

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033745.D
 Acq On : 19 Jan 2024 11:27
 Operator : SY/MD
 Sample : P1160-10
 Misc : 10.00g/10mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 XA319

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: VV033745.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.191	40	47	52	rBV	13639	13699	0.27%	0.031%
2	1.281	67	75	94	rBV	106428	137469	2.75%	0.312%
3	1.503	135	144	146	rBV2	10828	14777	0.30%	0.033%
4	1.532	147	153	165	rVB	73932	104038	2.08%	0.236%
5	2.053	302	315	329	rBV2	1121906	1790972	35.81%	4.058%
6	2.134	330	340	380	rVB	163694	448008	8.96%	1.015%
7	2.384	409	418	426	rBV2	16325	31834	0.64%	0.072%
8	2.442	427	436	457	rVB	141496	257191	5.14%	0.583%
9	2.622	485	492	493	rBV2	426	401	0.01%	0.001%
10	2.687	500	512	537	rBV	398280	704449	14.08%	1.596%
11	2.886	569	574	583	rBV3	702	1189	0.02%	0.003%
12	2.960	585	597	609	rBV3	6311	13500	0.27%	0.031%
13	3.468	753	755	760	rVB3	250	178	0.00%	0.000%
14	3.625	797	804	806	rBV2	202	232	0.00%	0.001%
15	3.664	811	816	827	rVB6	1077	1773	0.04%	0.004%
16	3.754	841	844	849	rVB2	233	181	0.00%	0.000%
17	3.815	850	863	903	rBV2	33968	137893	2.76%	0.312%
18	4.166	967	972	981	rBV5	580	658	0.01%	0.001%
19	4.268	981	1004	1039	rBV4	326928	1116047	22.31%	2.529%
20	4.477	1067	1069	1073	rVB2	318	203	0.00%	0.000%
21	4.584	1094	1102	1103	rBV4	286	300	0.01%	0.001%
22	4.838	1178	1181	1186	rVB2	259	234	0.00%	0.001%
23	4.953	1200	1217	1224	rBV2	400989	942563	18.84%	2.136%
24	5.005	1227	1233	1274	rVB2	727770	1873492	37.46%	4.245%
25	5.188	1288	1290	1297	rVB3	686	599	0.01%	0.001%
26	5.307	1324	1327	1329	rBV2	343	221	0.00%	0.001%
27	5.452	1369	1372	1380	rBV2	200	199	0.00%	0.000%
28	5.532	1383	1397	1441	rBV	326998	695273	13.90%	1.576%
29	5.828	1473	1489	1526	rBV	1101657	2198371	43.95%	4.982%
30	5.989	1527	1539	1569	rVB	204803	447952	8.96%	1.015%
31	6.159	1588	1592	1594	rVB3	564	386	0.01%	0.001%
32	6.227	1601	1613	1651	rBV	235044	496644	9.93%	1.125%
33	6.455	1679	1684	1690	rVB5	547	672	0.01%	0.002%
34	6.577	1712	1722	1750	rBV2	18453	51956	1.04%	0.118%
35	6.841	1801	1804	1810	rVB5	407	419	0.01%	0.001%
36	6.870	1810	1813	1816	rBV	327	234	0.00%	0.001%

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37	6.915	1816	1827	1831	rBV	143985	222560	4.45%	0.504%
38	6.953	1832	1839	1874	rVV	369634	729794	14.59%	1.654%
39	7.092	1874	1882	1895	rVV2	37568	88199	1.76%	0.200%
40	7.162	1895	1904	1917	rVV	260826	625403	12.50%	1.417%
41	7.243	1921	1929	1940	rVV	476452	906341	18.12%	2.054%
42	7.313	1941	1951	1988	rVB	1217186	2158536	43.16%	4.891%
43	7.580	2015	2034	2072	rBV2	688634	1473461	29.46%	3.339%
44	7.770	2080	2093	2124	rBV	513810	1077485	21.54%	2.442%
45	7.908	2126	2136	2149	rVB2	22015	39324	0.79%	0.089%
46	8.037	2163	2176	2179	rBV	88640	130904	2.62%	0.297%
47	8.178	2208	2220	2241	rBV	638244	1322251	26.44%	2.996%
48	8.281	2242	2252	2278	rVB	263038	504345	10.08%	1.143%
49	8.603	2349	2352	2361	rVV4	729	818	0.02%	0.002%
50	8.786	2397	2409	2433	rBV	434566	804931	16.09%	1.824%
51	8.908	2434	2447	2484	rVB	1053563	2028070	40.55%	4.596%
52	9.072	2485	2498	2523	rBV	1509415	2637772	52.74%	5.977%
53	9.226	2543	2546	2550	rBV4	311	207	0.00%	0.000%
54	9.291	2563	2566	2574	rVB	385	403	0.01%	0.001%
55	9.497	2612	2630	2672	rBV3	2192689	5001724	100.00%	11.334%
56	9.677	2672	2686	2708	rVV	105379	235240	4.70%	0.533%
57	9.757	2708	2711	2712	rVV	328	198	0.00%	0.000%
58	9.767	2712	2714	2718	rVB3	570	316	0.01%	0.001%
59	9.825	2729	2732	2733	rBV	448	235	0.00%	0.001%
60	9.879	2739	2749	2757	rVB3	2662	4344	0.09%	0.010%
61	9.947	2765	2770	2776	rVB3	317	411	0.01%	0.001%
62	10.062	2803	2806	2811	rVB	265	237	0.00%	0.001%
63	10.188	2818	2845	2850	rBV2	915840	2117782	42.34%	4.799%
64	10.323	2884	2887	2892	rVB5	1117	887	0.02%	0.002%
65	10.384	2904	2906	2909	rVB3	348	176	0.00%	0.000%
66	10.407	2909	2913	2917	rBV4	497	477	0.01%	0.001%
67	10.522	2945	2949	2950	rVV2	396	250	0.00%	0.001%
68	10.554	2950	2959	2972	rVB4	2775	5509	0.11%	0.012%
69	10.757	3015	3022	3031	rVV5	1839	2734	0.05%	0.006%
70	10.812	3031	3039	3046	rVV5	3784	5475	0.11%	0.012%
71	10.853	3046	3052	3060	rVB4	2939	4073	0.08%	0.009%
72	10.902	3060	3067	3074	rBV3	813	1227	0.02%	0.003%
73	11.120	3115	3135	3147	rBV	1320533	2086571	41.72%	4.728%
74	11.191	3147	3157	3160	rBV	560717	801391	16.02%	1.816%
75	11.564	3261	3273	3299	rBV	432829	687683	13.75%	1.558%
76	11.837	3348	3358	3368	rVB2	19992	32008	0.64%	0.073%

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77	12.194	3464	3469	3477	rVB	308	470	0.01%	0.001%
78	12.368	3507	3523	3545	rVV	236027	373957	7.48%	0.847%
79	12.693	3620	3624	3628	rVB2	272	269	0.01%	0.001%
80	12.712	3628	3630	3635	rBV2	220	176	0.00%	0.000%
81	12.792	3645	3655	3660	rBV4	1878	2448	0.05%	0.006%
82	12.831	3662	3667	3672	rVB4	838	992	0.02%	0.002%
83	13.072	3738	3742	3749	rBV4	660	815	0.02%	0.002%
84	13.197	3767	3781	3804	rBV	1146157	1749570	34.98%	3.965%
85	13.384	3826	3839	3848	rBV	2012119	3005202	60.08%	6.810%
86	13.439	3848	3856	3885	rVB	1164230	1760054	35.19%	3.988%
87	13.683	3926	3932	3943	rVB5	3300	4986	0.10%	0.011%
88	13.930	4007	4009	4012	rVB	295	177	0.00%	0.000%
89	13.988	4019	4027	4033	rBV5	479	733	0.01%	0.002%
90	14.043	4040	4044	4047	rBV3	319	266	0.01%	0.001%
91	14.258	4108	4111	4114	rVB2	295	202	0.00%	0.000%
92	14.297	4120	4123	4130	rBV2	232	268	0.01%	0.001%
93	14.345	4135	4138	4140	rBV2	411	256	0.01%	0.001%
94	14.413	4153	4159	4169	rVB3	1152	1484	0.03%	0.003%
95	14.757	4263	4266	4269	rBV2	1095	883	0.02%	0.002%
96	14.892	4305	4308	4311	rBV2	322	212	0.00%	0.000%
97	14.947	4320	4325	4329	rBV5	512	613	0.01%	0.001%
98	15.020	4343	4348	4351	rBV3	358	308	0.01%	0.001%
99	15.223	4404	4411	4412	rBV3	469	491	0.01%	0.001%
100	15.258	4419	4422	4424	rBV	538	372	0.01%	0.001%

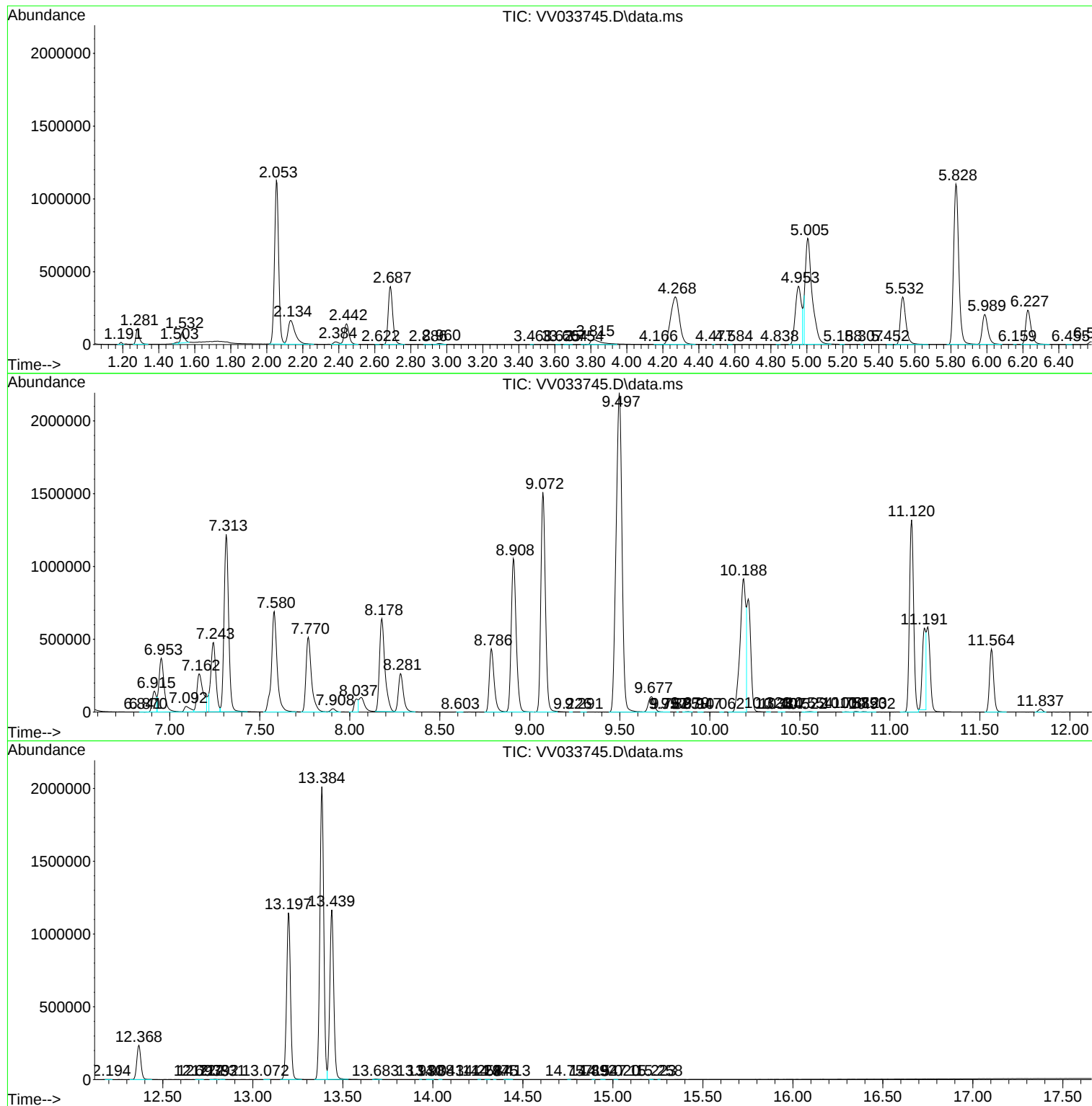
Sum of corrected areas: 44129163

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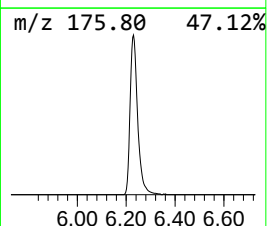
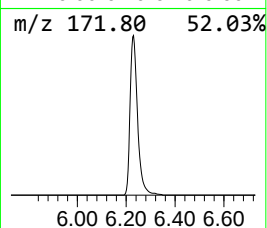
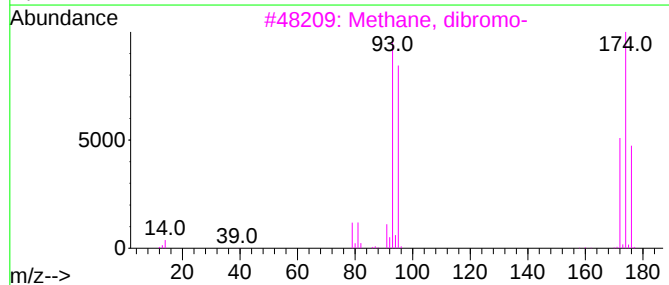
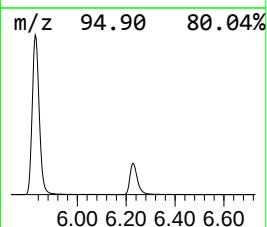
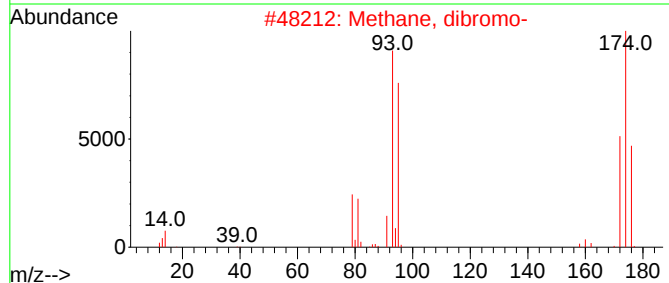
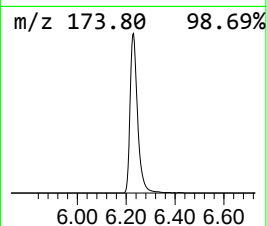
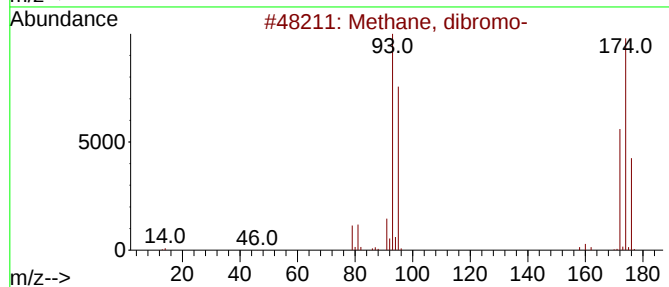
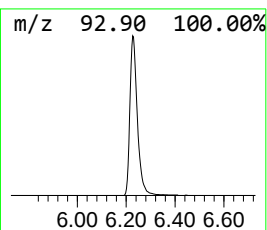
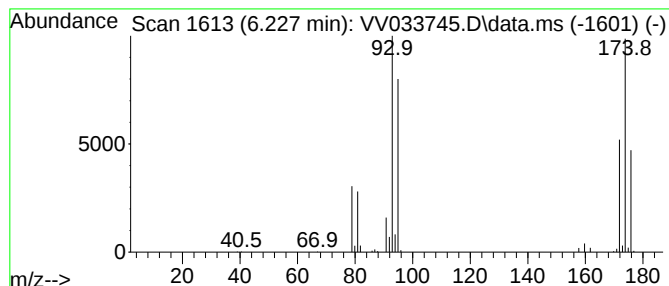
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methane, dibromo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.227	35.72 ug/L	496644	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	96
3			Methane, dibromo-	172	CH2Br2	000074-95-3	95
4			Methane, dibromo-	172	CH2Br2	000074-95-3	94
5			Phenol, 2-(methylsulfonyl)-	172	C7H8O3S	027489-33-4	9



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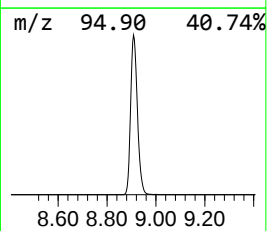
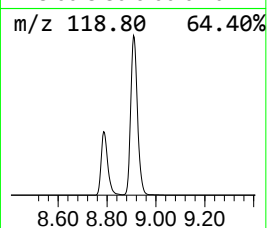
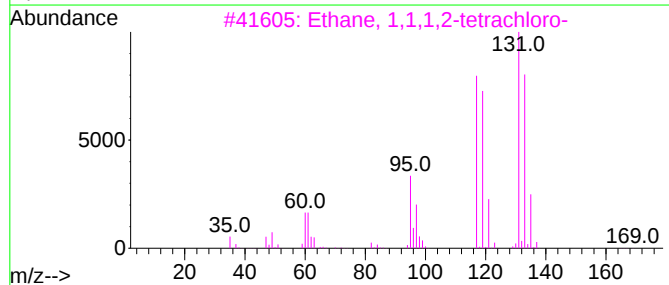
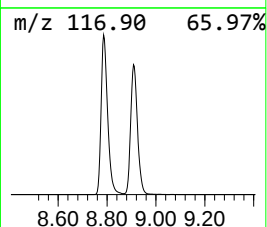
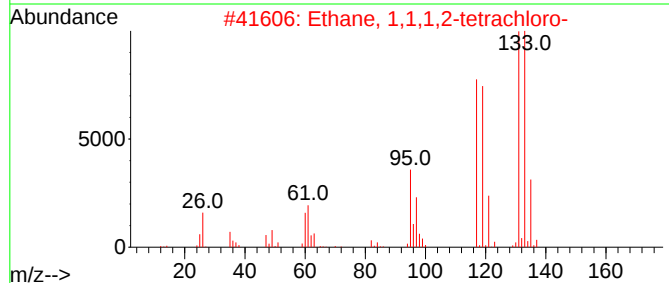
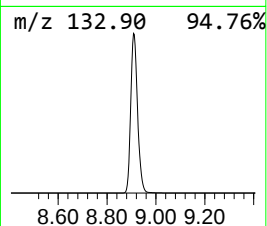
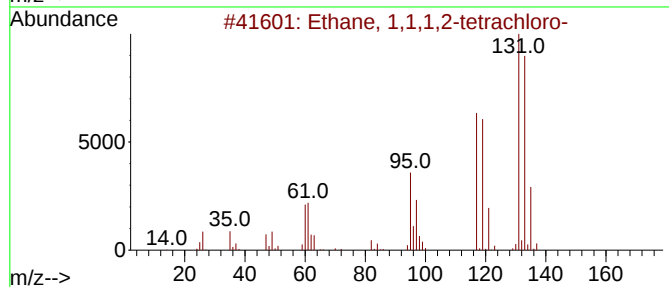
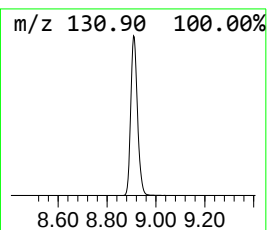
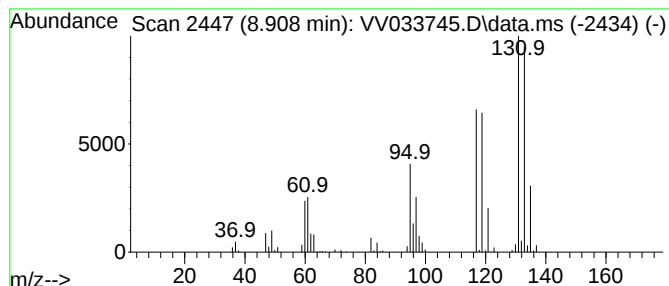
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.908	125.98 ug/L	2028070	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	86
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	72
5			Carbon Tetrachloride	152	CCl4	000056-23-5	11



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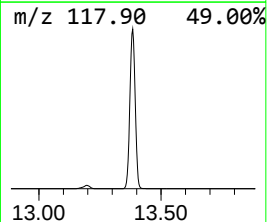
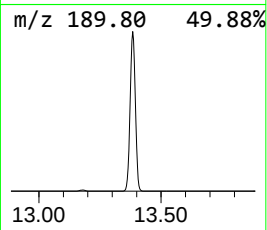
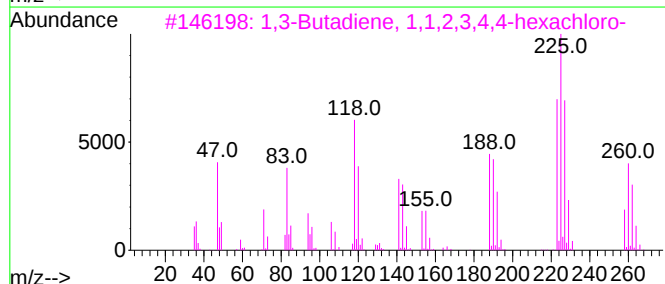
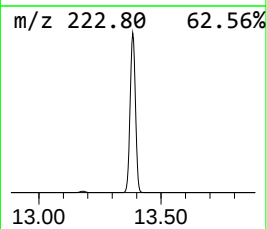
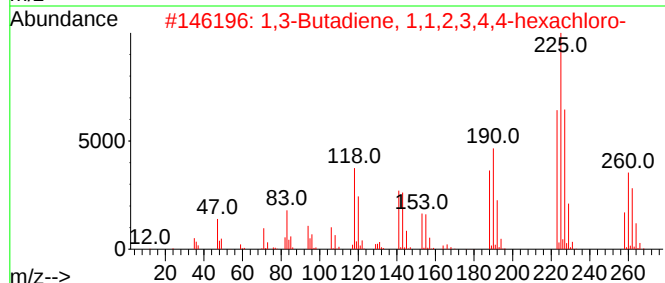
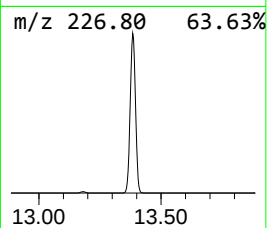
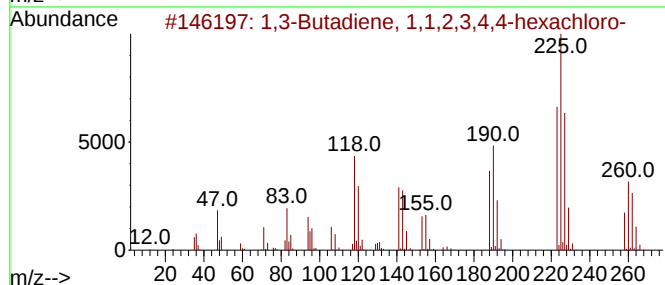
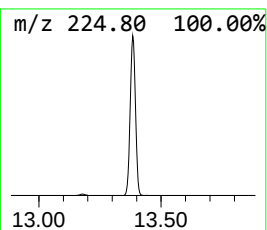
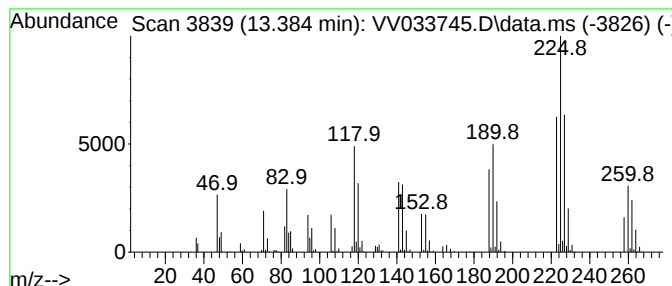
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.384	187.50 ug/L	3005200	1,4-Dichlorobenzene-d4	11.191

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\VV011924\
Data File : VV033745.D
Acq On : 19 Jan 2024 11:27
Operator : SY/MD
Sample : P1160-10
Misc : 10.00g/10mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
XA319

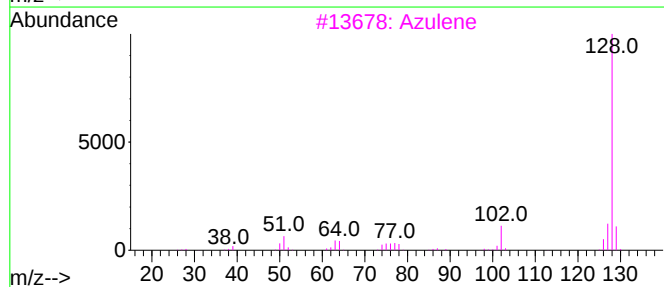
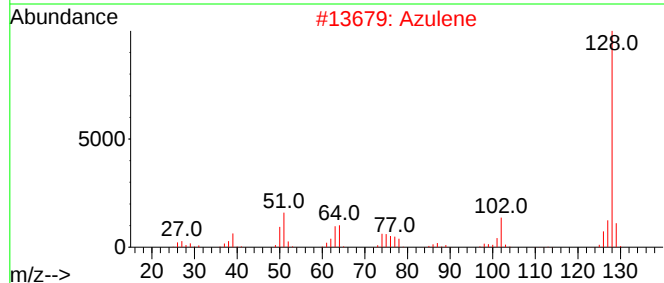
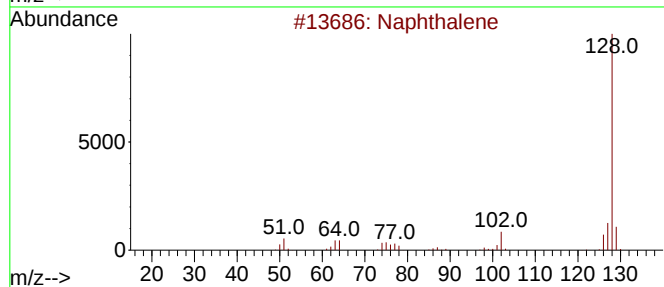
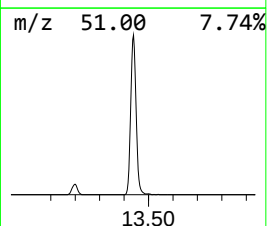
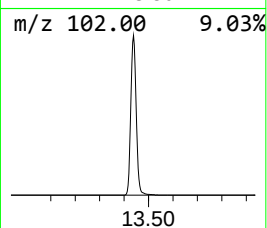
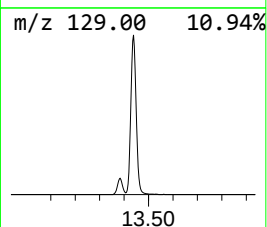
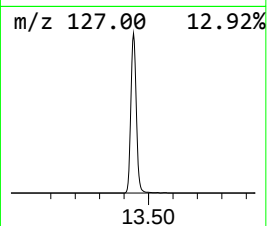
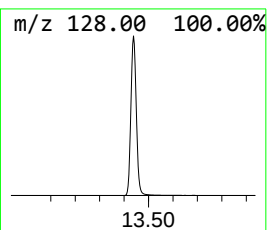
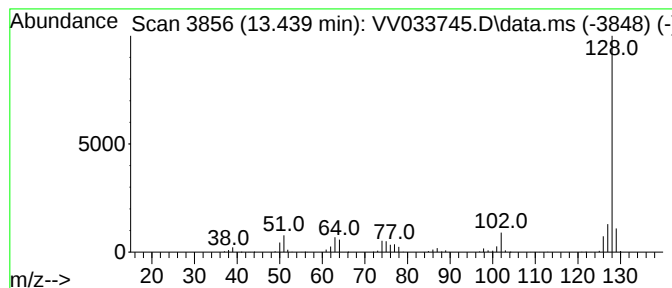
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Quant Title : VOC Analysis

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

Peak Number 6 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.438	109.81 ug/L	1760050	1,4-Dichlorobenzene-d4	11.191

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
Data File : VV033745.D
Acq On : 19 Jan 2024 11:27
Operator : SY/MD
Sample : P1160-10
Misc : 10.00g/10mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
XA319

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	35.7	ug/L	496644	1	5.532	695273	50.0
Ethane, 1,1,1,2...	8.908	126.0	ug/L	2028070	2	8.786	804931	50.0
1,3-Butadiene, ...	13.384	187.5	ug/L	3005200	3	11.191	801391	50.0
Azulene	13.438	109.8	ug/L	1760050	3	11.191	801391	50.0