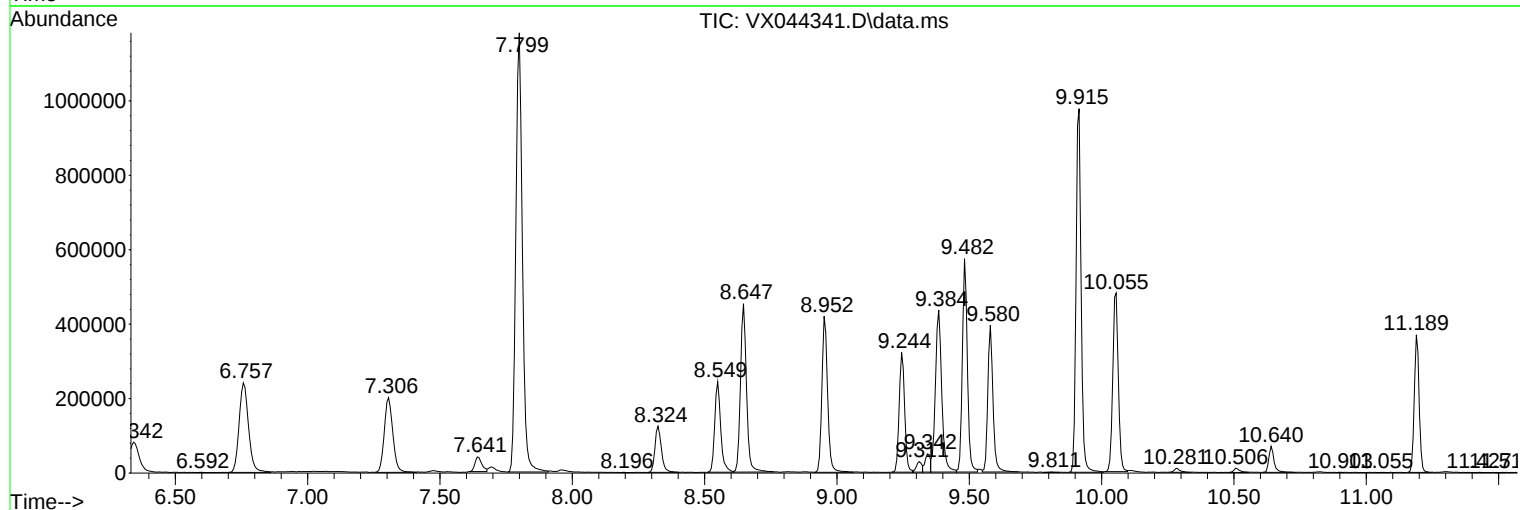
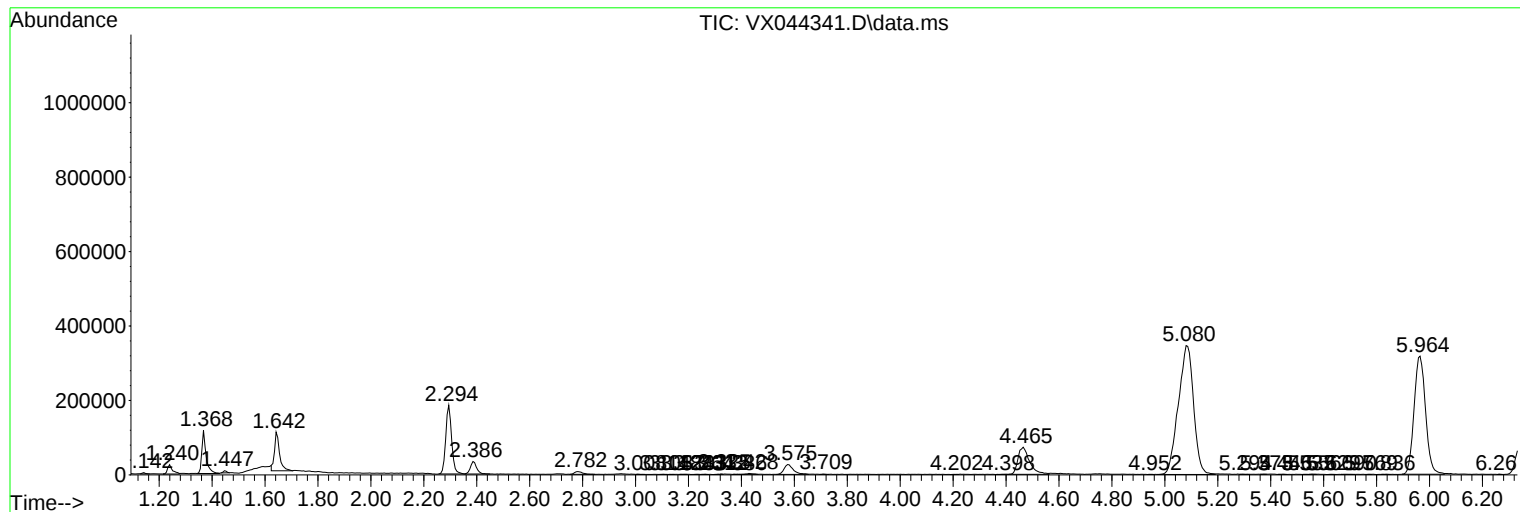
Sum of corrected areas: 14956036

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Instrument :
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ClientSampleId :
VLEB643

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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



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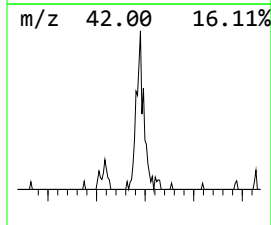
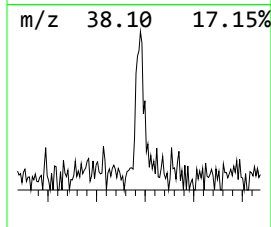
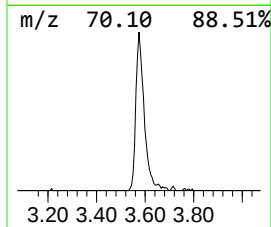
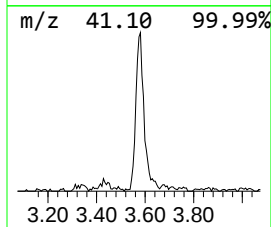
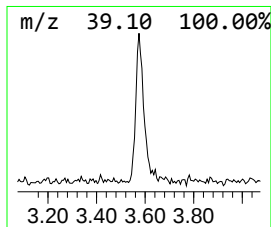
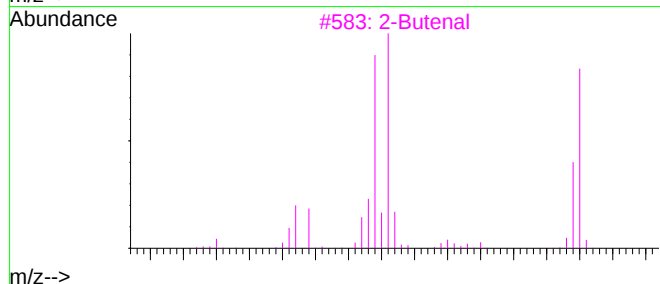
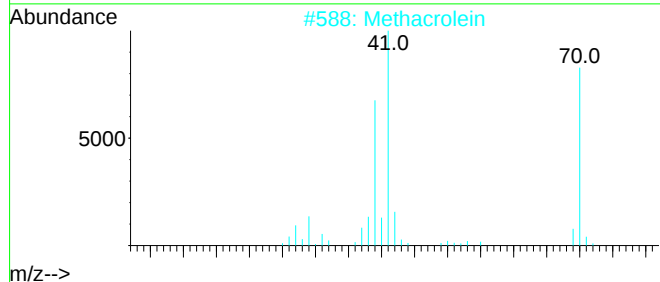
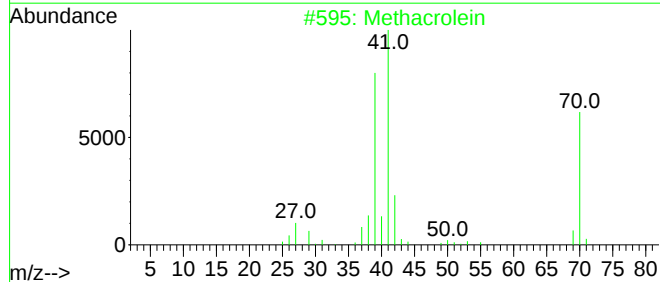
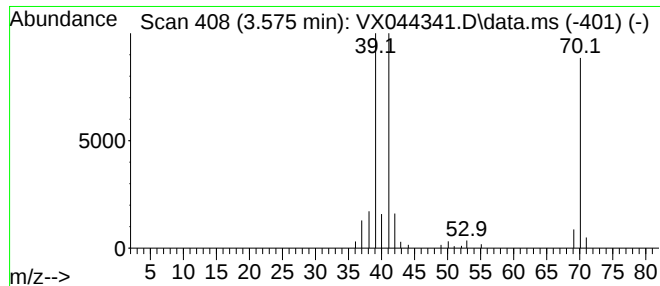
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Methacrolein Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.575	5.50 ug/L	65146	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methacrolein	70	C4H6O	000078-85-3	91
2	Methacrolein	70	C4H6O	000078-85-3	91
3	2-Butenal	70	C4H6O	004170-30-3	91
4	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	90
5	Methacrolein	70	C4H6O	000078-85-3	90



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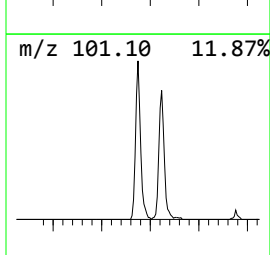
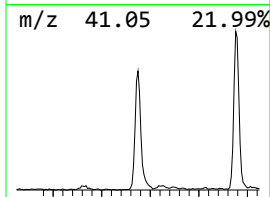
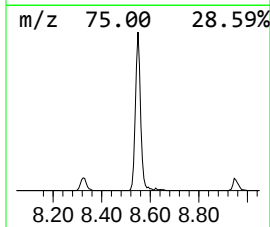
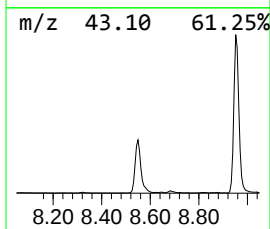
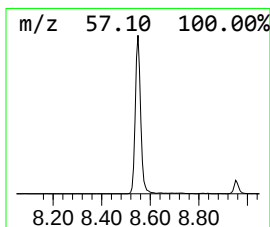
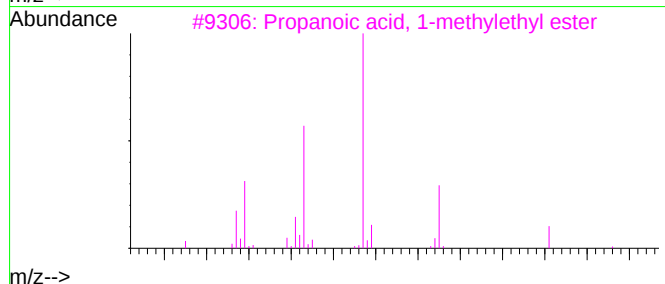
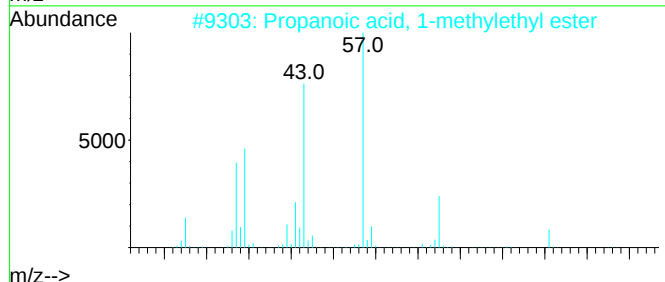
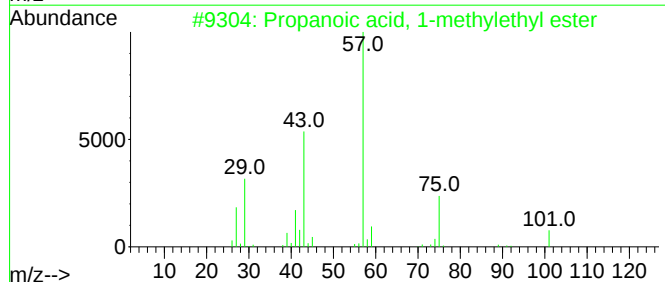
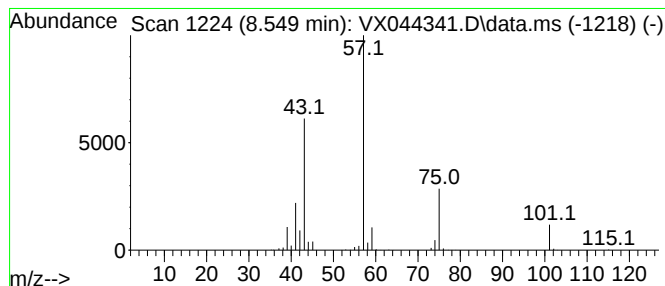
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	27.45 ug/L	383853	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	83
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45



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Quant Title : VOC Analysis

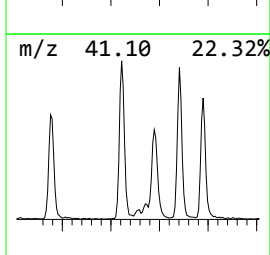
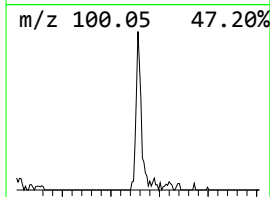
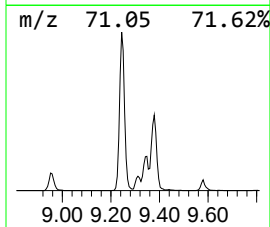
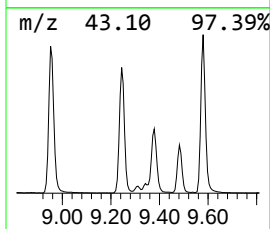
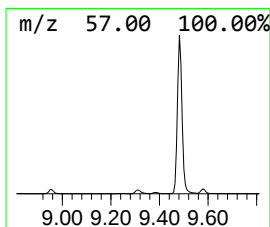
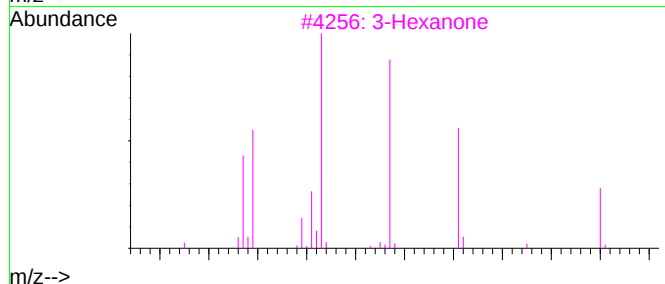
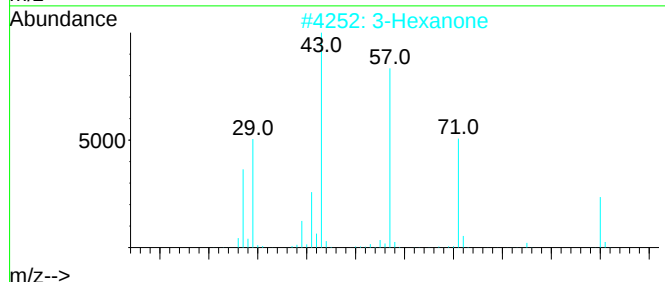
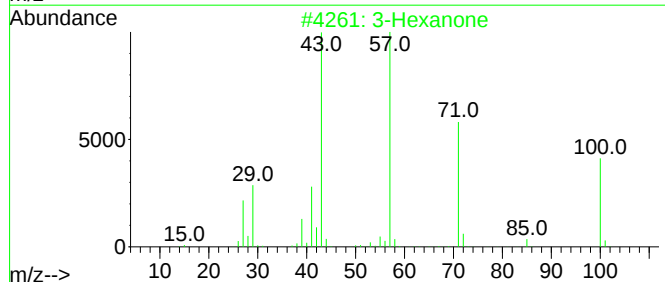
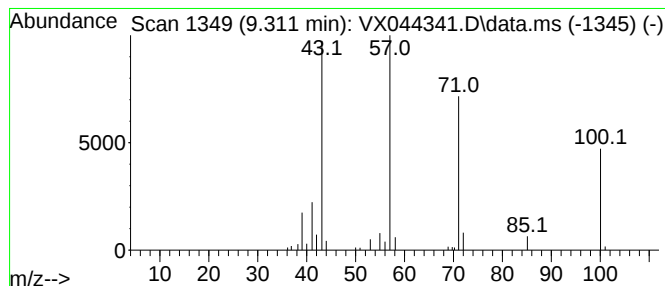
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 3-Hexanone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.311	2.95 ug/L	41243	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone	100	C6H12O	000589-38-8	91
2	3-Hexanone	100	C6H12O	000589-38-8	83
3	3-Hexanone	100	C6H12O	000589-38-8	78
4	3-Hexanone	100	C6H12O	000589-38-8	72
5	3-Hexanone	100	C6H12O	000589-38-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
Data File : VX044341.D
Acq On : 17 Dec 2024 11:12
Operator : JC/MD
Sample : PB165643TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB643

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

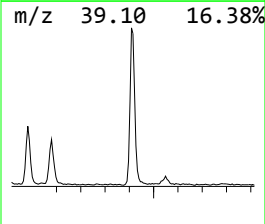
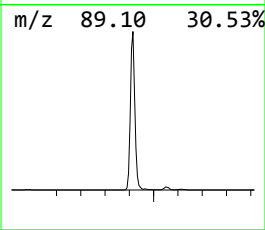
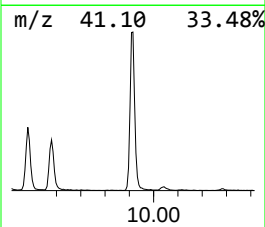
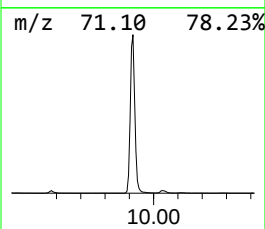
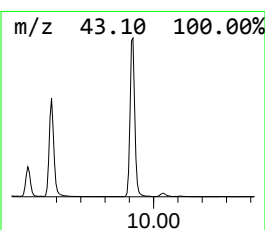
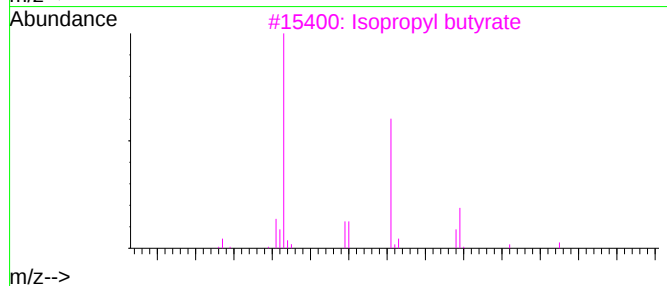
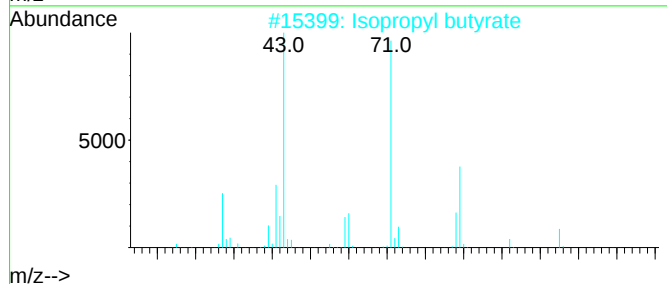
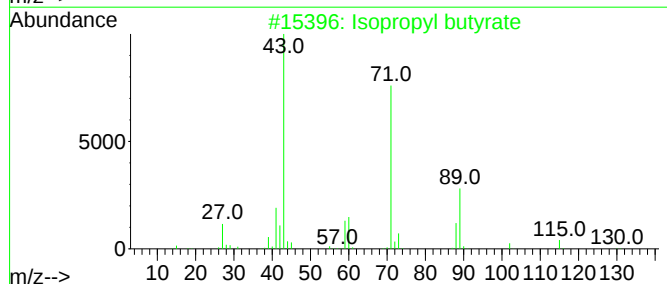
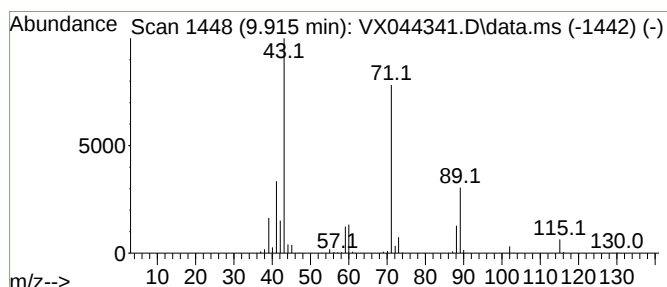
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 12 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	93.17 ug/L	1303020	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	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
Data File : VX044341.D
Acq On : 17 Dec 2024 11:12
Operator : JC/MD
Sample : PB165643TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB643

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

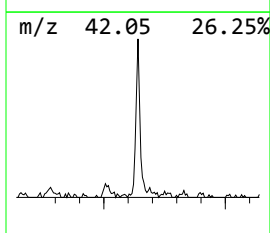
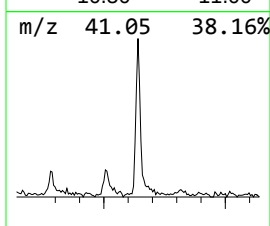
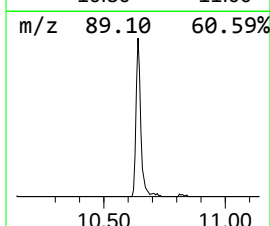
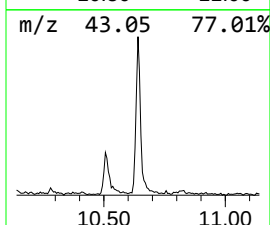
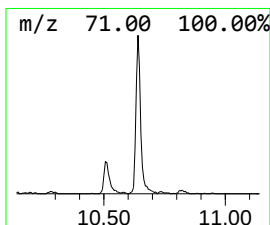
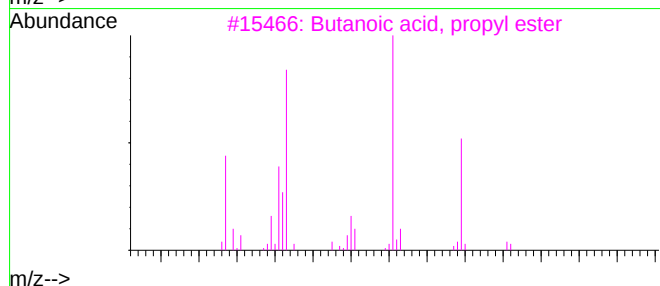
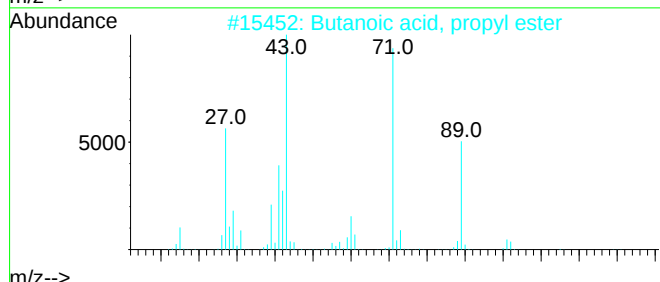
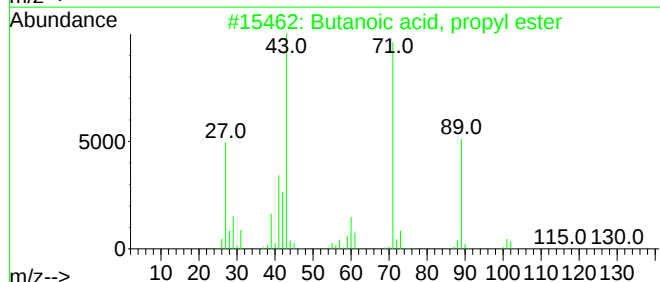
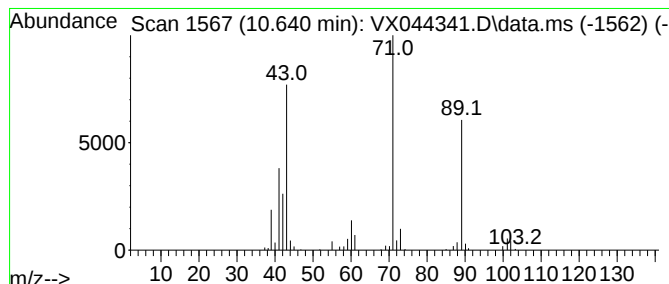
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 13 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	6.72 ug/L	93947	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, propyl ester	130	C7H14O2	000105-66-8	86
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
Data File : VX044341.D
Acq On : 17 Dec 2024 11:12
Operator : JC/MD
Sample : PB165643TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB643

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methacrolein	3.575	5.5	ug/L	65146	1	6.757	592446	50.0
Propanoic acid,...	8.549	27.4	ug/L	383853	2	10.055	699283	50.0
3-Hexanone	9.311	3.0	ug/L	41243	2	10.055	699283	50.0
Isopropyl butyrate	9.915	93.2	ug/L	1303020	2	10.055	699283	50.0
Butanoic acid, ...	10.640	6.7	ug/L	93947	2	10.055	699283	50.0