

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
 Data File : VV033562.D
 Acq On : 10 Jan 2024 15:53
 Operator : SY/MD
 Sample : P1016-02 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCML6

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033562.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.221	50	56	60	rBV4	2716	3671	0.08%	0.009%
2	1.278	67	74	87	rBV	198587	208217	4.54%	0.529%
3	1.529	145	152	168	rVB	150656	181038	3.95%	0.460%
4	2.063	307	318	328	rBV3	425602	715540	15.60%	1.818%
5	2.352	402	408	414	rBV3	3317	3992	0.09%	0.010%
6	2.446	425	437	461	rBV	691408	1143132	24.92%	2.904%
7	2.700	500	516	553	rBV2	1201159	2469819	53.85%	6.275%
8	3.111	630	644	669	rBV	416515	879660	19.18%	2.235%
9	3.442	744	747	749	rBV3	934	645	0.01%	0.002%
10	3.510	766	768	773	rBV4	410	318	0.01%	0.001%
11	3.593	789	794	796	rBV3	486	427	0.01%	0.001%
12	3.654	810	813	817	rBV3	579	373	0.01%	0.001%
13	3.812	844	862	892	rBV2	336132	1002423	21.86%	2.547%
14	4.249	981	998	1027	rBV	200407	511130	11.14%	1.299%
15	4.513	1064	1080	1101	rBV2	97068	250371	5.46%	0.636%
16	4.735	1132	1149	1174	rBV	173347	429702	9.37%	1.092%
17	4.957	1201	1218	1259	rBV2	503598	1344608	29.32%	3.416%
18	5.211	1290	1297	1316	rVB2	6979	16255	0.35%	0.041%
19	5.494	1381	1385	1386	rBV4	503	397	0.01%	0.001%
20	5.532	1386	1397	1431	rVV	410727	847683	18.48%	2.154%
21	5.741	1459	1462	1468	rVB4	643	676	0.01%	0.002%
22	5.834	1476	1491	1523	rBV	324965	667375	14.55%	1.696%
23	5.989	1526	1539	1567	rBV	294226	611986	13.34%	1.555%
24	6.227	1601	1613	1642	rBV	299862	594396	12.96%	1.510%
25	6.394	1657	1665	1670	rBV	97583	154385	3.37%	0.392%
26	6.571	1713	1720	1746	rVB	25245	57202	1.25%	0.145%
27	6.912	1814	1826	1832	rBV	193582	323185	7.05%	0.821%
28	6.953	1833	1839	1872	rVB	366498	657749	14.34%	1.671%
29	7.117	1881	1890	1895	rBV2	25873	39595	0.86%	0.101%
30	7.159	1895	1903	1918	rVV	141091	249740	5.45%	0.635%
31	7.243	1918	1929	1941	rVV	621074	1071078	23.35%	2.721%
32	7.314	1941	1951	1977	rVB	990406	1715124	37.40%	4.358%
33	7.551	2016	2025	2050	rBV	151823	274059	5.98%	0.696%
34	7.767	2080	2092	2113	rBV	855835	1435840	31.31%	3.648%
35	7.860	2114	2121	2127	rBV	32194	48308	1.05%	0.123%
36	7.905	2128	2135	2151	rVB	111034	188244	4.10%	0.478%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

37	7.976	2151	2157	2162	rBV3	4955	6282	0.14%	0.016%
38	8.021	2162	2171	2180	rBV	351076	581923	12.69%	1.478%
39	8.072	2180	2187	2199	rVB	596260	917535	20.01%	2.331%
40	8.175	2211	2219	2234	rVB	216931	374365	8.16%	0.951%
41	8.246	2235	2241	2261	rVB	30543	57016	1.24%	0.145%
42	8.474	2308	2312	2318	rVV4	603	607	0.01%	0.002%
43	8.535	2327	2331	2333	rBV4	605	432	0.01%	0.001%
44	8.619	2346	2357	2381	rBV	108268	174909	3.81%	0.444%
45	8.786	2397	2409	2411	rBV	682415	904170	19.71%	2.297%
46	8.908	2436	2447	2453	rBV	934691	1525288	33.26%	3.875%
47	8.944	2453	2458	2486	rVB	816929	1286549	28.05%	3.269%
48	9.069	2486	2497	2537	rVB	744381	1214444	26.48%	3.086%
49	9.281	2559	2563	2567	rBV5	783	608	0.01%	0.002%
50	9.333	2574	2579	2582	rBV6	1185	1194	0.03%	0.003%
51	9.407	2596	2602	2605	rBV5	854	825	0.02%	0.002%
52	9.481	2611	2625	2662	rBV4	2233463	4586382	100.00%	11.653%
53	9.664	2671	2682	2713	rVB	177711	299375	6.53%	0.761%
54	9.815	2726	2729	2733	rVB5	477	332	0.01%	0.001%
55	9.873	2739	2747	2755	rVV3	6206	9871	0.22%	0.025%
56	9.956	2770	2773	2777	rVB3	487	458	0.01%	0.001%
57	10.104	2816	2819	2820	rBV3	761	501	0.01%	0.001%
58	10.153	2820	2834	2839	rBV	383616	627509	13.68%	1.594%
59	10.207	2846	2851	2878	rVB	750449	1152346	25.13%	2.928%
60	10.477	2924	2935	2956	rBV	205761	313819	6.84%	0.797%
61	10.677	2989	2997	3000	rBV6	1710	2252	0.05%	0.006%
62	10.754	3014	3021	3029	rBV5	1718	2431	0.05%	0.006%
63	10.805	3029	3037	3041	rBV8	5200	6703	0.15%	0.017%
64	10.850	3041	3051	3070	rVB	398422	606274	13.22%	1.540%
65	11.021	3102	3104	3108	rVB5	588	328	0.01%	0.001%
66	11.085	3121	3124	3128	rBV4	486	314	0.01%	0.001%
67	11.127	3131	3137	3144	rBV9	1829	2843	0.06%	0.007%
68	11.188	3144	3156	3158	rBV	748552	996321	21.72%	2.531%
69	11.391	3215	3219	3226	rVB4	467	458	0.01%	0.001%
70	11.509	3253	3256	3258	rBV3	398	311	0.01%	0.001%
71	11.574	3258	3276	3298	rVV2	889313	2099153	45.77%	5.333%
72	11.834	3349	3357	3370	rVB6	8577	14224	0.31%	0.036%
73	12.169	3459	3461	3464	rVB2	761	361	0.01%	0.001%
74	12.194	3464	3469	3472	rBV4	622	517	0.01%	0.001%
75	12.214	3472	3475	3477	rBV2	632	470	0.01%	0.001%
76	12.365	3510	3522	3540	rBV	337866	538397	11.74%	1.368%

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 Title : VOC Analysis

77	12.493	3559	3562	3566	rVB4	414	303	0.01%	0.001%
78	12.529	3568	3573	3576	rBV3	317	359	0.01%	0.001%
79	12.587	3580	3591	3607	rBV2	15615	30363	0.66%	0.077%
80	12.834	3665	3668	3672	rVB6	467	369	0.01%	0.001%
81	12.918	3689	3694	3700	rBV5	366	388	0.01%	0.001%
82	13.072	3737	3742	3745	rBV5	443	379	0.01%	0.001%
83	13.198	3768	3781	3805	rBV	497583	780709	17.02%	1.984%
84	13.281	3805	3807	3811	rVB5	713	482	0.01%	0.001%
85	13.384	3826	3839	3848	rBV	855917	1306446	28.49%	3.319%
86	13.442	3848	3857	3885	rVB	494911	811540	17.69%	2.062%
87	13.686	3924	3933	3941	rBV2	9489	15133	0.33%	0.038%
88	13.937	4007	4011	4013	rBV2	653	469	0.01%	0.001%
89	13.960	4016	4018	4021	rBV2	679	407	0.01%	0.001%
90	14.101	4057	4062	4067	rBV5	891	960	0.02%	0.002%
91	14.149	4074	4077	4081	rBV3	689	461	0.01%	0.001%
92	14.268	4109	4114	4115	rBV4	469	443	0.01%	0.001%
93	14.316	4126	4129	4134	rBV4	611	509	0.01%	0.001%
94	14.561	4202	4205	4208	rBV3	580	516	0.01%	0.001%
95	14.625	4222	4225	4228	rVV4	683	395	0.01%	0.001%
96	14.641	4228	4230	4237	rVB7	569	722	0.02%	0.002%
97	14.844	4291	4293	4296	rBV3	461	312	0.01%	0.001%
98	14.905	4310	4312	4315	rVB3	803	448	0.01%	0.001%
99	15.053	4356	4358	4361	rBV3	596	422	0.01%	0.001%
100	15.117	4374	4378	4379	rBV3	848	574	0.01%	0.001%

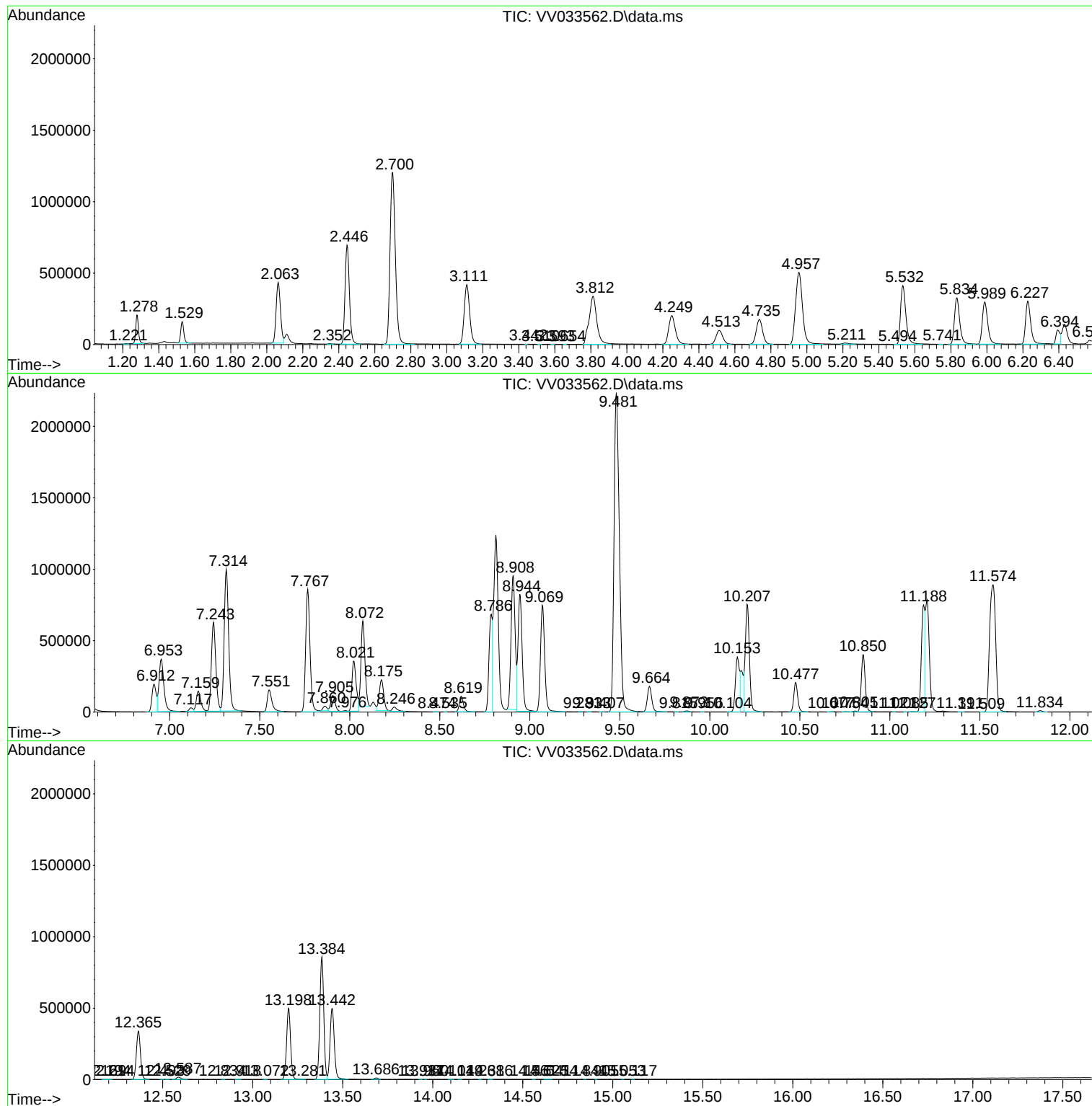
Sum of corrected areas: 39359549

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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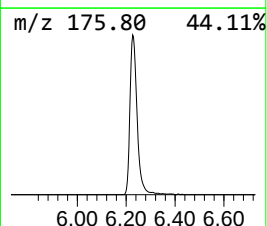
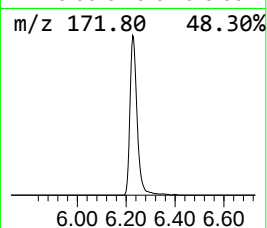
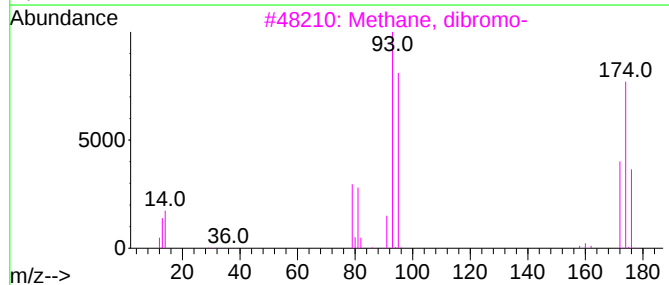
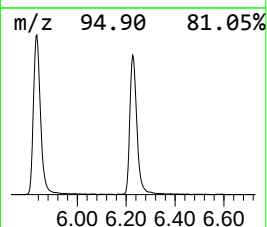
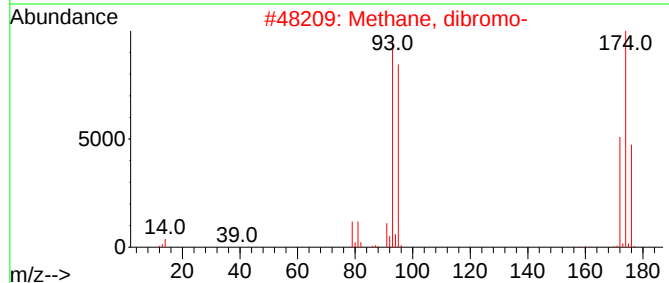
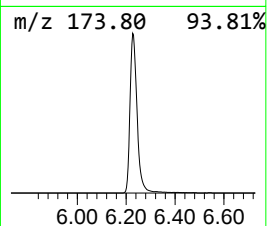
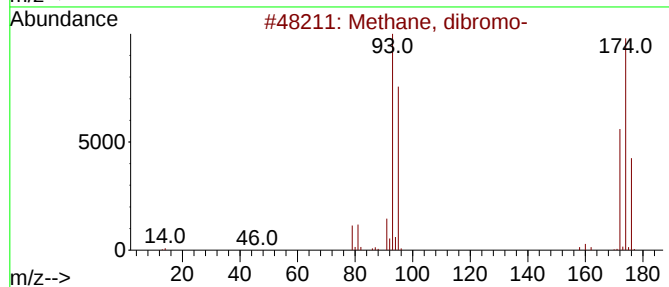
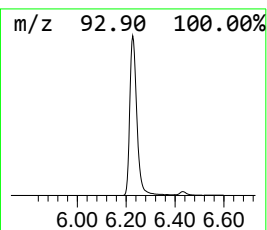
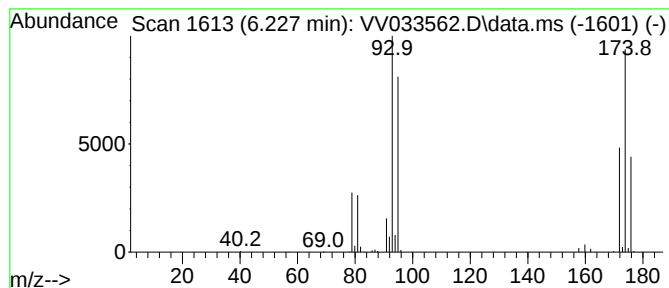
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methane, dibromo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.227	35.06 ug/L	594396	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, dibromo-	172	CH2Br2	000074-95-3	96
2			Methane, dibromo-	172	CH2Br2	000074-95-3	95
3			Methane, dibromo-	172	CH2Br2	000074-95-3	94
4			Methane, dibromo-	172	CH2Br2	000074-95-3	70
5			3-Chloro-6-methoxy-4-methylpyrid...	174	C6H7ClN2O2	050450-89-0	9



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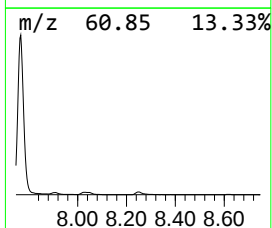
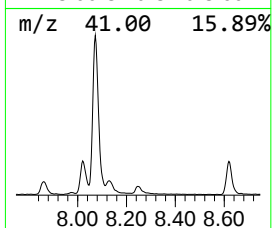
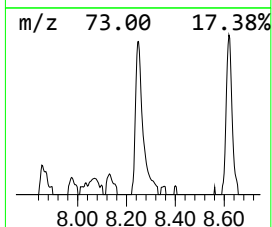
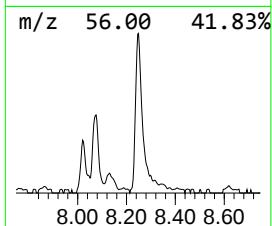
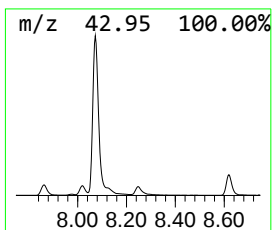
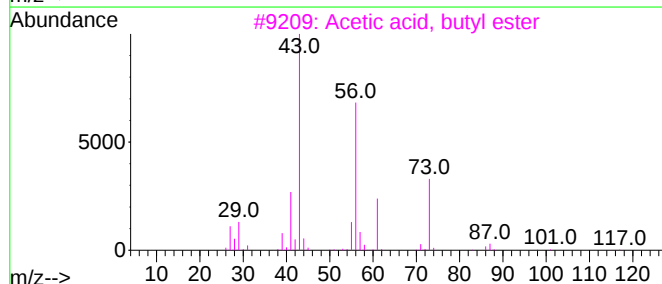
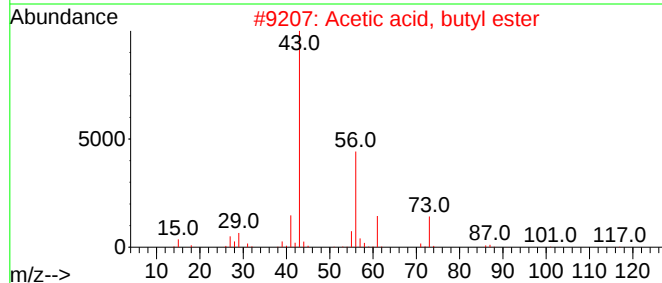
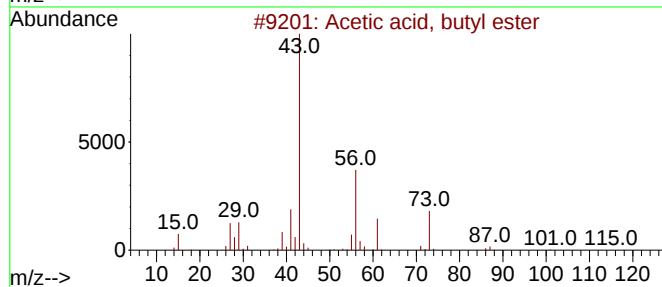
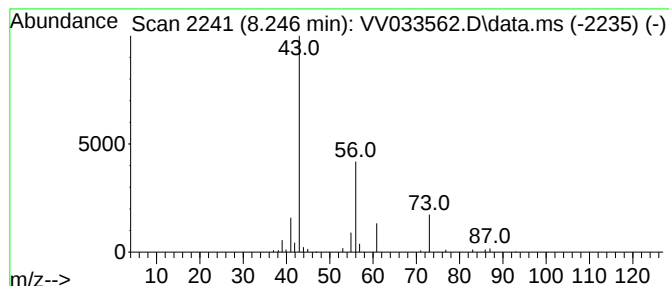
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.246	3.15 ug/L	57016	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5			Isobutyl acetate	116	C6H12O2	000110-19-0	39



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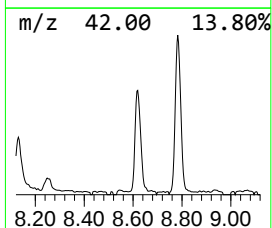
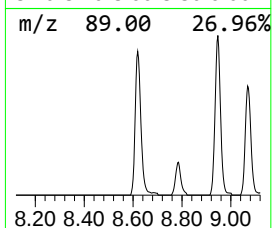
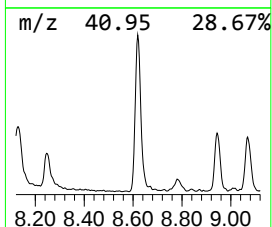
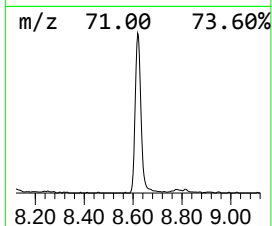
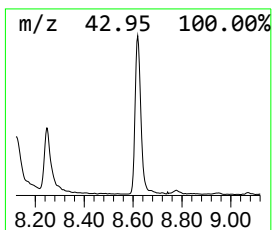
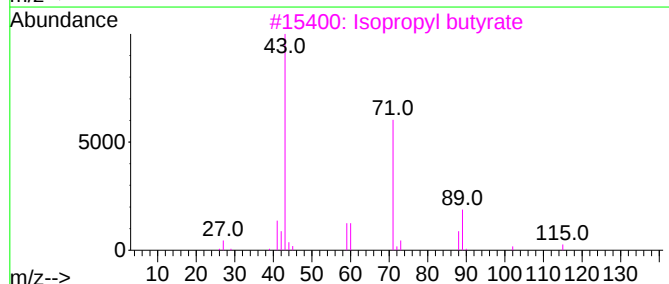
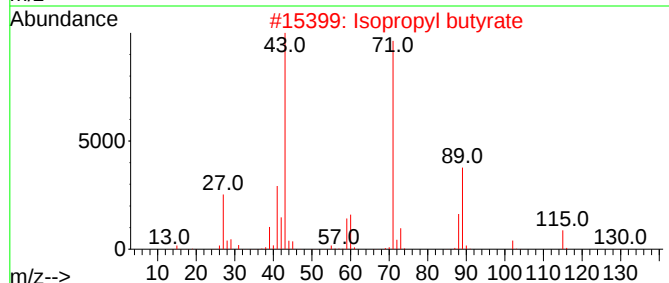
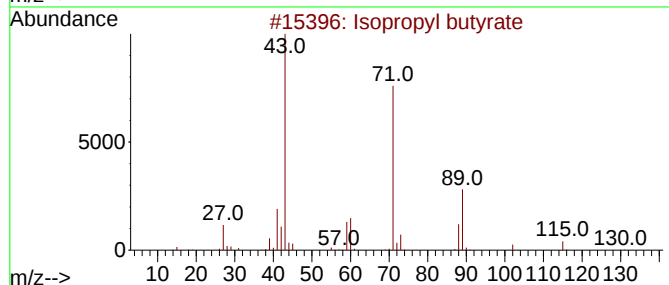
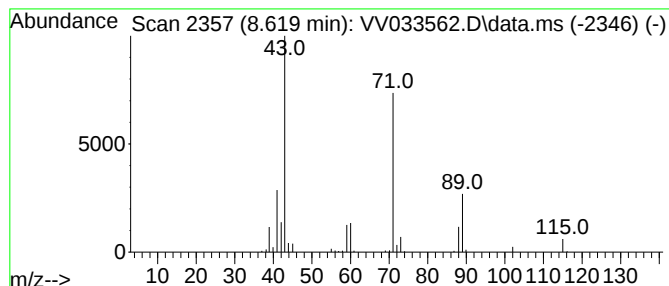
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	9.67 ug/L	174909	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
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_V\Data\VV011024\
Data File : VV033562.D
Acq On : 10 Jan 2024 15:53
Operator : SY/MD
Sample : P1016-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCML6

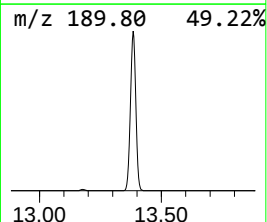
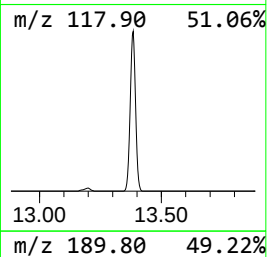
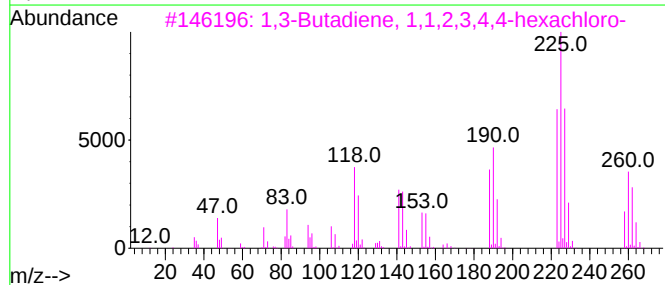
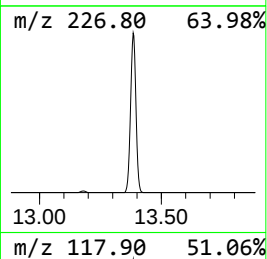
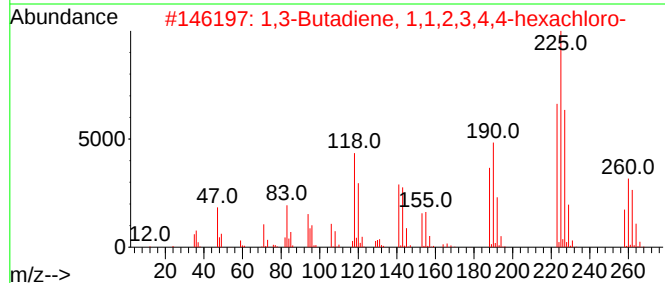
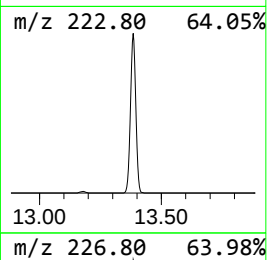
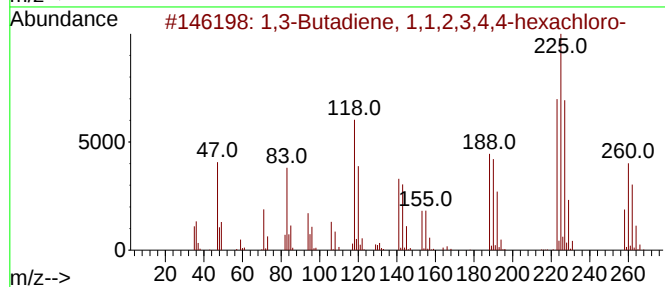
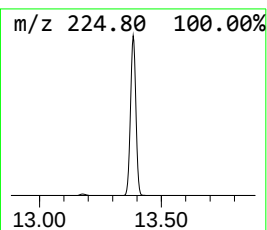
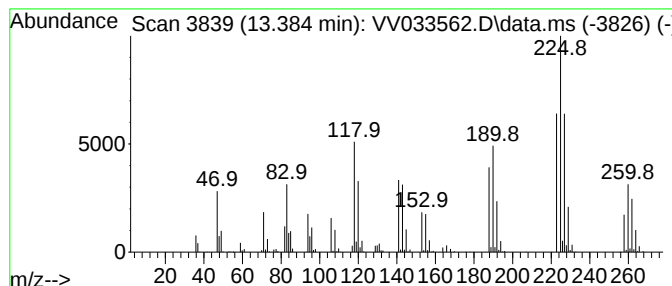
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Quant Title : VOC Analysis

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

Peak Number 5 1,3-Butadiene, 1,1,2,3,4,4-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.384	65.56 ug/L	1306450	1,4-Dichlorobenzene-d4	11.185

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
2			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
3			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
4			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
5			Tin(IV) chloride	260	Cl4Sn	007646-78-8	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033562.D
Acq On : 10 Jan 2024 15:53
Operator : SY/MD
Sample : P1016-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCML6

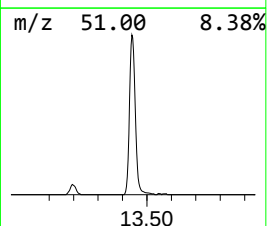
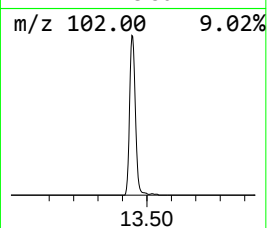
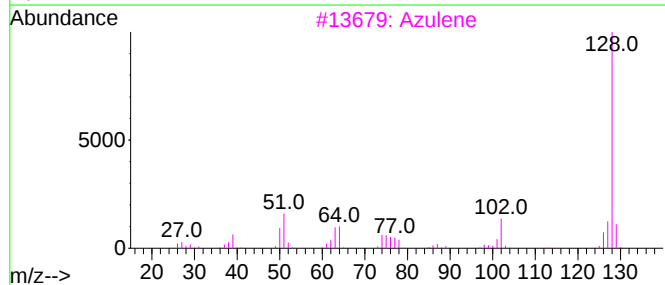
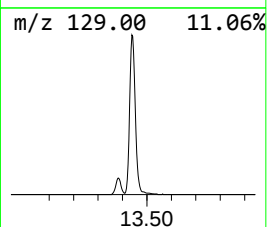
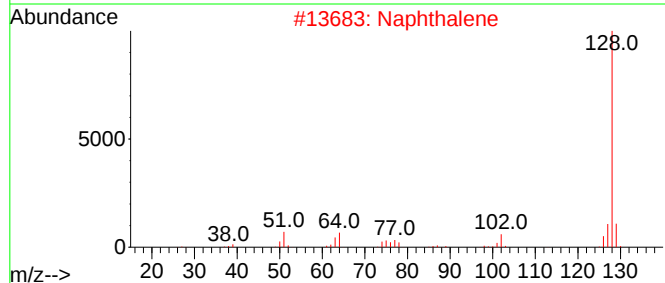
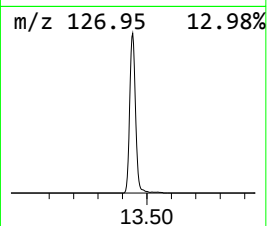
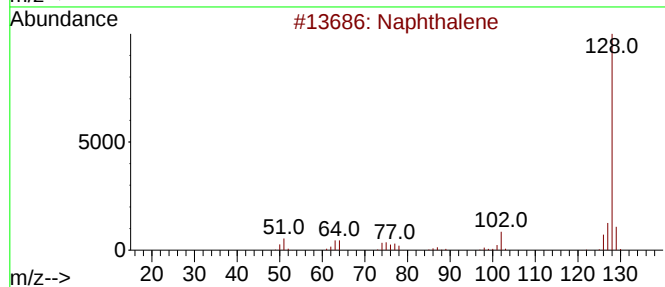
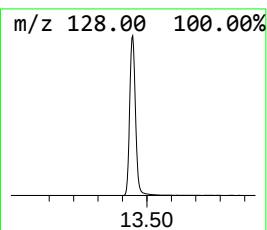
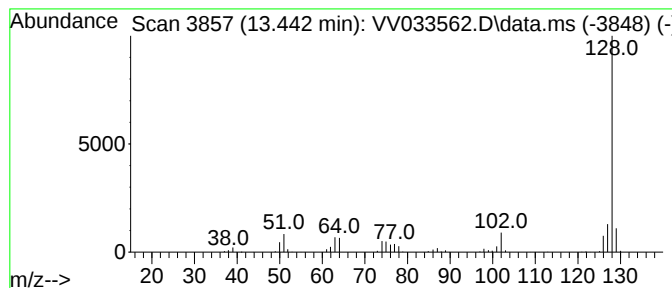
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.442	40.73 ug/L	811540	1,4-Dichlorobenzene-d4	11.185

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			Azulene	128	C10H8	000275-51-4	94
4			Naphthalene	128	C10H8	000091-20-3	93
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033562.D
Acq On : 10 Jan 2024 15:53
Operator : SY/MD
Sample : P1016-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCML6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.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
Methane, dibromo-	6.227	35.1	ug/L	594396	1	5.532	847683	50.0
Acetic acid, bu...	8.246	3.1	ug/L	57016	2	8.783	904170	50.0
Isopropyl butyrate	8.619	9.7	ug/L	174909	2	8.783	904170	50.0
1,3-Butadiene, ...	13.384	65.6	ug/L	1306450	3	11.185	996321	50.0
Azulene	13.442	40.7	ug/L	811540	3	11.185	996321	50.0