

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU073124\
 Data File : VU060279.D
 Acq On : 31 Jul 2024 13:13
 Operator : MD/SY
 Sample : P3287-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 XB509

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_U\Method\SFAMULM070224WMA.M
 Title : VOC Analysis

Signal : TIC: VU060279.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.518	64	71	83	rBV	38178	45096	3.87%	0.297%
2	1.596	87	95	113	rVV	117560	139685	11.98%	0.918%
3	1.901	182	190	208	rVB	78952	114440	9.81%	0.752%
4	2.560	381	395	408	rBV3	211465	400749	34.37%	2.635%
5	2.618	408	413	434	rVB	22559	40964	3.51%	0.269%
6	2.721	442	445	448	rBV2	392	276	0.02%	0.002%
7	2.782	458	464	468	rBV4	813	1055	0.09%	0.007%
8	3.036	530	543	568	rBV	106863	220621	18.92%	1.451%
9	3.161	577	582	584	rBV3	913	933	0.08%	0.006%
10	3.354	625	642	673	rBV	232137	540528	46.36%	3.554%
11	3.486	681	683	687	rVB	477	247	0.02%	0.002%
12	3.528	693	696	699	rVB2	408	267	0.02%	0.002%
13	3.612	716	722	729	rBV2	227	385	0.03%	0.003%
14	3.837	787	792	796	rBV2	260	309	0.03%	0.002%
15	4.097	866	873	878	rBV2	276	491	0.04%	0.003%
16	4.142	884	887	892	rVB	316	305	0.03%	0.002%
17	4.483	989	993	998	rBV	270	283	0.02%	0.002%
18	4.518	998	1004	1008	rBV2	301	389	0.03%	0.003%
19	4.557	1012	1016	1021	rBV2	247	288	0.02%	0.002%
20	4.615	1024	1034	1042	rBV2	75453	166921	14.32%	1.098%
21	4.920	1125	1129	1132	rVV2	401	367	0.03%	0.002%
22	5.055	1156	1171	1198	rBV3	150867	391575	33.58%	2.575%
23	5.525	1313	1317	1321	rBV	393	280	0.02%	0.002%
24	5.599	1335	1340	1345	rVB2	257	233	0.02%	0.002%
25	5.628	1345	1349	1351	rBV2	260	254	0.02%	0.002%
26	5.718	1357	1377	1390	rBV2	296137	796100	68.27%	5.235%
27	5.785	1391	1398	1422	rVB2	81219	169398	14.53%	1.114%
28	5.930	1440	1443	1447	rVB2	331	257	0.02%	0.002%
29	6.042	1471	1478	1480	rBV3	319	299	0.03%	0.002%
30	6.242	1527	1540	1563	rBV	281213	540340	46.34%	3.553%
31	6.534	1619	1631	1652	rBV	157807	304198	26.09%	2.000%
32	6.682	1664	1677	1696	rBV	185127	361733	31.02%	2.378%
33	6.782	1696	1708	1731	rVB	182730	355874	30.52%	2.340%
34	6.914	1739	1749	1768	rVB2	29252	55583	4.77%	0.365%
35	7.103	1802	1808	1811	rBV3	517	532	0.05%	0.003%
36	7.129	1814	1816	1822	rVB2	284	262	0.02%	0.002%

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37	7.168	1822	1828	1830	rBV2	273	231	0.02%	0.002%
38	7.216	1835	1843	1863	rBV2	12564	24922	2.14%	0.164%
39	7.283	1863	1864	1869	rVV2	519	385	0.03%	0.003%
40	7.335	1878	1880	1887	rVB3	374	322	0.03%	0.002%
41	7.367	1887	1890	1894	rBV2	258	287	0.02%	0.002%
42	7.399	1894	1900	1903	rVB2	460	402	0.03%	0.003%
43	7.560	1938	1950	1956	rBV	96084	165477	14.19%	1.088%
44	7.602	1957	1963	1982	rVB	132117	223238	19.14%	1.468%
45	7.721	1993	2000	2008	rBV4	3351	6105	0.52%	0.040%
46	7.782	2008	2019	2040	rVV	239629	420063	36.02%	2.762%
47	7.891	2042	2053	2065	rVV	373906	654270	56.11%	4.302%
48	7.962	2065	2075	2096	rVB	501090	863111	74.02%	5.675%
49	8.174	2127	2141	2147	rBV	70514	121600	10.43%	0.800%
50	8.335	2188	2191	2196	rBV2	218	240	0.02%	0.002%
51	8.393	2197	2209	2226	rBV	178500	302046	25.90%	1.986%
52	8.470	2231	2233	2239	rVB6	1064	999	0.09%	0.007%
53	8.547	2247	2257	2271	rBV2	75058	128731	11.04%	0.846%
54	8.627	2271	2282	2290	rBV	204894	352600	30.24%	2.318%
55	8.676	2291	2297	2324	rVV	198648	357257	30.64%	2.349%
56	8.801	2326	2336	2360	rVB	142856	246333	21.13%	1.620%
57	8.917	2360	2372	2391	rBV	81717	140001	12.01%	0.921%
58	9.203	2457	2461	2469	rBV4	447	577	0.05%	0.004%
59	9.412	2512	2526	2550	rBV	410861	703129	60.30%	4.623%
60	9.528	2550	2562	2587	rVB	359083	605269	51.91%	3.980%
61	9.692	2598	2613	2637	rBV	207855	362244	31.07%	2.382%
62	9.843	2657	2660	2664	rVB2	247	227	0.02%	0.001%
63	9.872	2664	2669	2671	rBV2	384	272	0.02%	0.002%
64	10.100	2726	2740	2767	rBV4	529137	1109863	95.18%	7.298%
65	10.283	2787	2797	2812	rBV2	54904	91935	7.88%	0.604%
66	10.470	2852	2855	2856	rBV	811	415	0.04%	0.003%
67	10.486	2856	2860	2864	rVB3	865	793	0.07%	0.005%
68	10.618	2897	2901	2905	rBV2	298	294	0.03%	0.002%
69	10.647	2905	2910	2917	rVB2	354	470	0.04%	0.003%
70	10.679	2917	2920	2926	rBV2	249	306	0.03%	0.002%
71	10.750	2929	2942	2953	rVV	260920	425745	36.51%	2.799%
72	10.814	2953	2962	2982	rVV	162383	264925	22.72%	1.742%
73	10.888	2982	2985	2989	rVB	390	317	0.03%	0.002%
74	10.910	2989	2992	2996	rBV2	419	251	0.02%	0.002%
75	10.997	3016	3019	3026	rBV2	525	539	0.05%	0.004%
76	11.084	3033	3046	3063	rBV	155786	244616	20.98%	1.608%

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77	11.299	3106	3113	3118	rVB3	591	770	0.07%	0.005%
78	11.367	3130	3134	3137	rBV2	324	268	0.02%	0.002%
79	11.463	3153	3164	3182	rVV	138089	216875	18.60%	1.426%
80	11.528	3182	3184	3189	rVB3	587	468	0.04%	0.003%
81	11.701	3234	3238	3244	rBV2	277	353	0.03%	0.002%
82	11.743	3244	3251	3259	rBV2	1575	2497	0.21%	0.016%
83	11.807	3259	3271	3297	rBV2	400401	739294	63.40%	4.861%
84	11.997	3326	3330	3334	rBV3	299	306	0.03%	0.002%
85	12.200	3376	3393	3413	rBV2	485368	1166053	100.00%	7.667%
86	12.331	3430	3434	3439	rVB3	725	618	0.05%	0.004%
87	12.354	3439	3441	3443	rBV	386	246	0.02%	0.002%
88	12.393	3449	3453	3455	rBV2	292	240	0.02%	0.002%
89	12.991	3627	3639	3658	rBV	57509	95081	8.15%	0.625%
90	13.836	3891	3902	3923	rBV2	116591	185110	15.87%	1.217%
91	13.955	3933	3939	3943	rBV4	526	536	0.05%	0.004%
92	14.013	3947	3957	3968	rVV	120706	185062	15.87%	1.217%
93	14.084	3968	3979	4007	rVV	72815	135447	11.62%	0.891%
94	14.280	4036	4040	4043	rBV4	559	500	0.04%	0.003%
95	14.328	4049	4055	4065	rVB5	3321	4311	0.37%	0.028%
96	14.492	4101	4106	4107	rBV	468	343	0.03%	0.002%
97	15.148	4308	4310	4313	rBV2	441	296	0.03%	0.002%
98	15.695	4478	4480	4482	rBV2	620	327	0.03%	0.002%
99	16.023	4579	4582	4585	rBV3	694	462	0.04%	0.003%
100	16.341	4678	4681	4684	rBV4	883	761	0.07%	0.005%

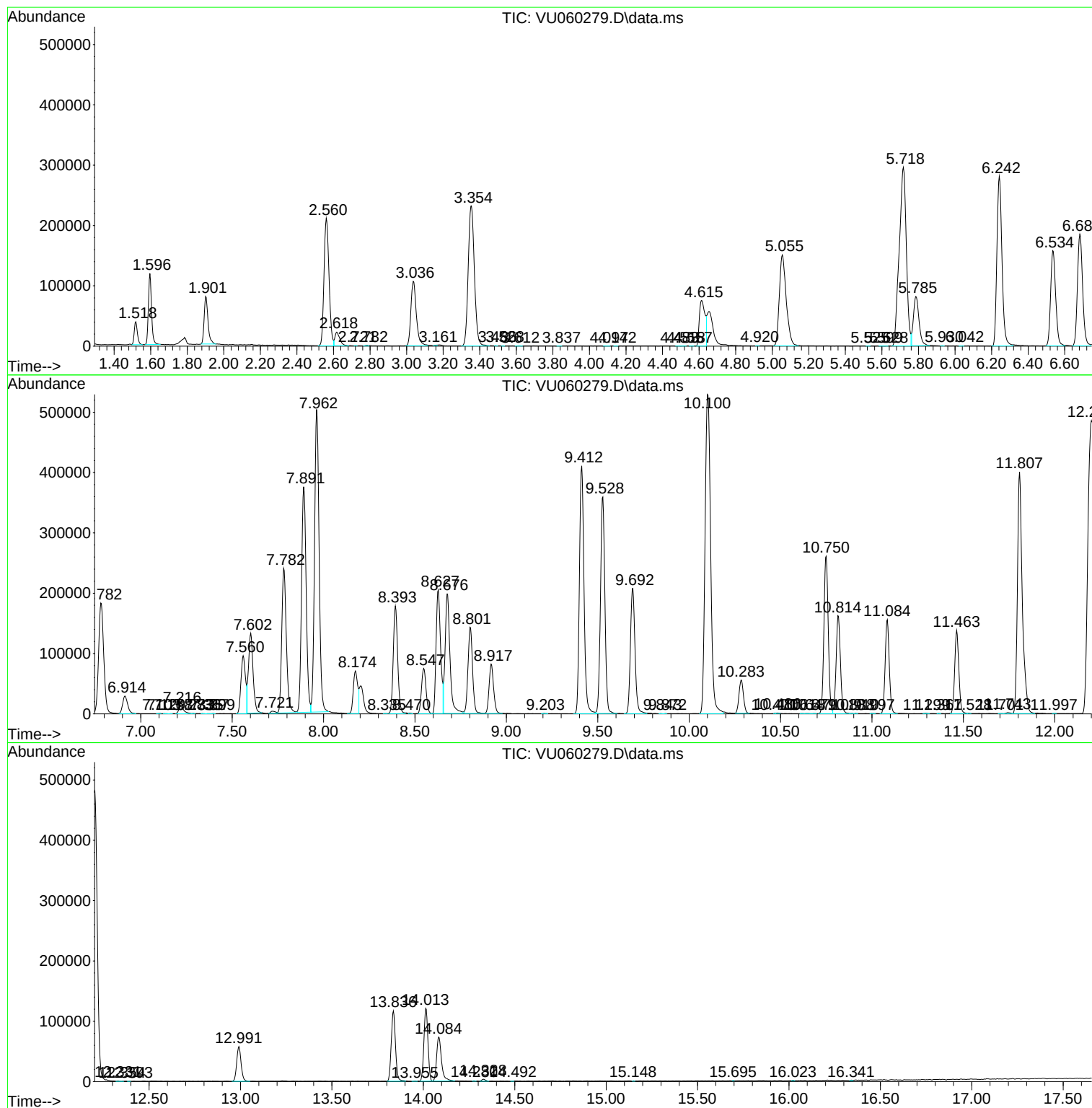
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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



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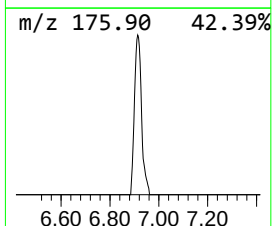
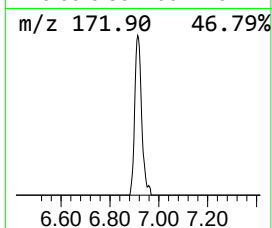
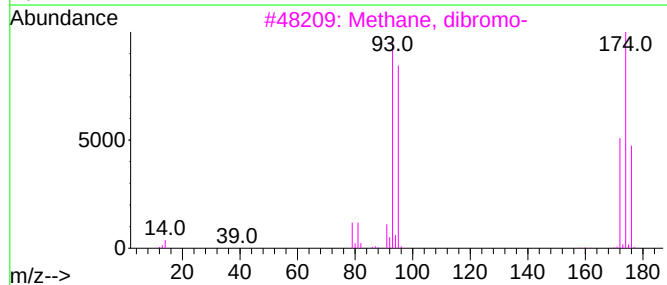
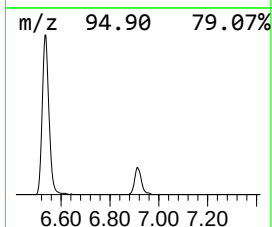
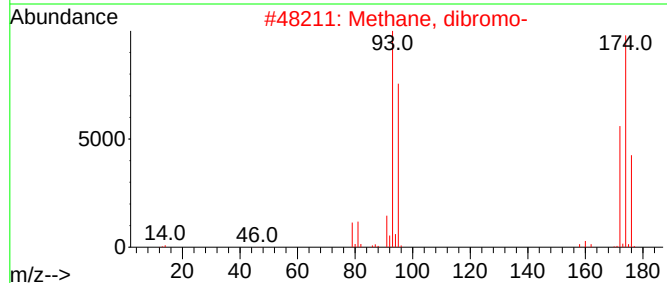
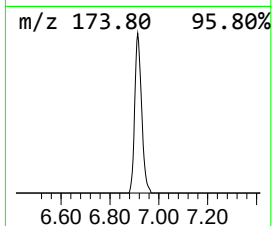
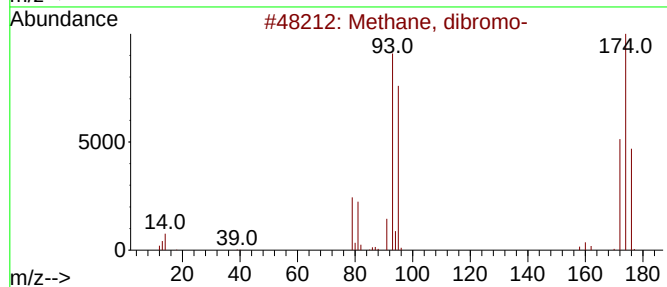
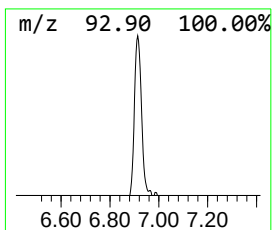
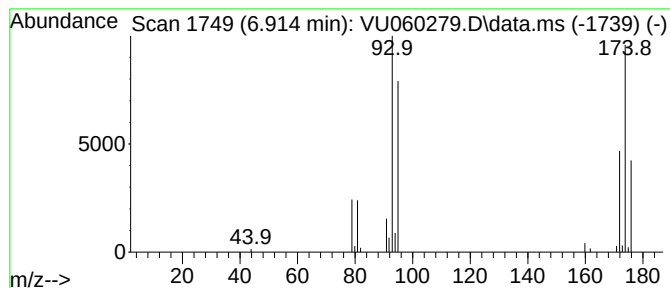
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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.
6.914	5.14 ug/L	55583	1,4-Difluorobenzene	6.242

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	91
5			Dimethyl selenodisulfide	174	C2H6S2Se	1000357-25-9	9



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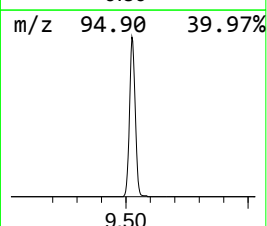
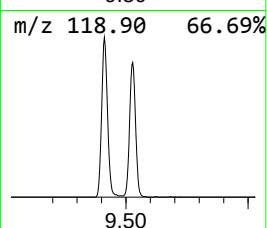
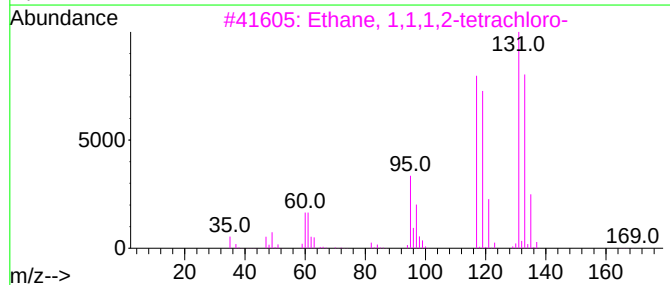
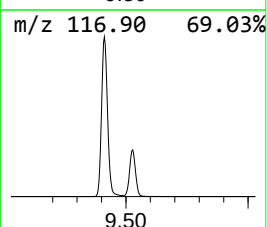
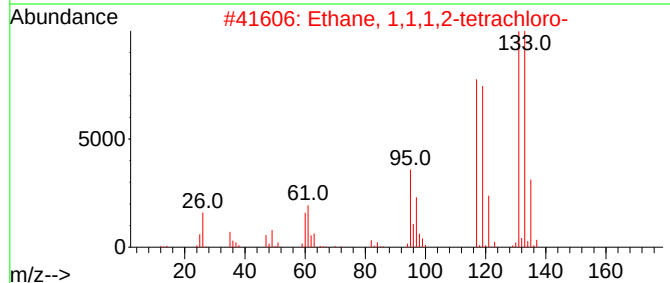
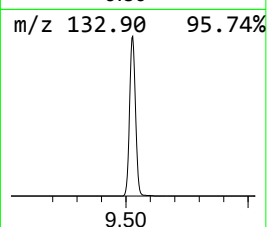
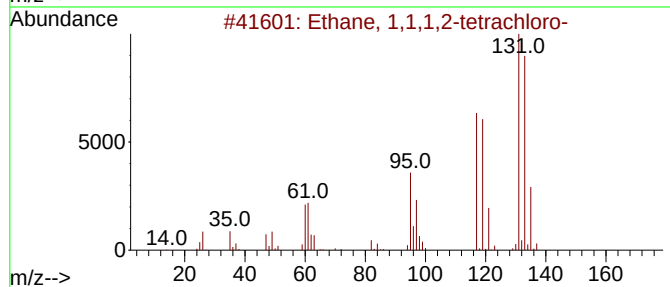
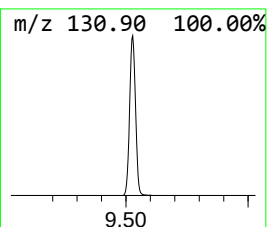
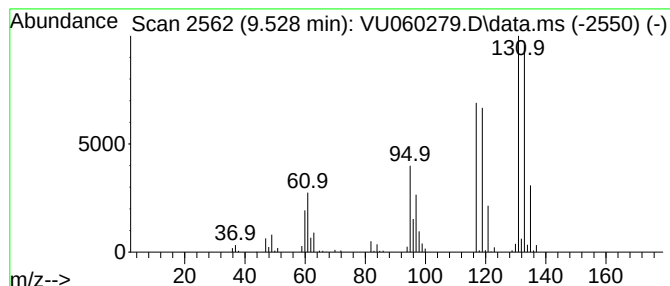
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.528	43.04 ug/L	605269	Chlorobenzene-d5	9.412

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	87
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	64
5			Trichloroacetyl chloride	180	C2Cl4O	000076-02-8	11



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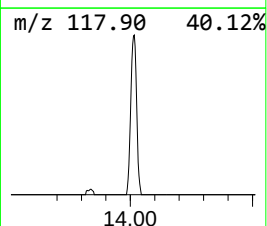
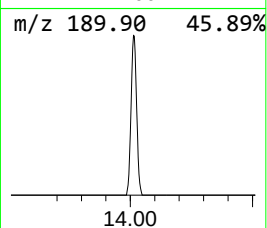
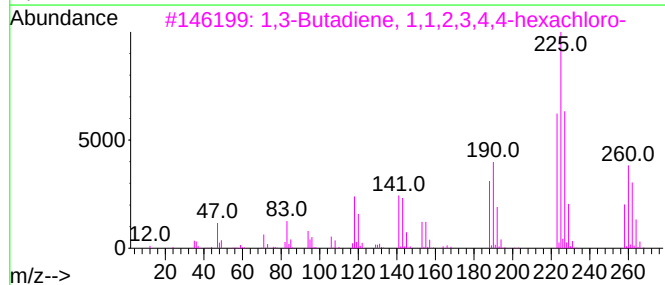
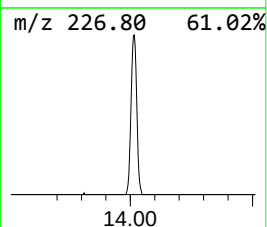
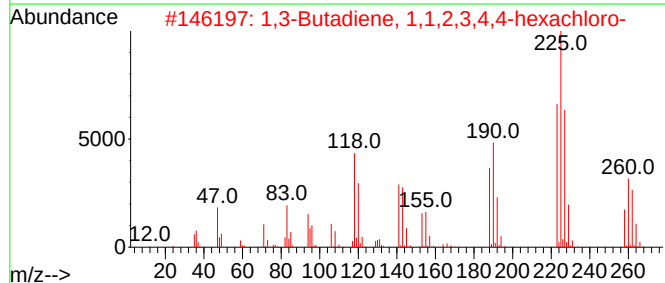
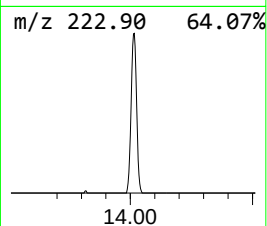
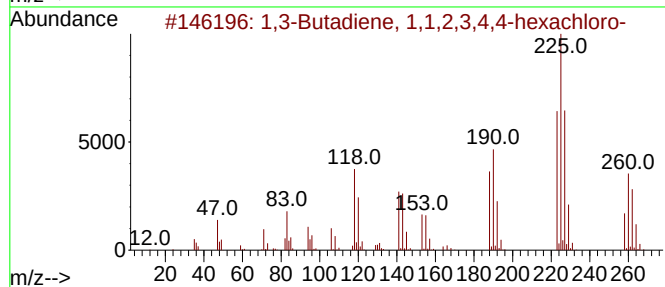
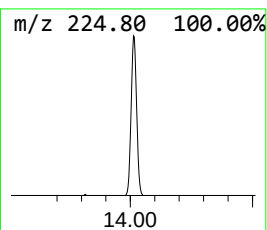
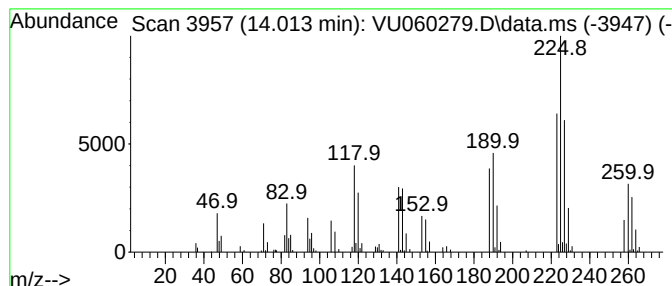
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.013	12.52 ug/L	185062	1,4-Dichlorobenzene-d4	11.807

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			Stannane, trimethylphenyl-	242	C9H14Sn	000934-56-5	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU073124\
Data File : VU060279.D
Acq On : 31 Jul 2024 13:13
Operator : MD/SY
Sample : P3287-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
XB509

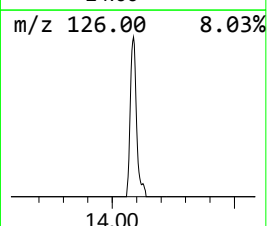
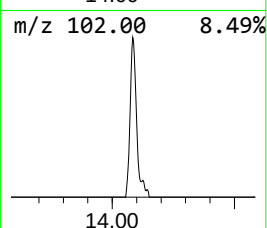
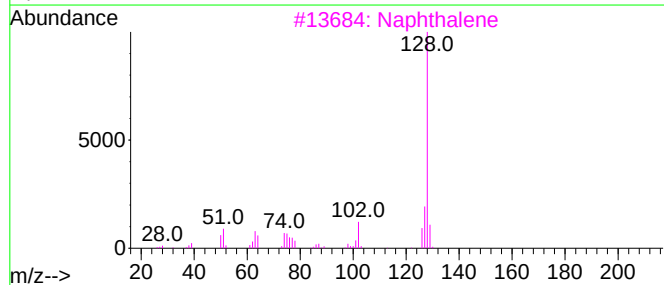
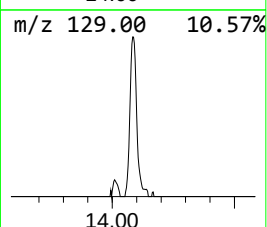
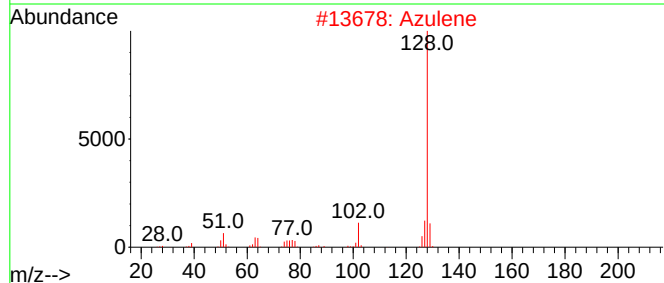
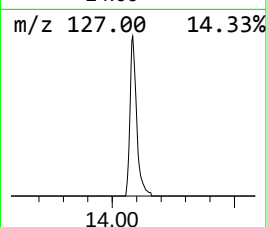
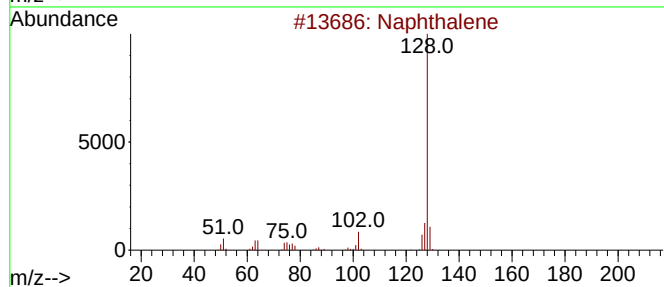
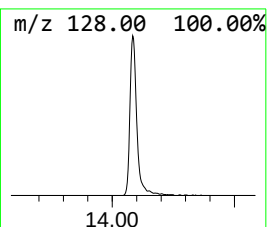
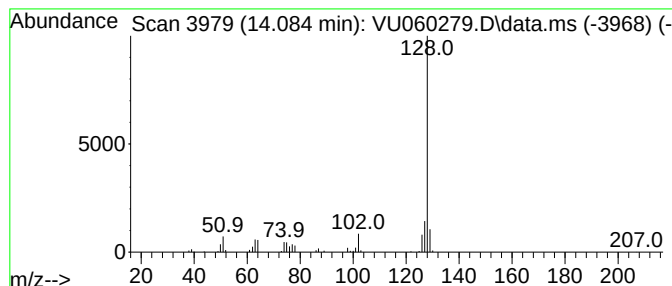
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Quant Title : VOC Analysis

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

Peak Number 4 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.084	9.16 ug/L	135447	1,4-Dichlorobenzene-d4	11.807

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			Naphthalene	128	C10H8	000091-20-3	91
4			Azulene	128	C10H8	000275-51-4	91
5			Naphthalene	128	C10H8	000091-20-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU073124\
Data File : VU060279.D
Acq On : 31 Jul 2024 13:13
Operator : MD/SY
Sample : P3287-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
XB509

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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-	6.914	5.1	ug/L	55583	1	6.242	540340	50.0
Ethane, 1,1,1,2...	9.528	43.0	ug/L	605269	2	9.412	703129	50.0
1,3-Butadiene, ...	14.013	12.5	ug/L	185062	3	11.807	739294	50.0
Azulene	14.084	9.2	ug/L	135447	3	11.807	739294	50.0